MANIPAL SCHOOL OF INFORMATION SCIENCES
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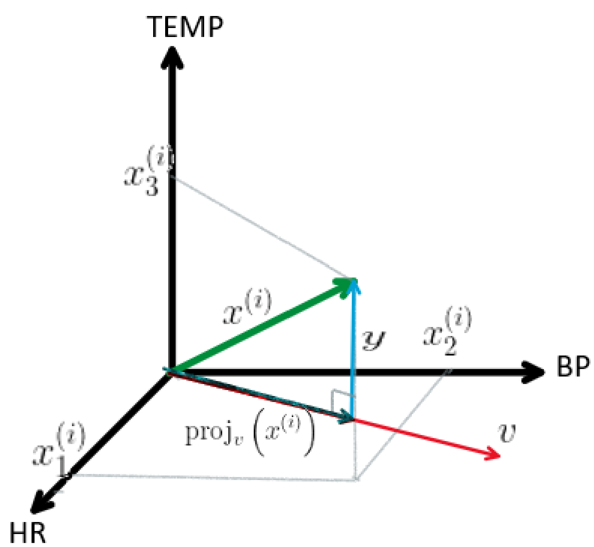
AML5101 | Applied Linear Algebra | In-class Problem Set-2

Consider the following data matrix:

	HR	BP	Temp
Patient-1	76	126	38.0
Patient-2	74	120	38.0
Patient-3	72	118	37.5
Patient-4	78	136	37.0

1. The projection of a sample vector $x^{(i)}$ along the direction specified by a vector v is intuitively a measure of how much of sample $x^{(i)}$ is contained along the direction given by v. A geometric presentation of the projection denoted as $\text{proj}\left(x^{(i)}\right)$ is given below:



We can derive an expression for the projection as follows:

$$\begin{cases} \text{proj}_v\left(x^{(i)}\right) & = cv, \text{for some unknown constant } c \text{ (why?)} \\ y & = x^{(i)} - \text{proj}_v\left(x^{(i)}\right) \text{ (why?)} \\ y \cdot v & = 0 \text{ (why?)} \end{cases}$$

$$\Rightarrow \left(x^{(i)} - \text{proj}_v\left(x^{(i)}\right)\right) \cdot v = 0$$

$$\Rightarrow \left(x^{(i)} - cv\right) \cdot v = 0$$

$$\begin{aligned}\Rightarrow x^{(i)}\cdot v - c(v\cdot v) &= 0\\ \Rightarrow c &= \frac{x^{(i)}\cdot v}{v\cdot v}\\ \Rightarrow \text{proj}_v\left(x^{(i)}\right) = cv &= \left(\frac{x^{(i)}\cdot v}{v\cdot v}\right)v.\end{aligned}$$

Note that the projection $\text{proj}_v\left(x^{(i)}\right)$ has two parts:

$$\text{proj}_v\left(x^{(i)}\right) = \left(\frac{x^{(i)}\cdot v}{v\cdot v}\right)v = \left(\frac{x^{(i)}\cdot v}{\|v\|^2}\right)v = \underbrace{\left(\frac{x^{(i)}\cdot v}{\|v\|}\right)}_{\text{shadow length}}\ \underbrace{\frac{v}{\|v\|}}_{\text{direction}}.$$

Note that the dot product $x^{(i)}\cdot v$ can also be seen as the matrix-vector product $\left(x^{(i)}\right)^{\mathrm{T}}v$. This means, the shadow length (also called the scalar projection) can be written as

$$\frac{\left(x^{(i)}\right)^{\mathrm{T}}v}{\|v\|}.$$

Calculate the scalar projection of the samples along the direction specified by the following vectors:

$$v = \begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}1\\1\\1\end{bmatrix}, \begin{bmatrix}-1\\-1\\-1\end{bmatrix}.$$

2. If the vector v, along which we want to project the samples, has unit magnitude, that is, if $\|v\| = 1$, then the scalar projection is simply

$$\frac{\left(x^{(i)}\right)^{\mathrm{T}}v}{\|v\|} = \left(x^{(i)}\right)^{\mathrm{T}}v.$$

So, we assume that the vector v has unit magnitude or convert it into a vector with unit magnitude; for example, go from $v = \begin{bmatrix}1\\1\\1\end{bmatrix}$ to $v = \frac{1}{\sqrt{3}}\begin{bmatrix}1\\1\\1\end{bmatrix}$ before calculating the scalar projection as $\left(x^{(i)}\right)^{\mathrm{T}}v$. Then, we can write down the scalar projections of all the four samples in a vector form as follows:

$$\begin{bmatrix}\left(x^{(1)}\right)^{\mathrm{T}}v\\ \left(x^{(2)}\right)^{\mathrm{T}}v\\ \left(x^{(3)}\right)^{\mathrm{T}}v\\ \left(x^{(4)}\right)^{\mathrm{T}}v\end{bmatrix}.$$

The quantity above is the same as (choose one): $Xv,\ X^{\mathrm{T}}v,\ v^{\mathrm{T}}X,\ v^{\mathrm{T}}X^{\mathrm{T}}$.

3. Calculate the mean sample from the data matrix. That is,

$$\mu = \frac{x^{(1)} + x^{(2)} + x^{(3)} + x^{(4)}}{4}.$$

4. The mean sample μ can also be calculated as (choose one):

$$\frac{1}{4}X\mathbf{1},\ \frac{1}{4}X^{\mathrm{T}}\mathbf{1},\ \frac{1}{4}\mathbf{1}^{\mathrm{T}}X,\ \frac{1}{4}\mathbf{1}^{\mathrm{T}}X^{\mathrm{T}},$$

   where $\mathbf{1}$ is the vector full of ones. In order to see this, note that

$$\mu = \frac{x^{(1)} \times 1 + x^{(2)} \times 1 + x^{(3)} \times 1 + x^{(4)} \times 1}{4}$$

   and relate this to a matrix-vector product.

5. Calculate the mean of the projected samples (that is, the scalar projections) where the projection is on to the direction of the vector $v = \begin{bmatrix}1\\1\\1\end{bmatrix}$.

6. Calculate the scalar projection of the mean sample μ on to the direction of the vector $v = \begin{bmatrix}1\\1\\1\end{bmatrix}$. Compare the answer to that of the previous question. What is your conclusion?

7. What do we conclude from the following?

$$\frac{1}{4}\left(v^{\mathrm{T}}x^{(1)} + v^{\mathrm{T}}x^{(2)} + v^{\mathrm{T}}x^{(3)} + v^{\mathrm{T}}x^{(4)}\right) = v^{\mathrm{T}}\frac{\left(x^{(1)} + x^{(2)} + x^{(3)} + x^{(4)}\right)}{4} = v^{\mathrm{T}}\mu.$$

8. Calculate the variance of the projected samples where the projection is on to the direction of the vector $v = \begin{bmatrix}1\\1\\1\end{bmatrix}$.

9. What does the following quantity represent?

$$\frac{1}{n}\sum_{i=1}^{n}\left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right)^2.$$

10. We expand the quantity from the previous step as follows (fill in the blanks):

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n}\left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right)^2 &= \frac{1}{n}\sum_{i=1}^{n}\left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right) \times \left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right)\\ &= \frac{1}{n}\sum_{i=1}^{n}\left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right) \times \left(\boxed{?}^{\mathrm{T}}v - \boxed{?}^{\mathrm{T}}v\right)\end{aligned}$$

$$= \frac{1}{n}\sum_{i=1}^{n}\left[\boxed{?}\left(x^{(i)}-\mu\right)\times\left(\left(x^{(i)}\right)^{\mathrm{T}}-\mu^{\mathrm{T}}\right)\boxed{?}\right]$$

$$= v^{\mathrm{T}}\left[\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)}-\mu\right)\left(\boxed{?}-\boxed{?}\right)^{\mathrm{T}}\right]v$$

11. We focus on the middle term that we derived at the end of the previous question. Fill in the blanks in the following (where we use the fact that $(a-b)^{\mathrm{T}} = a^{\mathrm{T}} - b^{\mathrm{T}}$):

$$\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)}-\mu\right)\left(x^{(i)}-\mu\right)^{\mathrm{T}} = \frac{1}{n}\begin{bmatrix}\boxed{?}-\mu & \boxed{?}-\mu & \dots & \boxed{?}-\mu\end{bmatrix}\times\begin{bmatrix}\left(x^{(?)}-\boxed{?}\right)^{\mathrm{T}}\\ \left(x^{(?)}-\boxed{?}\right)^{\mathrm{T}}\\ \vdots\\ \left(x^{(n)}-\boxed{?}\right)^{\mathrm{T}}\end{bmatrix}$$

$$= \frac{1}{n}\left(\begin{bmatrix}x^{(1)} & x^{(2)} & \dots & x^{(n)}\end{bmatrix}-\mu\begin{bmatrix}\boxed{?} & \boxed{?} & \dots & \boxed{?}\end{bmatrix}\right)\left(\begin{bmatrix}\boxed{?}^{\mathrm{T}}\\ \boxed{?}^{\mathrm{T}}\\ \vdots\\ \boxed{?}^{\mathrm{T}}\end{bmatrix}-\begin{bmatrix}1\\1\\ \vdots\\1\end{bmatrix}\boxed{?}^{\mathrm{T}}\right)$$

$$= \left(X^{\mathrm{T}}-\mu\mathbf{1}^{\mathrm{T}}\right)\left(\boxed{?}-\mathbf{1}\mu^{\mathrm{T}}\right).$$

Now we use the following facts:

- $\mu = \frac{1}{n}X^{\mathrm{T}}\mathbf{1}$,
- I represents the identity matrix with $IX = I$ and $XI = I$,
- $(ab)^{\mathrm{T}} = b^{\mathrm{T}}a^{\mathrm{T}}$,

to get

$$\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)}-\mu\right)\left(x^{(i)}-\mu\right)^{\mathrm{T}} = \frac{1}{n}\left(X^{\mathrm{T}}-\left(\frac{1}{n}X^{\mathrm{T}}\mathbf{1}\right)\mathbf{1}^{\mathrm{T}}\right)\left(X-\mathbf{1}\left(\frac{1}{n}X^{\mathrm{T}}\mathbf{1}\right)^{\mathrm{T}}\right)$$

$$= \frac{1}{n}\left(X^{\mathrm{T}}-\left(\frac{1}{n}X^{\mathrm{T}}\mathbf{1}\right)\mathbf{1}^{\mathrm{T}}\right)\left(X-\frac{1}{n}\mathbf{1}\boxed{?}^{\mathrm{T}}X\right)$$

$$= \frac{1}{n}\times\boxed{?}\underbrace{\left(I-\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\left(I-\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)}_{\text{See next question}}\boxed{?}.$$

12. Complete the steps below (note how the order of multiplication is maintained):

$$\left(I-\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\left(I-\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right) = I - I\times\left(\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)-\left(\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\times I+\left(\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)\left(\frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}\right)$$

$$= I - \frac{2}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}} + \frac{1}{n^2}\mathbf{1}\left(\underbrace{\mathbf{1}^{\mathrm{T}}\mathbf{1}}_{=?}\right)\mathbf{1}^{\mathrm{T}}$$
$$= I - \frac{1}{n}\boxed{?}\boxed{?}^{\mathrm{T}}.$$

13. Now use the results from (9), (10), (11) and (12) to show that the variance of the projected samples where the projection is on to the direction of a vector v is:

$$\frac{1}{n}\sum_{i=1}^{n}\left(v^{\mathrm{T}}x^{(i)} - v^{\mathrm{T}}\mu\right)^2 = v^{\mathrm{T}}\left[\frac{1}{n}\sum_{i=1}^{n}\left(x^{(i)} - \mu\right) \times \left(x^{(i)} - \mu\right)^{\mathrm{T}}\right] v = v^{\mathrm{T}}\left(\underbrace{\frac{1}{n}X^{\mathrm{T}}\boxed{?}X}_{\text{Covariance matrix}}\right)\mathrm{v}.$$

Now principal component analysis (PCA) is about finding the vector v that maximizes the variance of the projected samples given by the last term above. We will see that the vector v will turn out be the so called *eigenvector* of the covariance matrix.