

Applied Multivariate Analysis

Prof. Amit Mitra

Prof. Sharmishtha Mitra

Department of Mathematics and Statistics
Indian Institute of Technology, Kanpur

Lecture No. # 24

Principal Component Analysis

After we have considered construction of PCs, the principal components, which are in fact very special type of linear combinations of the original variables; we said that we are going to check the properties that we had stated in the very begin in the desirable properties of the principal components. The first one of them was that the total variability present in the original data should be equal to the total variability in principal components.

(Refer Slide Time: 00:49)

Property 1
Total variation of \underline{y} = Total variation of $\underline{X}^{p \times 1}$

Pf: Total variation of \underline{y} = $\text{trace Cov}(\underline{y})$
= $\text{trace Cov}(P' \underline{X})$
= $\text{trace}(P' \Sigma P)$
= $\text{trace}(P' P D_\lambda P' P)$
= $\text{trace } D_\lambda = \sum_{i=1}^p \lambda_i$

$y_1 = e_1' \underline{X}$
 $y_2 = e_2' \underline{X}$
 \vdots
 $y_p = e_p' \underline{X}$

$\underline{y} = \begin{pmatrix} e_1' \\ e_2' \\ \vdots \\ e_p' \end{pmatrix} \underline{X}$
 $\Rightarrow \underline{X} = P' \underline{y}$

So, let us start with our first property today that is property 1, we have total variation of Y that is of the principle components is equal to total variation of X. Now, at this point, we are still talking about the P dimensional vector of principal components, we have considered as many elements of this principal of or we have considered as many principal components as they are **are** the originally variables. And we have also defined

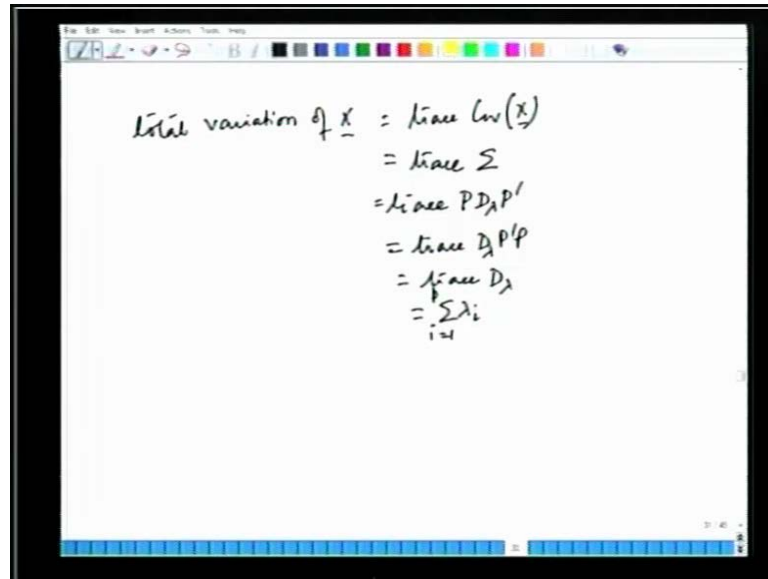
to total variation as the sum of the diagonal elements of the corresponding variance covariance matrix.

So, let us say that by having total variation of Y , what is this? By my definition of total variation of Y , it should be the trace of the variance covariance matrix of Y . Now we know that this is nothing but trace of **trace of** the variance covariance matrix of Y ; and what is Y ? Well Y is nothing but you know that Y is we have constructed the principal components in this way; Y is the linear combination; the first linear combination $e_1 X$, Y_2 is $e_2 X$, and similarly Y_t is nothing but $e_P X$.

So, this is in fact, if I want to write the Y vector, I can actually represent the whole thing; this is my Y vector, the collection of these $Y_1 Y_2$ to Y_P in the column form, and I have this as $e_1 e_2$ to e_P , all these are transpose, and I have this as x . So, this is, if you recall that this is nothing but our P transpose matrix, because this the P matrix is found, the column of the P matrix are nothing but the orthonormal eigen vectors e_1 to e_2 to e_P . So, this is nothing but $P X$, which also gives me prevalently that X is equal to $P Y$, but I can handle this situation this relation, so this is trace of nothing but covariance of P transpose X . Why do I do this, because I know, what is the variance covariance matrix of X .

And trace of covariance of this matrix is trace of P transpose σP , because I have assumed, I have taken that σ is the variance covariance matrix of the random variables X . And now, I use the spectral decomposition of σ , in terms of $P D \lambda$, so this is $P D \lambda P'$ we know, what are these matrices already? And since P is orthogonal matrix, its columns are made up of orthonormal eigen vectors, this is nothing but trace of $D \lambda$; and trace of $D \lambda$ is nothing but sum of λ_i , this is $\sum_{i=1}^P \lambda_i$.

(Refer Slide Time: 04:31)



The image shows a handwritten derivation on a whiteboard. The text is as follows:

$$\begin{aligned} \text{Total variation of } \underline{X} &= \text{trace}(\text{cov}(\underline{X})) \\ &= \text{trace } \Sigma \\ &= \text{trace } P D_{\lambda} P' \\ &= \text{trace } D_{\lambda} P' P \\ &= \text{trace } D_{\lambda} \\ &= \sum_{i=1}^p \lambda_i \end{aligned}$$

And what is total variation of X ? Well total variation of X is... Total variation represented by the original data that is X , well by definition it is trace of the covariance matrix of X , which is trace of sigma; and trace of sigma is nothing but trace of $P D$ lambda P prime. Again using the spectral decomposition of sigma, and I am using the fact the trace of $A B$ is trace of $B A$. So, this is nothing but trace of D lambda P prime P . Now P prime P now P prime P being an identity matrix I will have to consider only trace of D lambda and which is again equal to some of lambda i from 1 to P giving me the Property of the first property that total variation of Y is in fact equal to total variation of X .

(Refer Slide Time: 05:30)

Property 2...

y_1, \dots, y_p are uncorrelated with $\text{Var}(y_i) = \lambda_i$

Pf $y_i = e_i' X \quad \forall i = 1(1)p$

$$\text{Cov}(y_i, y_j) = \text{Cov}(e_i' X, e_j' X)$$

$$= e_i' \text{Cov}(X) e_j$$

$$= e_i' \sum e_j e_j' = e_i' P D P' e_j$$

$$= e_i' (e_1 \dots e_p) D_\lambda \begin{pmatrix} e_1' \\ \vdots \\ e_p' \end{pmatrix} e_j$$

$$\therefore \left. \begin{array}{l} \text{Cov}(y_i, y_j) = 0 \quad \forall i \neq j \\ \text{Var}(y_i) = \lambda_i \end{array} \right\} = \begin{pmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix} \begin{matrix} \rightarrow j^{\text{th}} \\ \rightarrow i^{\text{th}} \\ \rightarrow j^{\text{th}} \\ \rightarrow i^{\text{th}} \\ \rightarrow j^{\text{th}} \\ \rightarrow i^{\text{th}} \\ \rightarrow j^{\text{th}} \end{matrix}$$

$$= \begin{matrix} 0 & & & & & & \\ & \lambda_i & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \end{matrix}$$

The next one was we said that the principle component Y_1, Y_2, Y_P , they should be uncorrelated. So, let us see this, the principal components so constructed, they are boundary uncorrelated, so we have Y_1, Y_2 to Y_P are uncorrelated. We combine one more thing with this with variance of Y_i , the i th principal component is the i largest eigen value of the covariance matrix of X . So, we have Y_1, Y_2 to Y_P are uncorrelated with variance of, with variance of Y_i being λ_i , this is again very simple, because we have the i th principle component Y_i is nothing but e_i transpose X ; and this is true for all i from 1 to $2p$. So, that if I really have to consider, what is covariance matrix between Y_i and Y_j , where it is nothing but covariance between e_i prime X and e_j prime X .

So, this is in fact e_i prime covariance of X and e_j prime, and this covariance X is nothing but our sigma matrix, the matrix which is very important to us for calculation of eigen values and eigen vectors, and we use this spectral decomposed representation of this matrix to write e_i prime with $P D_\lambda P'$ and e_j prime, where the columns of P matrix, these are nothing but e_1 to e_P . Once I realize this, I can also realize very quickly that where if I write this as e_i transpose, and here I have e_1 to e_P , then I have a D_λ , and here I have transpose of this that is e_1 transpose to e_P transpose, and e_j here. Now since $e_i(s)$ are orthonormal eigen vectors, I am only going to have a 1 in the i th position, when this e_i transpose combines with the e_i here.

So, that 1 in the i eth position and 0 elsewhere D lambda, and then again I have... Now this is important, because this is in the i eth position, whereas this is in the j eth position. So, they are never matching, and I am as a result, I have a 0, this is j eth, and as a result, I have 0, if well if i is not equal to j , and well if it is equal to i is equal to j . So, 1 is going match with 1 here, and resultant element that is going to remain is this i eth element of D lambda and that is going to be lambda i , if i is equal to j . So, in 1 go, I can proof, I have been able to proof that this not only proofs that covariance of which implies that covariance of Y_i and Y_j is 0, for all i not equal to j and variance of Y_i , which is covariance between Y_i and Y with itself, this is equal to lambda i .

(Refer Slide Time: 09:20)

Property 3.

$$\text{Cov}(x_i, y_j) = e_{ij} \sqrt{\frac{\lambda_i}{\sigma_{ii}}}$$

$$e_{ij} : \text{The } i\text{th element of the } j\text{th eigenvector } (e_j)$$

Pf

$$y_j = e_{ij}' x \quad \forall j=1(p)$$

$$\underline{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_p \end{pmatrix} = \begin{pmatrix} e_1' x \\ \vdots \\ e_p' x \end{pmatrix} = \begin{pmatrix} e_1 \\ \vdots \\ e_p \end{pmatrix}' x = P' \underline{x}$$

$$P = (e_1 \dots e_p)$$

$$P = ((e_{ij}))$$

$$\underline{x} = P \underline{y}$$

$$\begin{pmatrix} x_1 \\ \vdots \\ x_p \end{pmatrix} = \begin{pmatrix} e_{11} & \dots & e_{1p} \\ \vdots & & \vdots \\ e_{p1} & \dots & e_{pp} \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_p \end{pmatrix}$$

The next property that we talk of is property 3. Well, we know covariance between X_i and X_j is σ_{ij} ; the ij eth element of the sigma matrix have constructed simple components in such a way such that the covariance between Y_i and Y_j that is the covariance between the i eth principal component, and the j eth principal component is 0, they are uncorrelated. Now, what about covariance between the original variable and principal components? Say I consider covariance between X_i , any X_i are not just the Y_i , but say any Y_j . So, let us look into that, because this relation, this covariance or this correlation coefficient that I am going to obtain from here is going to help me a lot in data interpretation.

So, this is the next Property that we are talking of that is covariance between X_i that is the i th original variable, and the j th principal component Y_j is $e_{ij} \sqrt{\lambda_i}$ by σ_{ii} . Now I know, what is λ_i ? It is the variance of the i th principal component, and σ_{ii} is the variance of the original variable x , but what is e_{ij} , where e_{ij} is the j th **sorry** the i th element of the j th eigen vector that is e_j **right**. This λ_i is λ_j because I am considering y_j here, so this is λ_j , variance of Y_j , this is σ_{ii} variance of X_i , and e_{ij} is coming from the j th eigen vector e_j , it is the i th element of that eigen vector. So our, again we start from the form of the principal component Y_j , let us try to express it in terms of X , then we are able to use the known results, and Y_j is nothing but $e_j^T X$. This is true for all j from 1 to P .

And then I have to consider, so well I know Y is again Y_1 to Y_P , and these are nothing but $e_1^T X$ to $e_P^T X$ **right**. So, this is nothing but $e^T X$ combine with X , and this is $P^T X$. So, I have Y is nothing but $P^T X$; P being orthogonal, I have X is equal to $P Y$. And then if I have to consider, well X is this like Y , it is also P dimensional, I have X_1 X_2 to X_P ; and I simply have the P matrix here; if you recall the P matrix is nothing but e_1 e_2 to e_P . And now I am saying that I am denoting the i th element of the j th eigen vector by e_{ij} .

So, I can open up this all these vectors **right**, so for e_1 , if I have to write the first element of the first eigen vector, I will write e_{11} , then the second element of the second this column vector, I am going to write e_{21} . So, this is exactly how I write up matrix P , if P is nothing but, and then P is nothing but represented by this e_{ij} , and I have e_{11} e_{21} in this way up to e_{p1} , and finally, the first element of the P th vector, P th eigen vector, which is e_{1P} , then the second element of e_P , which is e_{2P} , and then I have the last element of the P element of the P vector giving me e_{PP} , and then this is Y_1 to Y_P **right**.

(Refer Slide Time: 14:01)

$$\begin{aligned} \Rightarrow X_i &= \sum_{k=1}^p e_{ik} Y_k \\ \text{Cov}(X_i, Y_j) &= \text{Cov}\left(\sum_{k=1}^p e_{ik} Y_k, Y_j\right) & \text{Cov}(Y_k, Y_j) &= \begin{cases} 0 & k \neq j \\ \lambda_j & k = j \end{cases} \\ &= \text{Cov}(e_{ij} Y_j, Y_j) \\ &= e_{ij} \lambda_j \\ \text{Corr}_{X_i, Y_j} &= \frac{\text{Cov}(X_i, Y_j)}{\sqrt{V(X_i)} \sqrt{V(Y_j)}} = \frac{e_{ij} \lambda_j}{\sqrt{e_{ii}} \sqrt{\lambda_j}} \\ &= e_{ij} \sqrt{\frac{\lambda_j}{e_{ii}}} \end{aligned}$$

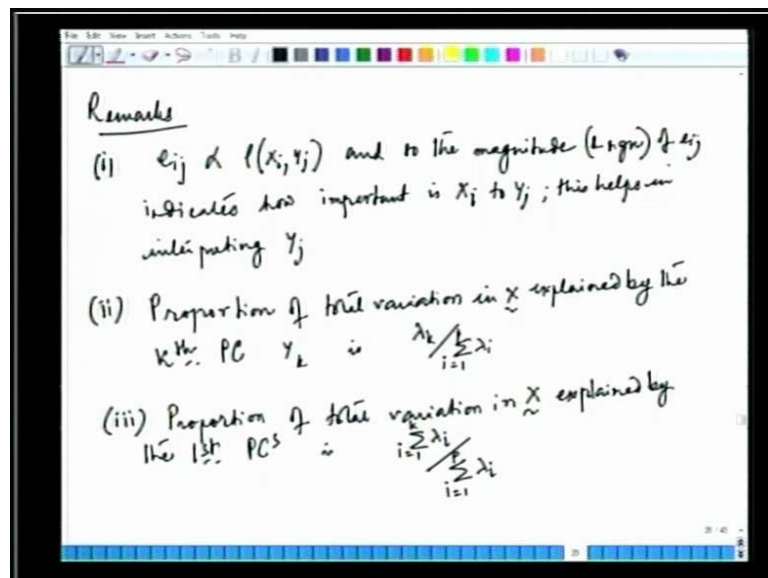
So, this gives me a new representation of X; I can say that X_i , if I consider the i th element of the X vector, it is nothing but sum of $e_{ik} Y_k$, and k the sum is over the common dimension obviously, it is P . So, now if I have to consider covariance between X_i and Y_j ; well, I will have to consider covariance between X_i , I am using this form of X_i , this is sum over k , and for Y_j , I am simply taking Y_j . Now, I can do this, because I know what already what is the covariance between **covariance between** any Y_k and Y_j . So, it is simple for me to handle this. Now I know that covariance between any Y_k and Y_j , where k is not equal to j is equal to 0. So, if I open up this sum, and consider the covariance with Y_j , the only term that will make a difference in the in this covariance will make a contribution rather in this differences the P th term that is when Y_P come terms with the coefficient e_{iP} ; others are all equal to 0, because I am considering covariance between Y_k and Y_j , and k is not equal to i .

So, this is basically nothing but covariance between $e_{ij} Y_j$, and then **sorry** this is going to give me **...** So, this is going to give me covariance between e_{ij} and e_{ik} , that is the only part that **that** is going to remain, and I have e_{ij} with Y_j and Y_j rest of this are not making any contribution, and covariance between Y_j and Y_j is of course, λ_j and e_{ij} remains as such giving me $e_{ij} \lambda_j$, because I know that covariance between Y_k and Y_j is 0 for all k not equal to j , and is λ_j , if k is equal to j . So, I am using this relation.

And then I have, I can also consider the correlation coefficient **correlation coefficient** between X_i and Y_j ; this is covariance $X_i Y_j$ by root variance of X_i times root variance of Y_j , I know all this; so, I can immediately write this as $e_{ij} \lambda_j$, and this is root of σ_{ii} , and this is root of λ_j . So, this is giving me e_{ij} with root λ_j by σ_{ii} . Let us go back to the statement, we had stated that now we have to make a small correction again here; this **this** is not actually the covariance, but in fact the correlation coefficient. The covariance being equal to $e_{ij} \lambda_j$; so if I consider the correlation coefficient between X_i and Y_j , then only I get this whole thing.

So from here, it is clear that this element e_{ij} , it plays a very significant role in the correlation coefficient between X_i and Y_j **right**, because its sign is going to determine the sign of the correlation coefficient, I have the rest of it is ratio of two standard deviation always positive. So, its sign as well as its magnitude are very important for me to interpret the relationship between the original variable and the principal components. If there are some more parameters, which can be now checked from whatever we have obtained, and let us list down few important of those parameters, which are very important, which are very useful for data interpretation part.

(Refer Slide Time: 18:32)



The first one is I have say we can note down this as some remark, so some notes. So, the first one is the one that we have just written that is e_{ij} that is the i th element of the j th eigen vector, this is proportional to correlation coefficient between X_i and Y_j ; and so

the magnitude of e_{ij} and sign also of e_{ij} indicates, how important is X_i to Y_j ; and this helps in interpreting, because after all these principal components that we have constructed, these are not some direct observable variables. These are linear combinations of a number of several variables. So to give, we have to give some interpretation in terms of the physical variables, and if we have certain relationship like this, it becomes little easier for us to give the interpretation as to how this are related. So, this helps in interpreting Y_j .

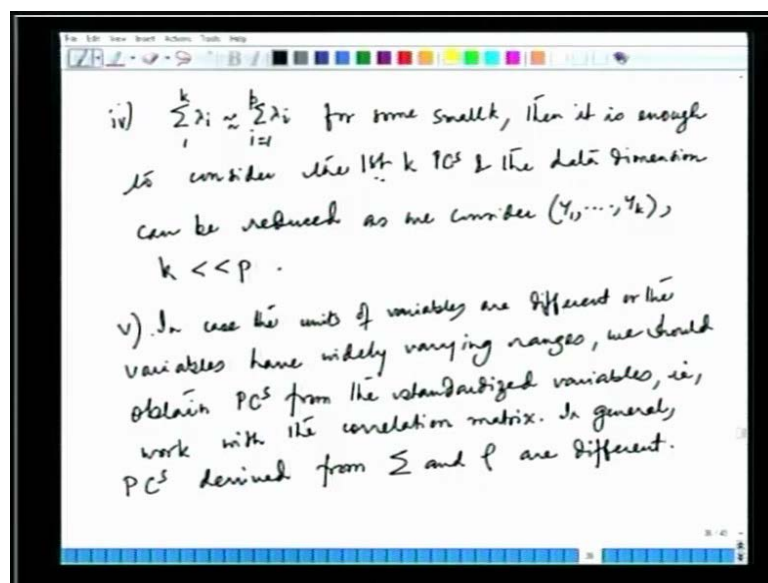
The second one is the proportion; now if you recall, we have now talked about one property of the principal components, which we said is very important that is though the total variation in X is equal to total variation in Y , ultimately to make the whole exercise fruitful one, I should have the total variation in Y , it should be explained by a very few number of total variation of a fewer number of the principal components that is you had recall we had written some thing like total variation in Y is approximately equal to the variation in Y_1 to Y_2 to Y_k , where k is a number, which is much smaller than the true dimension P .

Now, that we have not checked, because that is **that is** going to come out from actual data only when we have data, we can actually see that how this what is the effect or what is the extent to which this has been this approximation is effective. But before that, I can also say that the proportional of total variability or proportion of total variation in X explained by the k eth principal component **right**. What is a total variation in X ? It is sum of, sum the eigen values, and the variation explained by the k principal component is nothing but its variance, and that is equal to λ_k . So, this the proportion of total variation in X explained by the k eth PC Y_k is equal to λ_k by sum of λ_i , i from 1 to P .

And what do you want? Ideally, we would like to have this λ_1 by summation λ_k , a very large number. This should be as close to 1 as possible, then should come λ_2 by sum of λ_i (s) on in this way. As a value of k increases, we would like to have this factor to be smaller and smaller, so that I can stop at a small value of k , and say that if I consider these many principal components, it is good enough for me to explain the total variability present in the data.

Then again it is not necessary that I have to consider the principal component in isolation that I should say that one explains the highest variability, so I stop at 1, you know, I can consider 1 and 2, two-dimensional is also good enough for me. So, in that case, I have to look at the total variability explained by the first principal component, and the second sample component. So, in this way, that is another one more parameter that is of importance to me is proportion of total variation in X, explained by the first k principal components that is some of λ_i , i from 1 to k and this is the total variation some of λ_i from 1 to P all of them.

(Refer Slide Time: 23:54)



And then comes the important point that if I have sum of λ_i , i from 1 to k is approximately equal to some of λ_i from 1 to P. Then I will say, and that two for some small k, smaller the better, for some small k, then it is enough to consider the first k principal components, and the data dimension and the data dimension can be reduced k that was our goal, primary goal; the data dimension can be reduced as we consider a part of y that is we consider now the k dimensional vector $y_1 y_2$ to y_k , k is much smaller than P. Now one thing is we have to be careful about this is number 4, after the first three points, one thing we have to careful about we are saying that e_{ij} is a very important factor for me to explain the important, the association between X_i and y_{ij}

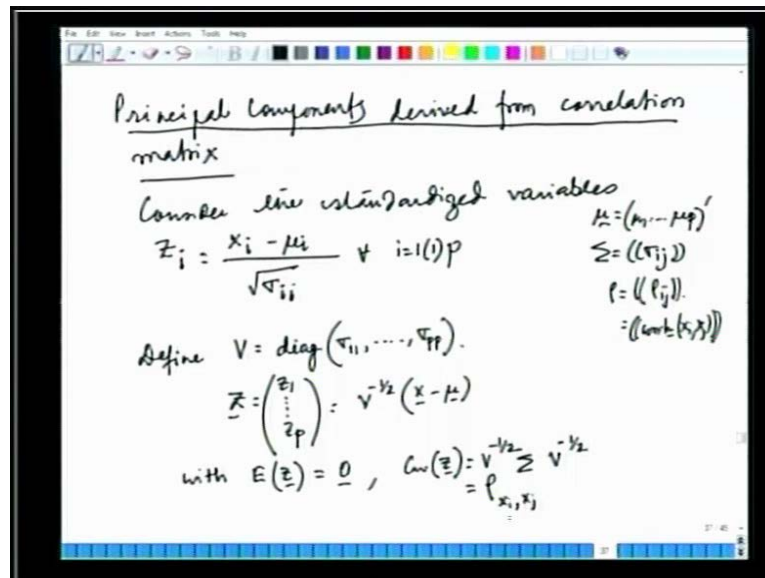
Now, if I have the data, e_{ij} is essentially the i eth element of the j eigen vector. Now if I have the data, which are in different units of measurement or data which have very

different and wide ranges of variation. Then if I consider the data as it is, and then focus on these $e_{ij}(s)$ and other measures, then the comparison would not be truly correct. What we have to do in such a situation is we have to try and make the measurements unit free and so that we get the true picture of association. So this point also to be noted down, before we actually do the excise of that. So, standardizing the variable; so in case of, in case the units of variables, units of measurements of the variables, so the units of variables are different or the variables, which is bound to happen in practical situations, we shall **we shall** consider variables from different fields, which we have, which are bound to have different units of measurements, and they can also have totally different and very high range of variation. So, this we should **and** are the variables have widely varying ranges we should obtain principal components from the standardized variables.

So, standardizing the variables means, essentially we will have to divide **the** we have to first take the difference of this variables from the corresponding means and divide by the corresponding standard deviations. Now initially, when we working with the plane, the raw data; our matrix of importance to us was the variance covariance matrix of X ; that is the sigma matrix. Now, you can easily realize that if we standardize the variables, the whole matrix of importance to us is now the correlation coefficient matrix of the variables. So now, we have to the everything is getting replaced by the correlation coefficient matrix rho, which **which work** initially we were worked with the sigma, the covariance matrix sigma.

Now, our matrix of importance is the correlation coefficient matrix rho. So, this is obtain from standardize variables; and we have to consider the that is work, we can put it like this, work with the correlation matrix, instead of the covariance matrix. Now, question remains that will the principal components be same, if we work with the sigma on the rho matrices? Now answer is no. In general the PC(s) derived from sigma and rho are different **right**.

(Refer Slide Time: 29:29)



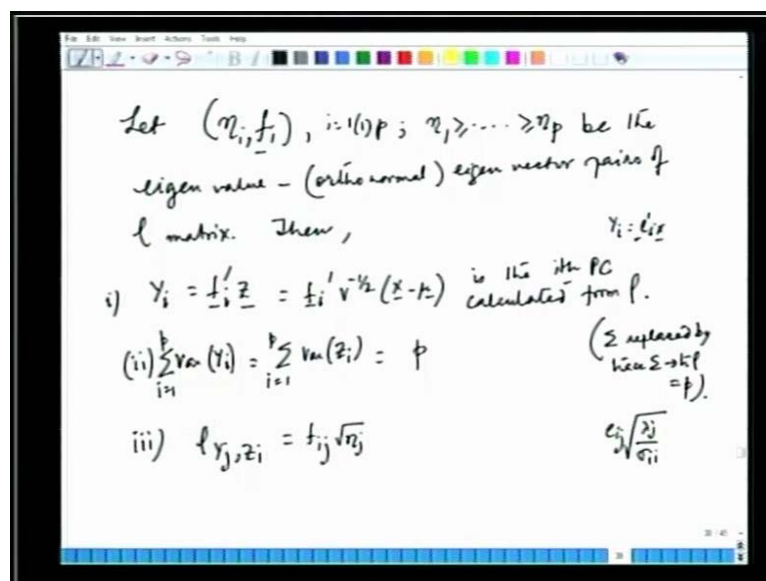
And now we consider calculation of principal components from the correlation matrix. So, I have principal components derived from correlation matrix. We really do not have **do not have** to do much here, we will see that how a simple transformation helps us and we will get all the results immediately from the once that we have really proved. So, first is we consider the standardize variables that is the first step; and use a very general notations set for those. So, I say that Z_i is nothing but X_i minus μ_i that is the mean of the i eth random variable, we had earlier say that the mean vector; well if you have to write the covariance of the term covariance with in terms of a expectation etcetera, we will have to use μ being the mean vector μ_1 to μ_p .

So, we have and σ , the variance covariance matrixes σ_{ij} **right**. So, this is X_i minus μ_i by root over σ_{ii} , for all the i from 1 to P ; there are P variables X_1 to X_P , I define P standardize variables Z_1 to Z_P . And now I just define a new matrix V , define V which is nothing but diagonal of the σ , diagonal elements of the σ matrix, so this is diagonal σ_{11} to σ_{pp} **right**. And then well I have z , how can I write this Z vectors, Z vector is nothing but Z_1 to Z_p **right**. In terms of the X vector, if I have to do it, well simply, it simply that now that I have defined what is V ; and the diagonal elements are all positives. So, V is a positive definite matrix, I considered the inverse square root of V , by speckle decomposition, by actually spectral decomposition of σ , this is good enough to give me this also, V square root inverse of V , and then rest of it is nothing but X minus μ .

So, I combine all these standardized variables in this Z vector, in this fashion using $X(s)$ $\mu(s)$ and these elements σ_{ii} $\sqrt{\sigma_{ii}}$ coming into the picture in this way. So, now, with that I have Z is, this. So, what is expectation Z as expected, because I have standardized this and got z. So, this is nothing but the null vector, because expectation X is μ , and what is variance covariance matrix of z? Well, this is V minus half, covariance of X minus μ which is same as covariance of X, which is σ , and then this is V minus half again. And what is that? Well, if σ is the variance covariance matrix or the dispersion matrix of something of X **right**, and you have these are getting **getting** divided by this, the ij eth element of σ matrix, what by what is it getting divided? Well, it is getting divided by this the element here that is it is getting multiplied here by σ_{ii} raise to the power minus half, and on the any other side its σ_{jj} raise to the power minus half.

So, in effect I am getting nothing but the correlation coefficients ρ of X ij **right**. So, ρ is nothing but ρ_{ij} , and what is ρ_{ij} ? It is the correlation coefficient matrix of X ij or this as ρ_{ij} , the matrix of correlation of X i and X j . Well, this was the matrix of covariance between X i and X j . So, you may write it X i X j as a subscript, but there is no need actually. Just like we have σ as covariance between X i j and ρ is the correlation matrix between X i and X j

(Refer Slide Time: 34:33)



And then if I consider the eigen value and orthonormal eigen vector that is I say there I had $\lambda_i e_i$, here let me have η_i and f_i , i from 1 to P . The same way as we had considered the λ s, I have λ η_1 greater than equal to up to η_P be the eigen value and orthonormal eigen vector pairs of ρ known; instead of σ , I had earlier λ_i and e_i eigen value eigen vector pair of σ ; I do not calculate the eigen values and corresponding Eigen vectors for σ . Now instead I calculate it for the correlation matrix ρ , and then I get this is pairs of ρ matrix, then **then** what is the i eth principal component? Let me use the same notation Y_i for its principal component, and then what is the i eth principal component? Well, originally if you recall I had Y_i is e_i times X e_i transpose X .

Then now using this notation I should have this as if I transpose Z **right**. And this is nothing but f_i transpose v inverse X minus μ . So, this is the i eth principal component calculated from ρ **right**. And if I have to consider the variance of this; well I consider the variance of some of the variance of first one, the first point to be noted is this. And then I have the total variation in **variation in** y that is sum of variance of Y_i from 1 to P , there are P of them as before, and then this is nothing but, because I had variance of Y_i equal to variance of X_i . So, similarly I should have this variance of Y_i this new Y_i , their variance, sum of their variances should be equal to variances of Z_i , i from 1 to P , and what is this? What is this matrix, actually this is giving me the correlation coefficient matrix, and then what are the diagonal elements, their diagonal elements are 1. So, some of them are actually equal to P . So σ , everywhere σ replace by ρ . Trace of σ , now I have trace of ρ , which is equal to P **right**.

And another point that to be noted is, what is the covariance between Y_j and Z_i ? So, as we had considered Y_j and X_i , well, there it was e_{ij} if you recall it was $e_{ij} \lambda_j$ by σ_i . So, here it is going to be f_{ij} , f_{ij} **right**; with λ_j is now being replaced by η_j , and σ_{ii} is now actually equal to 1, because I am considering the ρ matrix, instead of the σ matrix. So, we will continue with the calculation from a data, calculation of principal components from data after this. Now we consider the computational steps required for the calculation of the principal components. First we consider a situation, where we are calculating eigen value eigen vectors from the, from the σ matrix that is the covariance matrix. And next we will take up correlation matrixes, well.

(Refer Slide Time: 38:50)

Computational steps for calculation of PC's

$$\Sigma = \begin{pmatrix} 1 & -2 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad \begin{matrix} \lambda_1 = 5.83 \\ \lambda_2 = 2.0 \\ \lambda_3 = 0.17 \end{matrix}$$
$$\underline{e}_1 = \begin{pmatrix} 0.383 & -0.924 & 0 \end{pmatrix}$$
$$\underline{e}_2 = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix}$$
$$\underline{e}_3 = \begin{pmatrix} 0.924 & 0.383 & 0 \end{pmatrix}$$

PC's are

$$\begin{aligned} y_1 &= 0.383x_1 - 0.924x_2 \\ y_2 &= x_3 \\ y_3 &= 0.924x_1 + 0.383x_2 \end{aligned}$$

So, the first example that we considered here, this is the computational steps for calculation of PC(s) calculation of construction of PC(s). Now that we know the theory behind this, we actually know that the this important information, the important data that we required is nothing but the variance covariance matrix of the original variables sigma. So from here, we can calculate the eigen values, eigen vectors and the principal components also. So, that is what, that is what matters to me, and then I have the first example say the example 1, where I have the sigma matrix given to me as 1 minus 2 0 5 0 2, it is a symmetric matrix obviously, I know that the data dimension is 3, I have a 3 by 3 square matrix, which is symmetric and which is positive definite also **right**.

So, I calculate eigen values from here, the three eigen values, and I denote them as the first one is the highest one in this way. So, I calculate the three eigen values, and then I put them as lambda 1 is equal to 5.83 lambda 2, the second one in magnitude is 2 and lambda 3 is 0.17, all positive in decreasing order 5.832 and 0.17, I have to consider the corresponding, calculate the corresponding orthonormal eigen vector. First I get the eigen vectors, and then normalize them to get the orthonormal eigen vectors, and these are e 1 is the eigen vector, the orthonormal Eigen vector corresponding to lambda 1 equal to 5.83 is this one, its 0.383 minus 0.924 and then 0.

The second orthonormal eigen vector that is the eigen vector corresponding to the second highest eigen value, which is equal to 2, this is equal to 0 0 1 and e 3; similarly is 0.924

0.383 and 0. If I know this, I know all the three PCs, the PCs are well, the first one is Y_1 , it is $e_1^T X$. So, I know what are the coefficients with each of the X variables for the Y_1 for the first principal components? So, that is $0.383 X_1 - 0.924 X_2$ that is all, because the third coefficient is 0. The second principal component is identically equal to the third variable, the original variable X_3 ; and the third principal component is $0.924 X_1 + 0.383 X_2$, that is the third principal component. And if that is so, I am going to now see that how important these principal components are; how much of the total variation they can explain? So, this is the **the** five characteristic that we are talked about.

So, this tells me that I can reduce the data dimension from 3 to 2, because I see that the first 2 principal component, they are explaining 98 percent of the total variation, and this is the reduction of dimension by even 1 degree helps me a lot I can project this data on an $X-Y$ plane, and I can see various characteristics of this multivariate data **right**. And what about the covariance coefficient I have ρ_{X_i, Y_k} ; this is if you recall we have use a notation σ_{ij} , and this was e_{ij} , and I have $\sqrt{\lambda_j}$ by σ_{ii} .

So, that I have ρ_{X_1, Y_1} is 0.383, that is I am considering e_{ij} , and considering the j th Eigen vector; that is the first eigen vector, and the first element of that that is the 0.583, and I consider the **the** first eigen value, because j is equal to once. So, that is 5.83, and variance of the first that is the first element of the sigma matrix, and this is equal to 0.25; this tells me about the relative importance between X_1 , and Y_1 . Similarly, if I consider X_2 and Y_1 , what I get is that k remains 1 here, but i is 2.

So, I have thus first Eigen vector, but the second element from 8, and that is minus 0.924 the first Eigen value, and the second element second diagonal element of the sigma matrix giving me 5, and that is equal to minus 0.998. I can see that there is a direct relationship between X_1 and Y_1 , the first variable and the first principal component, whereas there is a negative relationship between X_2 and Y_1 , but nevertheless importance's are really high, there high in magnitude one is 0.925, another is minus 0.998. What about the third one X_3 with Y_1 will we have to consider the third element of the first eigen vector, and that is equal to 0.

So, there is no degree of a association between the first principal component, and the third original variable. So, in this way we can, if we 1, 2 go to the second principal

component, if you stick at the first principal component we need not go to the relation coefficient between the X_j 's X_i 's, and y_2 , but if we want to retain y_2 we should ideally, because the only when the first 2 are combine, we have 98 percent of variability explained. And then one can also consider **consider** the calculate the correlations between X_j 's - the different X_j with Y_2 .

(Refer Slide Time: 47:20)

$\Sigma = \begin{pmatrix} 1 & 4 \\ 4 & 101 \end{pmatrix}$
 $\lambda_1 = 100.16$
 $\lambda_2 = 0.84$
 $e_1 = \begin{pmatrix} 0.04 & 0.999 \\ 0.999 & -0.04 \end{pmatrix}$
 $e_2 = \begin{pmatrix} 0.999 & -0.04 \end{pmatrix}$
 $y_1 = 0.04x_1 + 0.999x_2$
 $y_2 = 0.999x_1 - 0.04x_2$
 y_1 explains $\frac{100.16}{101} \times 100 \approx 99\%$ of total variability
 $\left. \begin{aligned} \{x_1, y_1\} &= 0.04 \sqrt{\frac{100.16}{1}} = 0.4 \\ \{x_2, y_1\} &= 0.999 \sqrt{\frac{100.16}{101}} = 0.999 \end{aligned} \right\} x_2 \text{ is much more important to } y_1 \text{ than } x_1$

Let us take up the second example. And here we work with the, we will take a smaller matrix and work with both that is the dispersion as well as the correlation matrix. So, here first take consider this is case a, I have sigma this equal to 1 4 4 and 100; that is my variance covariance matrix. And my correlation coefficient matrix we can write it later on, when we consider case b. And what we have from here is the eigen values from this sigma matrix, I have two Eigen values lambda 1 and lambda 2, and these are 100.16 and 0.84. The corresponding orthonormal eigen vectors are e 1, this is 0.04 0.999 and e 2 is 0.999 minus 0.04. So, then I consider Y_1 and Y_2 ; Y_1 is nothing but I have to consider e_1 prime x , so which is $0.04 X_1$ plus $0.999 X_2$, e_2 is $0.99 X_1$ this the reverse relationship, and then minus with a negative sign here, and minus $0.04 X_2$ **right**.

So, then Y_1 explains, how much of the total variability it explains? The first eigen value lambda 1 by the some of it, which hardly makes a different, because I have 100.16 and 0.84 added to it, making this as 101, and this times 100 percent that is approximately equal to 99 percent of the total variability, **99 percent of total variability**. And Y_2

explains a rest of it. So no need to consider, no need to go to Y 2; if I consider Y 2, there is no reduction in the data dimension, and if I consider Y 2 now, this explain 100 percent. But at least from two dimensions, I have come down to one dimension that is the purpose, whether it really helps mean data dimension reduction. And then I consider the correlation coefficients also I have rho X 1 Y 1, this is important, and this is only the eigen vector the first eigen vector is coming into the picture, this is the e i j part that is e 1 1 here, and then I have the variance of the first, the standard division of the first eigen of the first principal component that is 100.16 by sigma i i sigma 11, that is 1. And this is giving me 0.0 4; 0.4 actual not 0. 0 4; and what about the correlation coefficient between Y 1 X 2; well this sigma now going to be 0.9 9 it is the first eigen value 100.16, but now it is the second variance sigma 22 and this is equal to 0.99 **right**

So, this terms may that X to is much more important the degree of association of Y 1 the only principal component that we are considering is much higher with second variable then with the first variable perfectly this no problem with that. So, X 2 is much more important to X Y 1 that an X 1. Now how, what is the true degree of this importance is a because of the much higher value of this second variance. So, look into questions like this, what we should do is actual standardize the variables and work with the correlation coefficient matrix rather than the covariance matrix. So, that is what we are going to do.

(Refer Slide Time: 51:51)

Case (b) $\rho = \begin{pmatrix} 1 & 0.4 \\ 0.4 & 1 \end{pmatrix}$

$Z_1 = \frac{X_1 - \mu_1}{\sqrt{\sigma_{11}}}, Z_2 = \frac{X_2 - \mu_2}{\sqrt{\sigma_{22}}}$

$\Sigma_Z = I_2$

$\eta_1 = 1.4, \quad f_1' = \begin{pmatrix} 0.707 & 0.707 \end{pmatrix}$

$\eta_2 = 0.6, \quad f_2' = \begin{pmatrix} 0.707 & -0.707 \end{pmatrix}$

$Y_1 = 0.707 Z_1 + 0.707 Z_2 = 0.707 \frac{(X_1 - \mu_1)}{\sqrt{\sigma_{11}}} + \frac{0.707(X_2 - \mu_2)}{\sqrt{\sigma_{22}}}$

$Y_2 = 0.707 Z_1 - 0.707 Z_2 = \dots$

Y_1 explains $\frac{1.4}{2.0} \times 100\% = 70\%$ of true variability

Y_2 explains 30% true variability

Now we consider case b part, where we have the correlation coefficient matrix calculated from the covariance matrix, just by that defining the V inverse, square root inverse of V matrix, and then we can easily get the correlation coefficient matrix, and that is equal to 1.4, I have and then what is this is 0.4 and 1 **right**. That is we are considering the standardized variables that is the standardize variables Z_1 is nothing but X_1 minus μ_1 by σ_{11} root of this. And Z_2 is nothing but X_2 minus μ_2 by root of σ_{22} . And then sigma Z matrix is actually the rho X matrix **right**. This is rho x, but I can also have the sigma Z matrix, and then this is nothing but this matrix, what I am getting here; 1 0.4 0.4 and 1 **right**.

And then I calculate the eigen values η_1 and η_2 from this rho matrix, and η_1 turns out 2 be 1.4 η_2 is 0.6 **right**. And the eigen vectors corresponding orthonormal eigen vectors f_1 prime and f_2 prime also have to be calculated; this is 0.707 0.707 and f_2 is 0.707 with minus 0.707 **right**. And then we have Y_1 , let us see that is the first thing that we going to check Y_1 explains; well what is Y_1 and Y_2 ; that is trivial. We need not write, but let us write here also Y_1 is nothing but if you want to write in terms of Z_1 and Z_2 , I should write it ideally as $0.707 Z_1$ plus $0.707 Z_2$, these are to be replaced by X_1 and X_2 and Y_2 is $0.707 Z_1$ minus $0.707 Z_2$. And Y_1 explains, and ideally then further you can write this as $0.707 X_1$ minus μ_1 by the element of the first **first** element of the sigma matrix that is 1, and you have $0.707 X_2$ minus μ_2 by second diagonal element that is root 100 and in this way **right**.

So, Y_1 explains what percentage of total variability it explains? Its own eigen value, its own variance, which is 1.4 divided by the total variability, which is sum of η_1 and η_2 that is 2 times 100 percent and that is equal to 70 percent of total variability. And if I consider Y_2 part of it, it explains if the rest of it **right**, because Y_1 and Y_2 will together consider the total variability. Now, that is what we see here the difference here, if you work with the covariance matrix, and the correlation matrix, when we had worked with the covariance matrix, we saw that Y_1 , the principal component can calculated from the covariance matrix explained 99 percent of the total variability, but here when we consider the correlation matrix, we see that Y_1 explains only about 70 percent of the total variation.

(Refer Slide Time: 56:23)

Consider coeff $\rho_{Y_1, Z_1} = 0.707 \sqrt{\frac{1.4}{1}} =$
 $\rho_{Y_1, Z_2} = 0.707 \sqrt{\frac{1.4}{1}} =$
Computation of PCs from data matrix

And let us look into the correlation coefficient part also, where we have correlation between if I have to consider the correlation coefficient of this is rho Y 1 with X 1. Well, I have to consider the first element of the first vector of the f vector that is 0.707. And then we have to consider the root of the first **root of the first** eigen value calculated from the correlation matrix that is going to be eta 1, which is root of 1.4; and then the variance, the first variance of X 1, this is well, this is actually equal to Z 1 **right**, and the variance here is nothing but 1. We can calculate this to get what is the correlation coefficient; and similarly I can have what is correlation coefficient between Y 1 and Z 2 **right**? So, this is going to be the e ij that is I am going to use the first element of the second vector, that is again 0.707. I will consider root of 4 and 1 here.

The interesting thing to see here is that Y 1 to Z 1 and Y 1 to Z 2, the degree of association is same, because I have the same value coming here, because of the fact that e 11 **right**; e 11 is equal to e 12, and I have the same eta i value coming here, and Z coming now from the correlation matrix have equal variances, which is equal to 1. So, that is precisely equal rho of Y 1 Z 1 is equal to rho of Y 1 and Z 2. A next example will be computation of PCs from data matrix; in these examples, what we had seen was that I did not have the data matrix, I only had the population variance covariance matrix given to me, that was good enough for me, I calculated the eigen values, eigen vectors, and then the principal components, and then I also talked about how much of the variabilities are getting, is getting explained by the principal component and so on and so forth.

But in reality, what we are going to have with going to have with us actually, the data, the **the** information on the multivariate data variables, and we are going to calculate our **...** We are going to calculate the whole sample covariance matrix from the data; and proceed for calculation of eigen value and eigen vector from that variance covariance matrix.