

## Sample Geometry and Random Sampling

Shyh-Kang Jeng

Department of Electrical Engineering/  
Graduate Institute of Communication/  
Graduate Institute of Networking and  
Multimedia

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## Outline

- The Geometry of the Sample
- Random Samples and the Expected Values of the Sample Mean and Covariance Matrix
- Generalized Variance
- Sample Mean, Covariance, and Correlation as Matrix Operations
- Sample Values of Linear Combinations of Variables

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## Questions

- How to represent a sample of size  $n$  from a  $p$ -variate population?
- What is the geometrical representation of sample mean and deviation?
- How to calculate lengths and angles of deviation vectors?
- What is the geometric meaning of the correlation coefficient?

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### Array of Data

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2k} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{j1} & x_{j2} & \cdots & x_{jk} & \cdots & x_{jp} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} & \cdots & x_{np} \end{bmatrix}$$

\*a sample of size  $n$  from a  $p$ -variate population

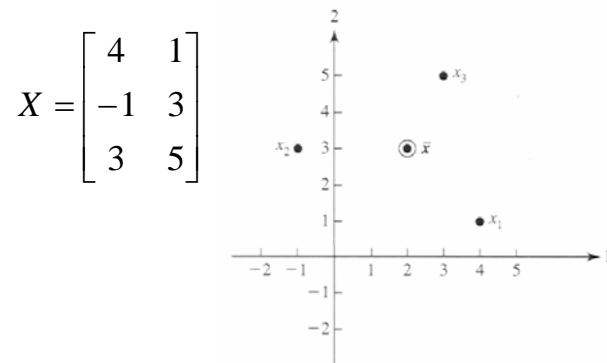
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### Row-Vector View

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2k} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{j1} & x_{j2} & \cdots & x_{jk} & \cdots & x_{jp} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} & \cdots & x_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \\ \vdots \\ \mathbf{x}_j' \\ \vdots \\ \mathbf{x}_n' \end{bmatrix}$$

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### Example 3.1



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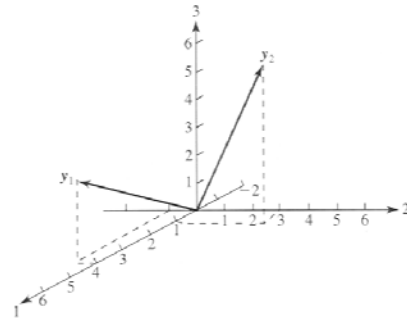
### Column-Vector View

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2k} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{j1} & x_{j2} & \cdots & x_{jk} & \cdots & x_{jp} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} & \cdots & x_{np} \end{bmatrix} = [\mathbf{y}_1 \mid \mathbf{y}_2 \mid \cdots \mid \mathbf{y}_p]$$

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### Example 3.2

$$X = \begin{bmatrix} 4 & 1 \\ -1 & 3 \\ 3 & 5 \end{bmatrix}$$



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X  
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### Geometrical Interpretation of Sample Mean and Deviation

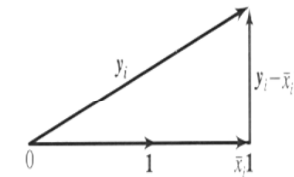
$$\mathbf{1}' = [1, 1, \dots, 1]$$

$$(\mathbf{y}_i' \frac{1}{\sqrt{n}} \mathbf{1}) \frac{1}{\sqrt{n}} \mathbf{1} = \frac{x_{1i} + x_{2i} + \dots + x_{ni}}{n} \mathbf{1} = \bar{x}_i \mathbf{1}$$

$$\bar{x}_i = \mathbf{y}_i' \frac{1}{n} \mathbf{1}$$

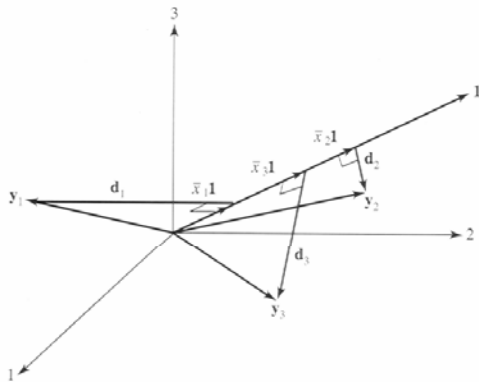
$$\mathbf{d}_i = \mathbf{y}_i - \bar{x}_i \mathbf{1}$$

$$= \begin{bmatrix} x_{1i} - \bar{x}_i \\ x_{2i} - \bar{x}_i \\ \vdots \\ x_{ni} - \bar{x}_i \end{bmatrix}$$



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### Decomposition of Column Vectors



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### Example 3.3

$$\mathbf{X} = \begin{bmatrix} 4 & 1 \\ -1 & 3 \\ 3 & 5 \end{bmatrix}, \bar{x}_1 = 2, \bar{x}_2 = 3$$

$$\bar{x}_1 \mathbf{1} = 2[1, 1, 1]' = [2, 2, 2]'$$

$$\bar{x}_2 \mathbf{1} = 3[1, 1, 1]' = [3, 3, 3]'$$

$$\mathbf{d}_1 = \mathbf{y}_1 - \bar{x}_1 \mathbf{1} = [4, -1, 3]' - [2, 2, 2]' = [2, -3, 1]'$$

$$\mathbf{d}_2 = \mathbf{y}_2 - \bar{x}_2 \mathbf{1} = [1, 3, 5]' - [3, 3, 3]' = [-2, 0, 2]'$$

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### Lengths and Angles of Deviation Vectors

$$L_{d_i}^2 = \mathbf{d}_i' \mathbf{d}_i = \sum_{j=1}^n (x_{ji} - \bar{x}_i)^2 = ns_{ii}$$

$$\mathbf{d}_i' \mathbf{d}_k = \sum_{j=1}^n (x_{ji} - \bar{x}_i)(x_{jk} - \bar{x}_k) = ns_{ik}$$

$$= L_{d_i} L_{d_k} \cos \theta_{ik}$$

$$= \sqrt{\sum_{j=1}^n (x_{ji} - \bar{x}_i)^2} \sqrt{\sum_{j=1}^n (x_{jk} - \bar{x}_k)^2} \cos \theta_{ik}$$

$$\cos \theta_{ik} = \frac{s_{ik}}{\sqrt{s_{ii}} \sqrt{s_{kk}}} = r_{ik}$$

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### Example 3.4

$$\mathbf{X} = \begin{bmatrix} 4 & 1 \\ -1 & 3 \\ 3 & 5 \end{bmatrix}$$

$$\mathbf{d}_1 = [2, -3, 1]', \quad \mathbf{d}_2 = [-2, 0, 2]'$$

$$\mathbf{d}_1' \mathbf{d}_1 = 14 = 3s_{11}, \quad \mathbf{d}_2' \mathbf{d}_2 = 8 = 3s_{22}$$

$$\mathbf{d}_1' \mathbf{d}_2 = -2 = 3s_{12}$$

$$r_{12} = \frac{s_{12}}{\sqrt{s_{11}} \sqrt{s_{22}}} = -0.189$$

$$\mathbf{S}_n = \begin{bmatrix} 14/3 & -2/3 \\ -2/3 & 8/3 \end{bmatrix}, \quad \mathbf{R} = \begin{bmatrix} 1 & -0.189 \\ -0.189 & 1 \end{bmatrix}$$

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### Questions

- What are random samples?
- What is the geometric interpretation of randomness?
- Result 3.1

## Random Matrix

$$\mathbf{X} = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1p} \\ X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'_1 \\ \mathbf{X}'_2 \\ \vdots \\ \mathbf{X}'_n \end{bmatrix}$$

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## Random Sample

- Row vectors  $\mathbf{X}'_1, \mathbf{X}'_2, \dots, \mathbf{X}'_n$  represent independent observations from a common joint distribution with density function  $f(\mathbf{x}) = f(x_1, x_2, \dots, x_p)$
- Mathematically, the joint density function of  $\mathbf{X}'_1, \mathbf{X}'_2, \dots, \mathbf{X}'_n$  is

$$f(\mathbf{x}_1)f(\mathbf{x}_2)\cdots f(\mathbf{x}_n)$$

$$f(\mathbf{x}_j) = f(x_{j1}, x_{j2}, \dots, x_{jp})$$

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## Random Sample

- Measurements of a single trial, such as  $\mathbf{X}'_j = [X_{j1}, X_{j2}, \dots, X_{jp}]$ , will usually be correlated
- The measurements from different trials must be independent
- The independence of measurements from trial to trial may not hold when the variables are likely to drift over time

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## Geometric Interpretation of Randomness

- Column vector  $\mathbf{Y}_k' = [X_{1k}, X_{2k}, \dots, X_{nk}]$  regarded as a point in  $n$  dimensions
- The location is determined by the joint probability distribution  $f(\mathbf{y}_k) = f(x_{1k}, x_{2k}, \dots, x_{nk})$
- For a random sample,  $f(\mathbf{y}_k) = f_k(x_{1k})f_k(x_{2k})\cdots f_k(x_{nk})$
- Each coordinate  $x_{jk}$  contributes equally to the location through the same marginal distribution  $f_k(x_{jk})$

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### Result 3.1

$\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$  are a random sample from a joint distribution that has mean vector  $\boldsymbol{\mu}$  and covariance matrix  $\boldsymbol{\Sigma}$ , then

$E(\bar{\mathbf{X}}) = \boldsymbol{\mu}$ , ( $\bar{\mathbf{X}}$  as an unbiased point estimate of  $\boldsymbol{\mu}$ )

$$\text{Cov}(\bar{\mathbf{X}}) = \frac{1}{n} \boldsymbol{\Sigma}, \quad E(\mathbf{S}_n) = \frac{n-1}{n} \boldsymbol{\Sigma}$$

$$E\left(\frac{n}{n-1} \mathbf{S}_n\right) = \boldsymbol{\Sigma}$$

( $\mathbf{S} = \frac{n}{n-1} \mathbf{S}_n$  as an unbiased point estimate of  $\boldsymbol{\Sigma}$ )

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### Proof of Result 3.1

$$\begin{aligned} E(\bar{\mathbf{X}}) &= E\left(\frac{1}{n} \mathbf{X}_1 + \frac{1}{n} \mathbf{X}_2 + \dots + \frac{1}{n} \mathbf{X}_n\right) \\ &= \frac{1}{n} E(\mathbf{X}_1) + \frac{1}{n} E(\mathbf{X}_2) + \dots + \frac{1}{n} E(\mathbf{X}_n) = \boldsymbol{\mu} \\ (\bar{\mathbf{X}} - \boldsymbol{\mu})(\bar{\mathbf{X}} - \boldsymbol{\mu})' &= \left(\frac{1}{n} \sum_{j=1}^n (\mathbf{X}_j - \boldsymbol{\mu})\right) \left(\frac{1}{n} \sum_{\ell=1}^n (\mathbf{X}_\ell - \boldsymbol{\mu})\right)' \\ &= \frac{1}{n^2} \sum_{j=1}^n \sum_{\ell=1}^n (\mathbf{X}_j - \boldsymbol{\mu})(\mathbf{X}_\ell - \boldsymbol{\mu})' \\ \text{Cov}(\bar{\mathbf{X}}) &= E(\bar{\mathbf{X}} - \boldsymbol{\mu})(\bar{\mathbf{X}} - \boldsymbol{\mu})' = \frac{1}{n^2} \sum_{j=1}^n \sum_{\ell=1}^n E(\mathbf{X}_j - \boldsymbol{\mu})(\mathbf{X}_\ell - \boldsymbol{\mu})' \end{aligned}$$

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### Proof of Result 3.1

$E(\mathbf{X}_j - \boldsymbol{\mu})(\mathbf{X}_\ell - \boldsymbol{\mu})' = 0$  for  $j \neq \ell$  because of independence.

$$\text{Cov}(\bar{\mathbf{X}}) = \frac{1}{n^2} \sum_{j=1}^n E(\mathbf{X}_j - \boldsymbol{\mu})(\mathbf{X}_j - \boldsymbol{\mu})' = \frac{1}{n^2} n \boldsymbol{\Sigma} = \frac{1}{n} \boldsymbol{\Sigma}$$

$$E(\mathbf{S}_n) = E\left(\frac{1}{n} \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})'\right)$$

$$\begin{aligned} &\sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})(\mathbf{X}_j - \bar{\mathbf{X}})' \\ &= \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})\mathbf{X}_j' - \sum_{j=1}^n (\mathbf{X}_j - \bar{\mathbf{X}})\bar{\mathbf{X}}' = \sum_{j=1}^n \mathbf{X}_j \mathbf{X}_j' - n \bar{\mathbf{X}} \bar{\mathbf{X}}' \end{aligned}$$

$$E(\mathbf{X}_j \mathbf{X}_j') = E((\mathbf{X}_j - \boldsymbol{\mu} + \boldsymbol{\mu})(\mathbf{X}_j - \boldsymbol{\mu} + \boldsymbol{\mu})') = \boldsymbol{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}'$$

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### Proof of Result 3.1

$$E(\bar{\mathbf{X}} \bar{\mathbf{X}}') = E((\bar{\mathbf{X}} - \boldsymbol{\mu} + \boldsymbol{\mu})(\bar{\mathbf{X}} - \boldsymbol{\mu} + \boldsymbol{\mu})') = \frac{1}{n} \boldsymbol{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}'$$

$$\begin{aligned} E(\mathbf{S}_n) &= \frac{1}{n} E\left(\sum_{j=1}^n \mathbf{X}_j \mathbf{X}_j' - n \bar{\mathbf{X}} \bar{\mathbf{X}}'\right) \\ &= \frac{1}{n} \left( n(\boldsymbol{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}') - n \left( \frac{1}{n} \boldsymbol{\Sigma} + \boldsymbol{\mu} \boldsymbol{\mu}' \right) \right) = \frac{n-1}{n} \boldsymbol{\Sigma} \end{aligned}$$

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## Some Other Estimators

The expectation of the  $(i, k)$ th entry of  $\frac{n}{n-1} \mathbf{S}_n$

$$E\left(\frac{n}{n-1} s_{ik}\right) = E\left(\frac{1}{n-1} \sum_{j=1}^n (X_{ji} - \bar{X}_i)(X_{jk} - \bar{X}_k)\right) = \sigma_{ik}$$

$$E(\sqrt{s_{ii}}) \neq \sqrt{\sigma_{ii}}, \quad E(r_{ik}) \neq \rho_{ik}$$

Biases  $E(\sqrt{s_{ii}}) - \sqrt{\sigma_{ii}}$  and  $E(r_{ik}) - \rho_{ik}$  can usually be ignored if size  $n$  is moderately large

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## Questions

- How to define a generalized sample variance?
- What is the geometric interpretation of a generalized sample variance for bivariate cases?
- What is the geometric interpretation of a generalized sample variance for multivariate cases?

## Questions

- What is the equation for points within a constant statistical distance  $c$  from the sample mean?
- Example 3.8
- Result 3.2
- Example 3.9
- Examples causing zero generalized variance

## Questions

- Example 3.10
- Result 3.3
- Result 3.4
- Generalized Sample Variance of Standardized Variables
- Example 3.11
- Total Sample Variance

## Generalized Sample Variance

Generalized Sample Variance =  $|\mathbf{S}|$

Example 3.7 : Employees and profits per employee for 16 largest publishing firms in US

$$\mathbf{S} = \begin{bmatrix} 252.04 & -68.43 \\ -68.43 & 123.67 \end{bmatrix}$$

$$|\mathbf{S}| = 26.487$$

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## Geometric Interpretation for Bivariate Case

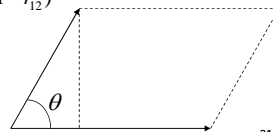
Area generated by two deviation vectors  $\mathbf{d}_1 = \mathbf{y}_1 - \bar{x}_1 \mathbf{1}$ ,  $\mathbf{d}_2 = \mathbf{y}_2 - \bar{x}_2 \mathbf{1}$

is  $area = L_{d_1} L_{d_2} \sin \theta = L_{d_1} L_{d_2} \sqrt{1 - \cos^2 \theta}$

$$L_{d_1} = \sqrt{\sum_{j=1}^n (x_{j1} - \bar{x}_1)^2} = \sqrt{(n-1)s_{11}}, \quad L_{d_2} = \sqrt{\sum_{j=1}^n (x_{j2} - \bar{x}_2)^2} = \sqrt{(n-1)s_{22}}$$

$$\cos \theta = r_{12}, \quad area = (n-1) \sqrt{s_{11}s_{22}(1-r_{12}^2)}$$

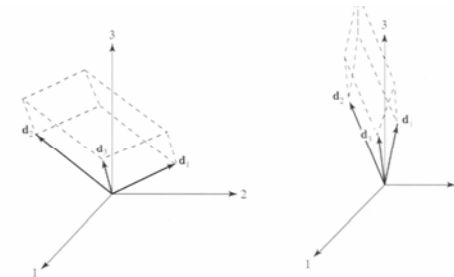
$$|\mathbf{S}| = \begin{vmatrix} s_{11} & \sqrt{s_{11}s_{22}}r_{12} \\ \sqrt{s_{11}s_{22}}r_{12} & s_{22} \end{vmatrix} = s_{11}s_{22}(1-r_{12}^2) \\ = (area)^2 / (n-1)^2$$



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## Generalized Sample Variance for Multivariate Cases

$$|\mathbf{S}| = (n-1)^{-p} (volume)^2$$



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### Interpretation in $p$ -space Scatter Plot

- ✦ Equation for points within a constant distance  $c$  from the sample mean

$$(\mathbf{x} - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) \leq c^2$$

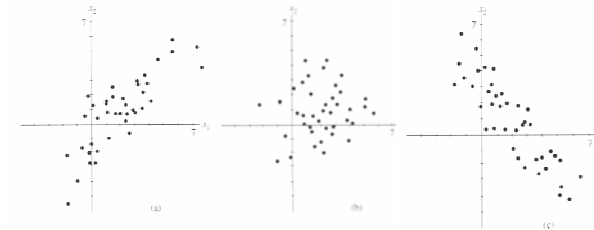
$$\text{Volume of } \{(\mathbf{x} - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) \leq c^2\}$$

$$= k_p |\mathbf{S}|^{1/2} c^p$$

A large volume corresponds to a large generalized variance

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### Example 3.8: Scatter Plots



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### Example 3.8: Sample Mean and Variance-Covariance Matrices

$$\mathbf{S} = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}, r = 0.8$$

$$\mathbf{S} = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}, r = 0$$

$$\mathbf{S} = \begin{bmatrix} 5 & -4 \\ -4 & 5 \end{bmatrix}, r = -0.8$$

$$\bar{\mathbf{x}}' = [2, 1], |\mathbf{S}| = 9 \text{ for all three cases}$$

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### Example 3.8: Eigenvalues and Eigenvectors

$$\begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix} : \lambda_1 = 9, \lambda_2 = 1$$

$$\mathbf{e}_1' = [1/\sqrt{2}, 1/\sqrt{2}], \mathbf{e}_2' = [1/\sqrt{2}, -1/\sqrt{2}]$$

$$\begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix} : \lambda_1 = 3, \lambda_2 = 3$$

$$\mathbf{e}_1' = [1, 0], \mathbf{e}_2' = [0, 1]$$

$$\begin{bmatrix} 5 & -4 \\ -4 & 5 \end{bmatrix} : \lambda_1 = 9, \lambda_2 = 1$$

$$\mathbf{e}_1' = [1/\sqrt{2}, -1/\sqrt{2}], \mathbf{e}_2' = [1/\sqrt{2}, 1/\sqrt{2}]$$

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### Example 3.8: Mean-Centered Ellipse

$$(\mathbf{x} - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) \leq c^2$$

$$(\mathbf{x} - \bar{\mathbf{x}})' \mathbf{S}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) = \frac{y_1^2}{\lambda_1} + \frac{y_2^2}{\lambda_2}$$

$\mathbf{S}^{-1}$ : eigenvalues  $\frac{1}{\lambda_1}, \frac{1}{\lambda_2}$ ; eigenvectors  $\mathbf{e}_1, \mathbf{e}_2$

$$(\because \mathbf{S}\mathbf{e} = \lambda\mathbf{e}, \quad \mathbf{e} = \lambda\mathbf{S}^{-1}\mathbf{e})$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \mathbf{e}_1' \\ \mathbf{e}_2' \end{bmatrix} \begin{bmatrix} x_1 - \bar{x}_1 \\ x_2 - \bar{x}_2 \end{bmatrix}$$

Choose  $c^2 = 5.99$  to cover approximately 95% observations

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### Example 3.8: Semi-major and Semi-minor Axes

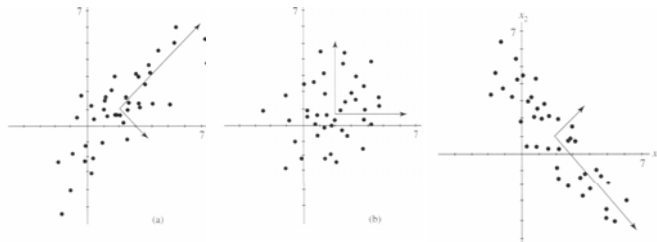
$$\mathbf{S} = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}, a = 3\sqrt{5.99}, b = \sqrt{5.99}$$

$$\mathbf{S} = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}, a = \sqrt{3}\sqrt{5.99}, b = \sqrt{3}\sqrt{5.99}$$

$$\mathbf{S} = \begin{bmatrix} 5 & -4 \\ -4 & 5 \end{bmatrix}, a = 3\sqrt{5.99}, b = \sqrt{5.99}$$

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### Example 3.8: Scatter Plots with Major Axes



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### Result 3.2

➤ The generalized variance is zero when the columns of the following matrix are linear dependent

$$\begin{bmatrix} \mathbf{x}_1' - \bar{\mathbf{x}}' \\ \mathbf{x}_2' - \bar{\mathbf{x}}' \\ \vdots \\ \mathbf{x}_n' - \bar{\mathbf{x}}' \end{bmatrix} = \begin{bmatrix} x_{11} - \bar{x}_1 & x_{12} - \bar{x}_2 & \cdots & x_{1p} - \bar{x}_p \\ x_{21} - \bar{x}_1 & x_{22} - \bar{x}_2 & \cdots & x_{2p} - \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} - \bar{x}_1 & x_{n2} - \bar{x}_2 & \cdots & x_{np} - \bar{x}_p \end{bmatrix} = \mathbf{X} - \mathbf{1}\bar{\mathbf{x}}'$$

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### Proof of Result 3.2

$$0 = a_1 \text{col}_1(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}') + \dots + a_p \text{col}_p(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$$

$$= (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a}, \quad \mathbf{a} \neq \mathbf{0}$$

$$(n-1)\mathbf{S} = (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$$

$$\therefore (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$$

$$= \begin{bmatrix} \mathbf{x}_1' - \bar{\mathbf{x}}' & \mathbf{x}_2' - \bar{\mathbf{x}}' & \dots & \mathbf{x}_p' - \bar{\mathbf{x}}' \end{bmatrix} \begin{bmatrix} \mathbf{x}_1' - \bar{\mathbf{x}}' \\ \mathbf{x}_2' - \bar{\mathbf{x}}' \\ \vdots \\ \mathbf{x}_n' - \bar{\mathbf{x}}' \end{bmatrix}$$

$$= \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'$$

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### Proof of Result 3.2

$$(n-1)\mathbf{S}\mathbf{a} = (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a} = 0$$

$$a_1 \text{col}_1(\mathbf{S}) + \dots + a_p \text{col}_p(\mathbf{S}) = 0 \Rightarrow |\mathbf{S}| = 0$$

if  $|\mathbf{S}| = 0, \exists \mathbf{a}$  such that  $\mathbf{S}\mathbf{a} = 0$

$$0 = (n-1)\mathbf{S}\mathbf{a} = (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a}$$

$$\mathbf{a}'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a} = 0$$

$$L^2_{(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a}} = 0 \Rightarrow (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a} = 0$$

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### Example 3.9

$$\mathbf{X} = \begin{bmatrix} 1 & 2 & 5 \\ 4 & 1 & 6 \\ 4 & 0 & 4 \end{bmatrix}, \bar{\mathbf{x}}' = [3, 1, 5], \mathbf{X} - \mathbf{1}\bar{\mathbf{x}}' = \begin{bmatrix} -2 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & -1 & -1 \end{bmatrix}$$

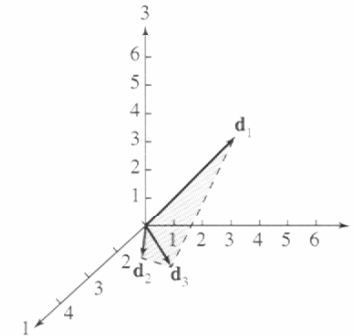
$$\mathbf{d}_1' = [-2, 1, 1], \mathbf{d}_2' = [1, 0, -1], \mathbf{d}_3' = [0, 1, -1]$$

$$\mathbf{d}_3 = \mathbf{d}_1 + 2\mathbf{d}_2 \Rightarrow |\mathbf{S}| = 0$$

$$\text{check : } \mathbf{S} = \begin{bmatrix} 3 & -3/2 & 0 \\ -3/2 & 1 & 1/2 \\ 0 & 1/2 & 1 \end{bmatrix} \Rightarrow |\mathbf{S}| = 0$$

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### Example 3.9



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## Examples Cause Zero Generalized Variance

### ➤ Example 1

- Data are test scores
- Included variables that are sum of others
- e.g., algebra score and geometry score were combined to total math score
- e.g., class midterm and final exam scores summed to give total points

### ➤ Example 2

- Total weight of chemicals was included along with that of each component

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## Example 3.10

$$\mathbf{X} = \begin{bmatrix} 1 & 9 & 10 \\ 4 & 12 & 16 \\ 2 & 10 & 12 \\ 5 & 8 & 13 \\ 3 & 11 & 14 \end{bmatrix}, \mathbf{X} - \mathbf{1}\bar{\mathbf{x}}' = \begin{bmatrix} -2 & -1 & -3 \\ 1 & 2 & 3 \\ -1 & 0 & -1 \\ 2 & -2 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \mathbf{S} = \begin{bmatrix} 2.5 & 0 & 2.5 \\ 0 & 2.5 & 2.5 \\ 2.5 & 2.5 & 5.0 \end{bmatrix}$$

$$|\mathbf{S}| = 0 \Rightarrow \mathbf{S}\mathbf{a} = \mathbf{0}$$

Eigenvector corresponding to zero eigenvalues of S

$$\Rightarrow \mathbf{a}' = [1, 1, -1]$$

$$\therefore 1(x_{j1} - \bar{x}_1) + 1(x_{j2} - \bar{x}_2) - (x_{j3} - \bar{x}_3) = 0$$

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## Result 3.3

- If the sample size is less than or equal to the number of variables ( $n \leq p$ ) then  $|\mathbf{S}| = 0$  for all samples

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## Proof of Result 3.3

The  $n$  row vectors of  $\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}'$  sum to the zero vector

$$\text{because } \sum_{j=1}^n x_{jk} = \sum_{j=1}^n \bar{x}_k$$

Thus the rank of  $\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}'$  is less than or equal to  $n - 1$ , i.e., less than or equal to  $p - 1$ , because of  $n \leq p$

$$\text{Since } (n - 1)\mathbf{S} = (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}'),$$

$$(n - 1)\text{col}_k(\mathbf{S}) = (\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')'\text{col}_k(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$$

$$= (x_{1k} - \bar{x}_k)\text{row}_1(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')' + \cdots + (x_{nk} - \bar{x}_k)\text{row}_n(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$$

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### Proof of Result 3.3

$\therefore \text{row}_1(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')$  is a linear combination of the remaining row vectors  
 $\text{col}_k(\mathbf{S})$  is a linear combination of at most  $n-1$  linear independent of transpose of row vectors  
 The rank of  $\mathbf{S}$  is thus less than or equal to  $n-1$ , i.e., less than or equal to  $p-1$ .  
 Since  $\mathbf{S}$  is a  $p$  by  $p$  matrix,  $|\mathbf{S}| = 0$

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### Result 3.4

- Let the  $p$  by 1 vectors  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ , where  $\mathbf{x}_j'$  is the  $j$ th row of the data matrix  $\mathbf{X}$ , be realizations of the independent random vectors  $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n$ .
- If the linear combination  $\mathbf{a}'\mathbf{X}_j$  has positive variance for each non-zero constant vector  $\mathbf{a}$ , then, provided that  $p < n$ ,  $\mathbf{S}$  has full rank with probability 1 and  $|\mathbf{S}| > 0$
- If, with probability 1,  $\mathbf{a}'\mathbf{X}_j$  is a constant  $c$  for all  $j$ , then  $|\mathbf{S}| = 0$

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### Proof of Part 2 of Result 3.4

$\mathbf{a}'\mathbf{X}_j = a_1X_{j1} + a_2X_{j2} + \dots + a_pX_{jp} = c$  with probability 1,  
 $\mathbf{a}'\mathbf{x}_j = c$  for all  $j$ . The sample mean for it is

$$\sum_{j=1}^n (a_1x_{j1} + a_2x_{j2} + \dots + a_px_{jp}) / n = \mathbf{a}'\bar{\mathbf{x}} = c$$

$$(\mathbf{X} - \mathbf{1}\bar{\mathbf{x}}')\mathbf{a} = a_1 \begin{bmatrix} x_{11} - \bar{x}_1 \\ \vdots \\ x_{n1} - \bar{x}_1 \end{bmatrix} + \dots + a_p \begin{bmatrix} x_{1p} - \bar{x}_p \\ \vdots \\ x_{np} - \bar{x}_p \end{bmatrix}$$

$$= \begin{bmatrix} \mathbf{a}'\mathbf{x}_1 - \mathbf{a}'\bar{\mathbf{x}} \\ \vdots \\ \mathbf{a}'\mathbf{x}_n - \mathbf{a}'\bar{\mathbf{x}} \end{bmatrix} = \begin{bmatrix} c - c \\ \vdots \\ c - c \end{bmatrix} = \mathbf{0} \Rightarrow |\mathbf{S}| = 0$$

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### Generalized Sample Variance of Standardized Variables

Generalized sample variance of the standardized variables =  $|\mathbf{R}|$

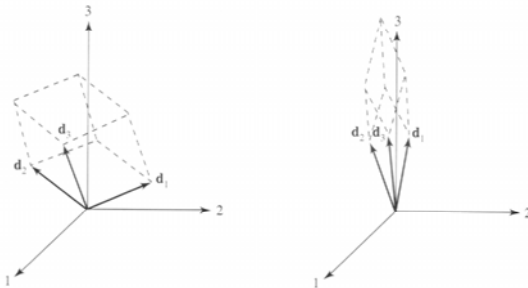
$$\frac{y_i - \bar{y}_i}{\sqrt{s_{ii}}} = \begin{bmatrix} \frac{x_{1i} - \bar{x}_i}{\sqrt{s_{ii}}} & \frac{x_{2i} - \bar{x}_i}{\sqrt{s_{ii}}} & \dots & \frac{x_{ni} - \bar{x}_i}{\sqrt{s_{ii}}} \end{bmatrix},$$

$$|\mathbf{R}| = (n-1)^{-p} (\text{volume})^2, |\mathbf{S}| = (s_{11}s_{22} \dots s_{pp}) |\mathbf{R}|$$

$|\mathbf{R}|$  is large when all  $r_{ik}$  are nearly zero, and is small when one or more  $r_{ik}$  are nearly +1 or -1

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### Volume Generated by Deviation Vectors of Standardized Variables



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### Example 3.11

$$\mathbf{S} = \begin{bmatrix} 4 & 3 & 1 \\ 3 & 9 & 2 \\ 1 & 2 & 1 \end{bmatrix}, \quad \mathbf{R} = \begin{bmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 2/3 \\ 1/2 & 2/3 & 1 \end{bmatrix}$$

$$s_{11} = 4, \quad s_{22} = 9, \quad s_{33} = 1$$

$$|\mathbf{S}| = 14, \quad |\mathbf{R}| = \frac{7}{18}, \quad |\mathbf{S}| = s_{11}s_{22}s_{33}|\mathbf{R}|$$

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### Total Sample Variance

$$\text{Total Sample Variance} = s_{11} + s_{22} + \cdots + s_{pp}$$

Pays no attention to the orientation of the residual vectors

$$\text{Example 3.7: } \mathbf{S} = \begin{bmatrix} 252.04 & -68.43 \\ -68.43 & 123.67 \end{bmatrix}$$

$$\text{Total sample variance} = 375.71$$

$$\text{Example 3.9: } \mathbf{S} = \begin{bmatrix} 3 & -3/2 & 0 \\ -3/2 & 1 & 1/2 \\ 0 & 1/2 & 1 \end{bmatrix}$$

$$\text{Total sample variance} = 5$$

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### Outline

- The Geometry of the Sample
- Random Samples and the Expected Values of the Sample Mean and Covariance Matrix
- Generalized Variance
- Sample Mean, Covariance, and Correlation as Matrix Operations
- Sample Values of Linear Combinations of Variables

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## Questions

- How to compute sample mean by matrix operation?
- How to compute sample covariance matrix by matrix operation?
- How to compute sample correlation coefficient matrix by matrix operation?

## Sample Mean as Matrix Operation

$$\begin{aligned}\bar{\mathbf{x}} &= \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{bmatrix} = \begin{bmatrix} \mathbf{y}'_1 \mathbf{1}/n \\ \mathbf{y}'_2 \mathbf{1}/n \\ \vdots \\ \mathbf{y}'_p \mathbf{1}/n \end{bmatrix} = \frac{1}{n} \begin{bmatrix} x_{11} & x_{21} & \cdots & x_{n1} \\ x_{12} & x_{22} & \cdots & x_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1p} & x_{2p} & \cdots & x_{np} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \\ &= \frac{1}{n} \mathbf{X} \mathbf{1}\end{aligned}$$

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## Covariance as Matrix Operation

$$\begin{aligned}\begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \\ \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \end{bmatrix} &= \mathbf{1} \bar{\mathbf{x}}' = \frac{1}{n} \mathbf{1} \mathbf{1}' \mathbf{X} \\ \begin{bmatrix} x_{11} - \bar{x}_1 & x_{12} - \bar{x}_2 & \cdots & x_{1p} - \bar{x}_p \\ x_{21} - \bar{x}_1 & x_{22} - \bar{x}_2 & \cdots & x_{2p} - \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} - \bar{x}_1 & x_{n2} - \bar{x}_2 & \cdots & x_{np} - \bar{x}_p \end{bmatrix} &= \mathbf{X} - \mathbf{1} \mathbf{1}' \mathbf{X}\end{aligned}$$

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## Covariance as Matrix Operation

$$\begin{aligned}(n-1)\mathbf{S} &= \begin{bmatrix} x_{11} - \bar{x}_1 & x_{21} - \bar{x}_1 & \cdots & x_{n1} - \bar{x}_1 \\ x_{12} - \bar{x}_2 & x_{22} - \bar{x}_2 & \cdots & x_{n2} - \bar{x}_2 \\ \vdots & \vdots & \ddots & \vdots \\ x_{1p} - \bar{x}_p & x_{2p} - \bar{x}_p & \cdots & x_{np} - \bar{x}_p \end{bmatrix} \times \\ &\quad \begin{bmatrix} x_{11} - \bar{x}_1 & x_{12} - \bar{x}_2 & \cdots & x_{1p} - \bar{x}_p \\ x_{21} - \bar{x}_1 & x_{22} - \bar{x}_2 & \cdots & x_{2p} - \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} - \bar{x}_1 & x_{n2} - \bar{x}_2 & \cdots & x_{np} - \bar{x}_p \end{bmatrix} \\ &= \left( \mathbf{X} - \frac{1}{n} \mathbf{1} \mathbf{1}' \mathbf{X} \right)' \left( \mathbf{X} - \frac{1}{n} \mathbf{1} \mathbf{1}' \mathbf{X} \right)\end{aligned}$$

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## Covariance as Matrix Operation

$$\begin{aligned}
 & \left( \mathbf{X} - \frac{1}{n} \mathbf{1}\mathbf{1}'\mathbf{X} \right)' \left( \mathbf{X} - \frac{1}{n} \mathbf{1}\mathbf{1}'\mathbf{X} \right) \\
 &= \mathbf{X}' \left( \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \right)' \left( \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \right) \mathbf{X} \\
 & \left( \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \right)' \left( \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \right) = \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' - \frac{1}{n} \mathbf{1}\mathbf{1}' + \frac{1}{n^2} \mathbf{1}\mathbf{1}'\mathbf{1}\mathbf{1}' \\
 &= \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \quad (\because \mathbf{1}'\mathbf{1} = n) \\
 & \mathbf{S} = \frac{1}{n-1} \mathbf{X}' \left( \mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}' \right) \mathbf{X}
 \end{aligned}$$

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## Sample Standard Deviation Matrix

$$\begin{aligned}
 \mathbf{D}^{1/2} &= \begin{bmatrix} \sqrt{s_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{s_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{s_{pp}} \end{bmatrix}, \mathbf{D}^{-1/2} = \begin{bmatrix} 1/\sqrt{s_{11}} & 0 & \cdots & 0 \\ 0 & 1/\sqrt{s_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/\sqrt{s_{pp}} \end{bmatrix} \\
 \mathbf{R} &= \begin{bmatrix} \frac{s_{11}}{\sqrt{s_{11}}\sqrt{s_{11}}} & \frac{s_{12}}{\sqrt{s_{11}}\sqrt{s_{22}}} & \cdots & \frac{s_{1p}}{\sqrt{s_{11}}\sqrt{s_{pp}}} \\ \frac{s_{21}}{\sqrt{s_{22}}\sqrt{s_{11}}} & \frac{s_{22}}{\sqrt{s_{22}}\sqrt{s_{22}}} & \cdots & \frac{s_{2p}}{\sqrt{s_{22}}\sqrt{s_{pp}}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{s_{p1}}{\sqrt{s_{pp}}\sqrt{s_{11}}} & \frac{s_{p2}}{\sqrt{s_{pp}}\sqrt{s_{22}}} & \cdots & \frac{s_{pp}}{\sqrt{s_{pp}}\sqrt{s_{pp}}} \end{bmatrix} = \mathbf{D}^{-1/2} \mathbf{S} \mathbf{D}^{-1/2} \\
 \mathbf{S} &= \mathbf{D}^{1/2} \mathbf{R} \mathbf{D}^{1/2}
 \end{aligned}$$

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## Questions

- Result 3.5
- Result 3.6



### Result 3.5

$$\mathbf{b}'\mathbf{X} = b_1X_1 + b_2X_2 + \cdots + b_pX_p$$

$$\mathbf{c}'\mathbf{X} = c_1X_1 + c_2X_2 + \cdots + c_pX_p$$

$$\text{Sample mean of } \mathbf{b}'\mathbf{X} = \mathbf{b}'\bar{\mathbf{x}}$$

$$\text{Sample variance of } \mathbf{b}'\mathbf{X} = \mathbf{b}'\mathbf{S}\mathbf{b}$$

$$\text{Sample covariance of } \mathbf{b}'\mathbf{X} \text{ and } \mathbf{c}'\mathbf{X} = \mathbf{b}'\mathbf{S}\mathbf{c}$$

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### Proof of Result 3.5

$$\mathbf{b}'\mathbf{x}_j = b_1x_{j1} + b_2x_{j2} + \cdots + b_px_{jp}$$

$$\text{Sample mean} = \frac{\mathbf{b}'\mathbf{x}_1 + \mathbf{b}'\mathbf{x}_2 + \cdots + \mathbf{b}'\mathbf{x}_n}{n} = \mathbf{b}'\bar{\mathbf{x}}$$

$$(\mathbf{b}'\mathbf{x}_j - \mathbf{b}'\bar{\mathbf{x}})^2 = \mathbf{b}'(\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'\mathbf{b}$$

$$\begin{aligned} \text{Sample variance} &= \frac{1}{n-1} \sum_{j=1}^n (\mathbf{b}'\mathbf{x}_j - \mathbf{b}'\bar{\mathbf{x}})^2 \\ &= \frac{1}{n-1} \mathbf{b}' \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'\mathbf{b} = \mathbf{b}'\mathbf{S}\mathbf{b} \end{aligned}$$

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### Proof of Result 3.5

$$\begin{aligned} \text{Sample covariance} &= \frac{1}{n-1} \sum_{j=1}^n (\mathbf{b}'\mathbf{x}_j - \mathbf{b}'\bar{\mathbf{x}})(\mathbf{c}'\mathbf{x}_j - \mathbf{c}'\bar{\mathbf{x}}) \\ &= \frac{1}{n-1} \mathbf{b}' \sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}})(\mathbf{x}_j - \bar{\mathbf{x}})'\mathbf{c} = \mathbf{b}'\mathbf{S}\mathbf{c} \end{aligned}$$

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### Result 3.6

$$\mathbf{A}\mathbf{X} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ a_{21} & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{q1} & a_{q2} & \cdots & a_{qp} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_p \end{bmatrix}$$

$$\text{Sample mean of } \mathbf{A}\mathbf{X} = \mathbf{A}\bar{\mathbf{x}}$$

$$\text{Sample covariance matrix} = \mathbf{A}\mathbf{S}\mathbf{A}'$$

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