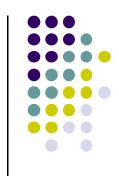
다변량통계방법론

2021년 2학기 고려대학교 통계학과 대학원

Ch 1. Aspects of Multivariate Analysis



Multivariate analysis: statistical analysis for data with simultaneous measurements on p > 1 variables. HC15 644 2/2 HS

- Investigation of the dependence among variables

- Prediction

- Hypothesis testing ANOVA

Examples of multivariate analysis

- Data reduction and simplification

- Sorting and grouping observation Enterior, cluster analysis. on 43478

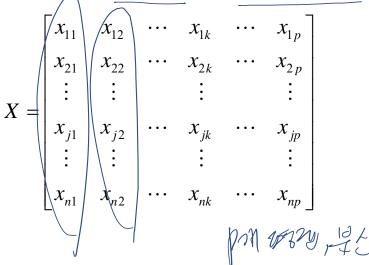
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- Arrays
 - x_{ik} : measurement of the kth variable on the jth item
 - Data with *n* measurements of *p* variables

	Variable 1	Variable 2		Variable k	•••	Variable <i>p</i>
Item 1:	x_{11}	<i>x</i> ₁₂		x_{1k}	•••	x_{1p}
Item 2:	<i>x</i> ₂₁	<i>x</i> ₂₂	•••	x_{2k}	•••	x_{2p}
:	:	:		÷		:
Item <i>j</i> :	x_{j1}	x_{j2}	•••	x_{jk}	•••	x_{jp}
:	:	:		÷		:
Item <i>n</i> :	x_{n1}	x_{n2}	•••	x_{nk}	•••	x_{np}

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- Data is expressed as a matrix *X* with *n* rows and *p* columns:





- Sample mean:
$$\bar{x}_k = \frac{1}{n} \sum_{j=1}^n x_{jk}, \quad k = 1, 2, ..., p$$

- Sample variance:
$$s_k^2 = s_{kk} = \frac{1}{n} \sum_{j=1}^n (x_{jk} - \overline{x}_k)^2, \quad k = 1, 2, ..., p$$

- Sample covariance:
$$s_{ik} = \frac{1}{n} \sum_{j=1}^{n} \left(x_{ji} - \overline{x}_i \right) \left(x_{jk} - \overline{x}_k \right), \quad i = 1, 2, ..., p, k = 1, 2, ..., p$$



- Sample correlation coefficient (or Pearson's product-moment correlation coefficient):

$$r_{ik} = \frac{S_{ik}}{\sqrt{S_{ii}} \sqrt{S_{kk}}} = \frac{\sum_{j=1}^{n} (x_{ji} - \overline{x}_i)(x_{jk} - \overline{x}_k)}{\sqrt{\sum_{j=1}^{n} (x_{ji} - \overline{x}_i)^2} \sqrt{\sum_{j=1}^{n} (x_{jk} - \overline{x}_k)^2}}, \quad i = 1, ..., p, k = 1, ..., p$$

- Sum of squares of the deviations from the mean:

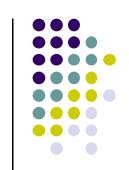
$$w_{kk} = \sum_{j=1}^{n} (x_{jk} - \overline{x}_k)^2, \quad k = 1, 2, ..., p$$

- Sum of cross-product deviations:

$$w_{ik} = \sum_{j=1}^{n} (x_{ji} - \overline{x}_i)(x_{jk} - \overline{x}_k), \quad i = 1, 2, ..., p, k = 1, 2, ..., p$$



• Descriptive statistics (continued) The descriptive statistics from n observations on p variables are summarized as



- Sample means:
$$\overline{x} = \begin{bmatrix} \overline{x}_1 \\ \overline{x}_2 \\ \vdots \\ \overline{x}_p \end{bmatrix}$$

- Sample variances and covariances: $S_n = \begin{bmatrix} s_{21} \\ \vdots \\ s_{p1} \end{bmatrix}$

- Sample correlations: $R = \begin{bmatrix} r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{bmatrix}$

140 29 27 121 221 0129 0129 (p-dimensional scatterplot (n points in p dimensions)

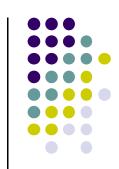
- The p measurements $(x_{i1}, x_{i2}, \dots, x_{ip})$ on the jth item represent the coordinates of a point in p-dimensional space.

- The coordinate axes correspond to the variables.

n-dimensional scatterplot (p points in n dimensions)

- The n observations of the p variables can be regarded as p points in *n*-dimensional space.

- The coordinate axes correspond to the observations.





- Euclidean distance
 - The straight-line distance from point $P = (x_1, x_2, \dots x_p)$ to the origin $O = (0,0,\dots 0)$

$$d(O,P) = \sqrt{x_1^2 + x_2^2 + \dots + x_p^2}$$

- Euclidean distance between two arbitrary points P and Q with coordinates P = $(x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$

$$d(P,Q) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \dots + (x_p - y_p)^2}$$

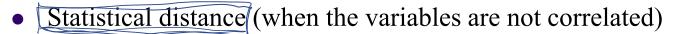
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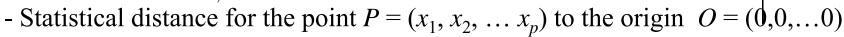
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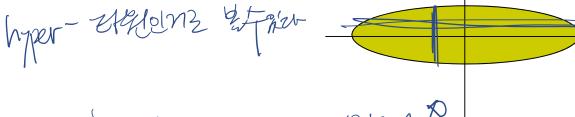


$$d(O,P) = \sqrt{\frac{x_1^2}{s_{11}} + \frac{x_2^2}{s_{22}} + \dots + \frac{x_p^2}{s_{pp}}}$$

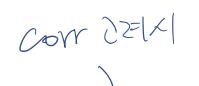
- Statistical distance between two arbitrary points P and Q with coordinates P $= (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$

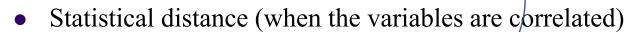
$$d(P,Q) = \sqrt{\frac{(x_1 - y_1)^2}{(s_{11})^2} + \frac{(x_2 - y_2)^2}{(s_{22})^2} + \dots + \frac{(x_p - y_p)^2}{(s_{pp})^2}} = c^2$$

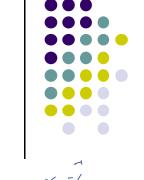
- All points P with a constant squared distance from Q lie on a hyper-ellipsoid centered at Q whose major and minor axes are parallel to the coordinate axes.

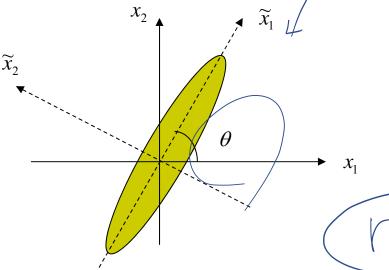


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- Rotate the original coordinate system through the angle θ while keeping the scatter fixed and label the rotated axes \widetilde{x}_1 and \widetilde{x}_2 .

- Note that
$$\widetilde{x}_1 = x_1 \cos(\theta) + x_2 \sin(\theta)$$
, $\widetilde{x}_2 = -x_1 \sin(\theta) + x_2 \cos(\theta)$.

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• Statistical distance (when the variables are correlated) (continued)

$$- d(O,P) = \sqrt{\frac{\tilde{x}_1^2}{\tilde{s}_{11}} + \frac{\tilde{x}_2^2}{\tilde{s}_{22}}}$$
$$= \sqrt{a_{11}x_1^2 + a_{22}x_2^2 + 2a_{12}x_1x_2}.$$



$$- (d^{2})(O,P) = [x_{1} \quad x_{2}] \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix} = x'Ax = c^{2}.$$

- This is called the Mahalanobis distance.

Mahalanobis distance of



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- Statistical distance (when the variables are correlated) (continued)
 - The statistical distance between the point $P = (x_1, x_2, \dots x_p)$ to the origin O = (0,0,...0)

$$d(O,P) = \sqrt{a_{11}x_1^2 + a_{22}x_2^2 + \dots + a_{pp}x_p^2 + 2a_{12}x_1x_2 + +2a_{13}x_1x_3 + \dots + 2a_{p-1,p}x_{p-1}x_p}.$$

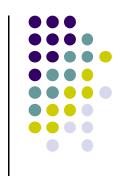
- The statistical distance between two arbitrary points P and Q with coordinates $P = (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$ is expressed by

$$d(P,Q) = \sqrt{\frac{a_{11}(x_1 - y_1)^2 + a_{22}(x_2 - y_2)^2 + \dots + a_{pp}(x_p - y_p)^2 + 2a_{12}(x_1 - y_1)(x_2 - y_2)}{+ 2a_{13}(x_1 - y_1)(x_3 - y_3) + \dots + 2a_{p-1,p}(x_{p-1} - y_{p-1})(x_p - y_p)}},$$

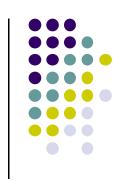
where the a's are numbers such that the distances are always nonnegative.

- Note that these distances are completely determined by the coefficients (weights) a_{ik} , i=1,2,...,p, k=1,2,...,p, shown as a rectangular array

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{12} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & & \vdots \\ a_{1p} & a_{2p} & \cdots & a_{pp} \end{bmatrix}$$
 so that $d^2(O, P) = x'Ax$.



- The entries in the array specify the distance functions.
 - The a_{ik} 's cannot be arbitrary numbers; they must be such that the computed distance is nonnegative for every pair of points.
- Other measures of distance is also possible. Any distance measure d(P,Q) between two points P and Q is valid provided that it satisfies the following properties, where R is any other intermediate point:
- -d(P,Q) = d(Q,P); $-d(P,Q) > 0 \text{ if } P \neq Q;$ -d(P,Q) = 0 if P = Q; $-d(P,Q) \leq d(P,R) + d(R,Q) \text{ (triangle inequality)}.$



• Minkowski distance between two arbitrary points P and Q with coordinates $P = (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$

$$d(P,Q) = \left[\sum_{i=1}^{p} |x_i - y_i|^m\right]^{\frac{1}{m}}$$

- For m = 1, it is called the "city-block" distance.
- For m = 2, it is the Euclidean distance.
- Canberra distance between two arbitrary points P and Q with coordinates $P = (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$

$$d(P,Q) = \sum_{i=1}^{p} \frac{|x_i - y_i|}{(x_i + y_i)}$$



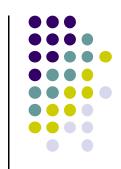
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• For *p* binary variables and two observations *P* and *Q* with values $P = (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$,

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$$(x_i - y_i)^2 = \begin{pmatrix} 0 & \text{if } x_i = y_i. \\ 1 & \text{if } x_i \neq y_i. \end{pmatrix}$$

$$-d(P,Q) = \sum_{i=1}^{p} (x_i - y_i)^2$$

- This Euclidean distance measures the number of discordance.



- Gower distance between two arbitrary points P and Q with values $P = (x_1, x_2, \dots x_p)$ and $Q = (y_1, y_2, \dots y_p)$
 - For categorical variables,

$$d_i = \begin{cases} 0 & \text{if } x_i = y_i. \\ 1 & \text{if } x_i \neq y_i. \end{cases}$$

- For numeric variables,

$$d_i = \frac{\left| x_i - y_i \right|}{R_i},$$

where R_i is the range of the *i*th variable.

$$-d(P,Q) = \frac{\sum_{i=1}^{p} \delta_{i} d_{i} w_{i}}{\sum_{i=1}^{p} \delta_{i} w_{i}}$$

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