Displays for Statistics 5401/8401

Lecture 6

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Class Web Page

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Lecture 6

Multivariate population mean vector

Suppose  $X = [X_1, X_2, ... X_D]'$  is a random vector (X1, ..., X are p jointly distributed random variables).

The population mean vector (true mean, expectation) of X is

$$\mu_{x} = E[X] = [\mu_{1}, \mu_{2}, ..., \mu_{p}]',$$

$$\mu_{i} = E[X_{i}], j = 1, ..., p$$

 $\mu_{\rm v}$  has the same dimensions as X (p × 1).

Note:

Statistics 5401

**x** is the vector of <u>univariate</u> sample means

 $\mu_{x}$  is the vector of the <u>univariate</u> population means.

Statistics 5401

September 19, 2005

Statistics 5401

Lecture 6

September 19, 2005

September 19, 2005

The population mean or expectation of a <u>random matrix</u>  $Y = [y_{ij}]$  is the matrix  $\mu_{Y} = [\mu_{y_{ij}}] = [E[y_{ij}]].$ 

It can be useful to equate a n by p matrix, say  $X = [X_1, X_2, ..., X_n]$ , to the np by 1 vector

$$\operatorname{vec}(\mathbf{X}) \equiv \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \vdots \\ \mathbf{X}_n \end{bmatrix}, \operatorname{np} \times 1$$

Clearly

$$\mu_{\text{vec}(\mathbf{x})} = \text{vec}(\mu_{\mathbf{x}})$$

that is the matrix is "unravelled" or unrolled column by column. This is what vector(x) creates when x is a matrix.

Population variance matrix Vocabulary

The **population covariance** between X, and  $X_{k}$ ,  $j \neq k$ , is

•  $\sigma_{ik} \equiv E[(X_i - \mu_i)(X_k - \mu_k)].$ 

**Properties** 

- $\sigma_{ik} = \sigma_{ki}$  (symmetry)
- $\sigma_{ik} > 0 \Leftrightarrow positive association$
- $\sigma_{ik} < 0 \iff$  negative association

The population variance is

- $\sigma_j^2 = \sigma_{jj} = E[(X_j \mu_j)^2] \ge 0$   $|\sigma_{jk}| \le \sqrt{\{\sigma_{jj}\sigma_{kk}\}}, \sigma_{jk}^2 \le \sigma_{jj}^2 \sigma_{kk}^2$
- $-1 \le \rho_{ik} \le 1$ ,  $\rho_{ik} = \sigma_{ik} / \sqrt{\{\sigma_{ij}\sigma_{kk}\}}$ =  $cov[X_i, X_k]/{SD[X_i]SD[X_k]}$ ,  $SD[X_i] = \sqrt{\sigma_{ii}}$

 $\rho_{\mbox{\tiny jk}}$  is the population (true) correlation between  $X_i$  and  $X_k$ .

Statistics 5401

The population *covariance matrix* or variance matrix of  $X = [X_1, ..., X_n]$ ' is the p×p matrix

Lecture 6

$$V[x] = \sum_{x} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \dots & \sigma_{1p} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} & \dots & \sigma_{2p} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} & \dots & \sigma_{3p} \\ \dots & \dots & \dots & \dots & \dots \\ \sigma_{1p} & \sigma_{2p} & \sigma_{3p} & \dots & \sigma_{pp} \end{bmatrix}$$

- $\Sigma$  is symmetric ( $\Sigma$ ' =  $\Sigma$ )
- The diagonal elements  $\sigma_{_{ij}}$  of  $\Sigma$  are variances (o<sup>2</sup>)
- The off-diagonal o<sub>ik</sub>, j ≠ k are covariances.
- When  $\mathbf{a} = [\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_p]'$  is constant so  $\mathbf{a}' \mathbf{x}$ is a linear combination, with variance  $V[a'x] = a'\Sigma a \ge 0$ . Hence  $\Sigma$  is positive semi-definite

Statistics 5401

September 19, 2005

## Population correlation matrix

The population (Pearson) correlation between X, and X, is

$$\rho_{jk} \equiv \sigma_{jk}^{\prime} / \sqrt{(\sigma_{jj} \sigma_{kk})} = \rho_{kj} = \text{cov}[Z_j, Z_k].$$

Standardized  $X_i$  is  $Z_i = (X_i - \mu_i) / \sqrt{\sigma_{ii}}$ .

Note:  $\rho_{ik} = 0 \iff \sigma_{ik} = 0$ 

The symmetric p by p matrix

$$\mathbf{R} = \begin{bmatrix} 1 & \rho_{12} & \rho_{13} & \dots & \rho_{1p} \\ \rho_{12} & 1 & \rho_{23} & \dots & \rho_{2p} \\ \rho_{13} & \rho_{23} & 1 & \dots & \rho_{3p} \\ \dots & \dots & \dots & \dots \\ \rho_{1p} & \rho_{2p} & \rho_{3p} & \dots & 1 \end{bmatrix} = \mathbf{D}^{-1} \mathbf{\Sigma} \mathbf{D}^{-1}$$

is the population correlation matrix

- = diag[ $\sqrt{\sigma_{11}}$ , $\sqrt{\sigma_{22}}$ ,..., $\sqrt{\sigma_{pp}}$ ]
- $\mathbf{D}^{-1}$  = diag[1/ $\sqrt{\sigma}_{11}$ ,1/ $\sqrt{\sigma}_{22}$ ,...,1/ $\sqrt{\sigma}_{00}$ ].

When  $\Sigma$  = diag[ $\sigma_{11}, \sigma_{22}, ..., \sigma_{pp}$ ] is diagonal,

- $\rho_{ii} = 0$ ,  $i \neq j$
- $R = I_p = diag[1, 1,..., 1].$

I hope I don't need to say this:

It is important to distinguish these population variances and covariances from the sample variances and covariances

- $s_{ij} = \sum_{1 \le i \le n} (X_{ij} \overline{X}_j)^2 / (n-1)$  is not the
- $s_{ik} = \sum_{1 \le i \le n} (X_{ij} \overline{X}_i)(X_{ik} \overline{X}_k)/(n-1)$  is not the same as  $\sigma_{ik}$

and to distinguish the population variance matrix  $\Sigma$  from the sample variance matrix S.

You never test a null hypothesis about the value of x or S.

To state that a test statistic tests the null hypothesis  $H_n$ :  $\overline{\mathbf{x}} = \mathbf{0}$  is nonsense. Probably what is meant is  $H_0$ :  $\mu = 0$ .

Statistics 5401

Lecture 6

September 19, 2005

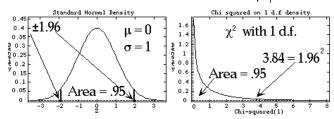
## Univariate normal Distribution

X is  $N(\mu, \sigma^2)$  means X is normal with mean  $\mu$  and variance  $\sigma^2$ . Its density is

$$f(x,\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left[\frac{(x-\mu)^2}{\sigma^2}\right]} = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$

where  $z = (x - \mu)/\sigma$  (standardized x). Facts:

- z is <u>standard normal</u> N(0,1<sup>2</sup>)
- $z^2 = \frac{(x-\mu)^2}{\sigma^2}$  is  $\chi_1^2$  (chi-squared, 1 DF) Densities of Z and  $\chi_{_{\scriptscriptstyle 1}}^{^{2}}$



The total area under each curve is 1.

The area under the  $\chi_1^2$  curve to the left of  $3.84 = 1.96^2$  is

$$P(\chi_1^2 \le 3.84) = P(|z| \le 1.96) = .95$$

# Multivariate normal distribution Notation

Lecture 6

$$\mathbf{x} = [x_1, x_2, ..., x_p]$$
 is  $N_p(\mathbf{μ}, \mathbf{Σ})$ ,

- μ p×1 vector
- **Σ** p×p positive definite symmetric matrix.

*Density* of  $N_{p}(\mu, \Sigma)$  random vector  $\mathbf{x}$ :

$$f(\mathbf{x}, \mathbf{\Sigma}, \mu) = \frac{e^{-\frac{1}{2}[(\mathbf{x} - \mu)' \mathbf{\Sigma}^{-1}(\mathbf{x} - \mu)]}}{(2\pi)^{p/2} \sqrt{\det(\mathbf{\Sigma})}} = \frac{e^{-\frac{1}{2}Q(\mathbf{x} - \mu, \mathbf{\Sigma})}}{(2\pi)^{p/2} \sqrt{\det(\mathbf{\Sigma})}}$$

#### Multivariate Normal Facts

- $E[x] = \mu$  p parameters
- $V[x] = \Sigma$  p(p+1)/2 parameters, p variances, (p-1)/2 covariances
- $Q(x \mu, \Sigma) \equiv (x \mu)' \Sigma^{-1}(x \mu)$ =  $trace(\Sigma^{-1}(x - \mu)(x - \mu)') \sim \chi_p^2$

When  $p = 1 (N(\mu, \sigma^2))$ 

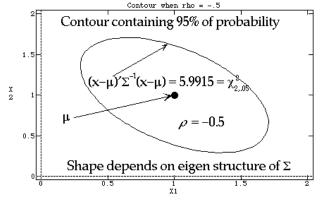
- $\mu = \mu, \Sigma = \sigma^2$
- $(\mathbf{x} \mathbf{\mu})'\mathbf{\Sigma}^{-1}(\mathbf{x} \mathbf{\mu}) = ((\mathbf{x} \mathbf{\mu})/\sigma)^2 = \chi_1^2$

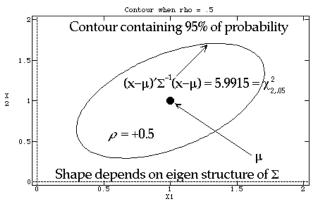
Statistics 5401

Lecture 6

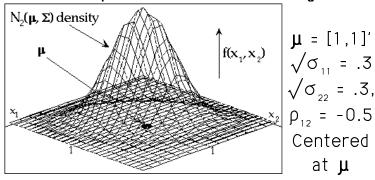
September 19, 2005

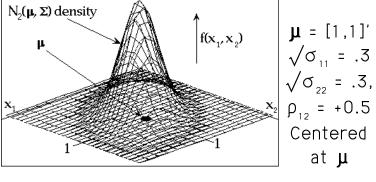
# All contours (level curves) are ellipses centered at $\mu$ = [1,1]' like these:





## Shape of bivariate density





- The mode (maximum) is at μ
- Every  $\underline{\text{contour}}$  (level curve) is an  $\underline{\text{ellipse}}$  centered at  $\mu$

1

Statistics 5401 Lecture 6

September 19, 2005

#### Standard Multivariate Normal

When z is  $N_{\scriptscriptstyle D}(0, I_{\scriptscriptstyle D})$ , its density is

$$f(\mathbf{z}) = \frac{e^{-\frac{1}{2}z'\mathbf{z}}}{(2\pi)^{p/2}} = \frac{e^{-\frac{1}{2}\sum_{i=1}^{p}z_i^2}}{(2\pi)^{p/2}} = \frac{e^{-\frac{z_1^2}{2}}}{\sqrt{2\pi}} \frac{e^{-\frac{z_2^2}{2}}}{\sqrt{2\pi}} \dots \frac{e^{-\frac{z_p^2}{2}}}{\sqrt{2\pi}},$$

That is

- $\mu_1 = \mu_2 = \dots = \mu_n = 0$
- $\sigma_{11} = \sigma_{22} = \dots = \sigma_{nn} = 1$
- $\sigma_{ij} = 0$ ,  $i \neq j \Rightarrow \rho_{ij} = 0$
- The z<sub>i</sub>'s are <u>independent</u> N<sub>1</sub>(0, 1<sup>2</sup>)
   because

$$f(\mathbf{z}) = f(z_1) \times f(z_2) \times \dots \times f(z_p)$$

• Q( $\mathbf{z} - \boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z$ ) = ( $\mathbf{z} - \mathbf{0}$ )' $\mathbf{I}_p^{-1}(\mathbf{z} - \mathbf{0}) = \sum_{1 \le i \le p} \mathbf{Z}_i^2$  is distributed as  $\chi_p^2$  by a standard univariate result.

September 19, 2005

## Properties of Multivariate Normal

Lecture 6

The following properties are basically mathematical theorems. They are important in part because they provide a basis assessing or testing multivariate normality. If a sample of data appears not to satisfy one of these properties, it is evidence the sample is not from a multivariate normal population.

- 1. All marginal distributions are normal.
- Each x<sub>i</sub>, ignoring other x's, is N<sub>1</sub>(μ<sub>i</sub>,σ<sub>ii</sub>)
- Any subset of variables, ignoring other x's, is *multivariate* normal.

Application: If a univariate sample consisting of the values of x, does not appear to come from a normal population, then the multivariate data is probably not multivariate normal.

Specifically, when  $\mathbf{x}' = [\mathbf{x}_1', \mathbf{x}_2']$ , where  $\mathbf{x}_1$ is a  $p_1$  by 1 vector,  $\mathbf{x}_2$  is a  $p_2$  by 1 vector than you can partition  $\Sigma$  and  $\mu$ :

$$\Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ & & \\ \Sigma_{21} = \Sigma_{12}, & \Sigma_{22} \end{bmatrix}, \quad \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad p_1$$

$$p_1 \qquad p_2$$

where

Statistics 5401

- $\mu_1$  is  $p_1 \times 1$  and  $\mu_2$  is  $p_2 \times 1$
- $\Sigma_{11}$  is  $p_1 \times p_1$  and  $\Sigma_{22}$  is  $p_2 \times p_2$
- $\Sigma_{12}$  is  $p_1 \times p_2$  and  $\Sigma_{21} = \Sigma_{12}$  is  $p_2 \times p_1$

This property states

$$\mathbf{X}_{\scriptscriptstyle 1}$$
 is  $N_{\scriptscriptstyle p_{\scriptscriptstyle 1}}(\boldsymbol{\mu}_{\scriptscriptstyle 1},\;\boldsymbol{\Sigma}_{\scriptscriptstyle 11}),\;\mathbf{X}_{\scriptscriptstyle 2}$  is  $N_{\scriptscriptstyle p_{\scriptscriptstyle 2}}(\boldsymbol{\mu}_{\scriptscriptstyle 2},\;\boldsymbol{\Sigma}_{\scriptscriptstyle 22})$ 

Statistics 5401 September 19, 2005

13

- All conditional distributions are normal.
- Distribution of  $p_2 \times 1$   $\mathbf{x}_2$  given  $p_1 \times 1$   $\mathbf{x}_1$  is  $N_{p_2}(\mu_2 + \beta_{2\cdot 1}'(x_1 - \mu_1), \Sigma_{22\cdot 1}),$

That is.

$$E[\mathbf{x}_{2} | \mathbf{x}_{1}] = \mu_{2} + \beta_{2} \cdot \mathbf{1}'(\mathbf{x}_{1} - \mu_{1}), \quad p_{2} \text{ by } 1$$
  
 $V[\mathbf{x}_{2} | \mathbf{x}_{1}] = \Sigma_{2} \cdot \mathbf{1}, \quad p_{2} \text{ by } p_{2}$ 

- This is a linear regression of  $\ \mathbf{X}_{_{2}}$  on  $\ \mathbf{X}_{_{1}}$
- Application: if the dependence of one variable, say  $x_{_{i}}$ , on another, say  $x_{_{k}}$ , is not linear, then X is probably not multivariate normal.
- $\beta_{2\cdot 1} = \Sigma_{11}^{-1}\Sigma_{12}$ ,  $p_1 \times p_2$  is a matrix of population regression coefficients.

Statistics 5401

•  $V[\mathbf{x}_2 \mid \mathbf{x}_1] = \mathbf{\Sigma}_{221}$  does not depend on  $\mathbf{x}_1$ .

14

•  $\Sigma_{22\cdot 1} \equiv \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12} = \Sigma_{22} - \beta_{2\cdot 1}'\Sigma_{11}\beta_{2\cdot 1}$ =  $V[\mathbf{x}_2 - E[\mathbf{x}_2 | \mathbf{x}_1]]$ =  $V[\mathbf{x}_{2} - \boldsymbol{\mu}_{2} - \boldsymbol{\beta}_{2}]'(\mathbf{x}_{1} - \boldsymbol{\mu}_{1})]$ 

That is,

$$\Sigma_{22\cdot 1} = \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$$
 is the variance matrix of the

residuals =  $\mathbf{x}_2$  -  $E[\mathbf{x}_2 | \mathbf{x}_1]$ .

Application: If regression diagnostics in a linear regression of one variable on the others indicate non-constant variance, that indicates the data do not come from a multivariate normal population.

### Bivariate case

When p = 2 and  $p_1 = p_2 = 1$ , these are

- $\beta_{2.1} = \sigma_{12}/\sigma_{11}$  (simple linear regression)
- $\sigma_{22.1} = \sigma_{22} \sigma_{12}^2 / \sigma_{11} = \sigma_{22} \beta_{2.1}^2 \sigma_{11}$  $= (1 - \rho_{12}^{2})\sigma_{22}$

3. Linear combinations are normal

- $\mathbf{a}'\mathbf{x} = \sum_{1 \le i \le p} a_i \mathbf{x}_i \text{ is } \mathbf{N}_1(\mathbf{a}'\mathbf{\mu}, \mathbf{a}'\mathbf{\Sigma}\mathbf{a})$
- $A'x = [a_1'x,...,a_q'x]'$  is  $N_q(A'\mu, A'\Sigma A)$ when  $A = [a_1,...,a_q]$  is p by q whose columns define linear combinations.

**Example:** If  $\{d_i\}$ ,  $d_i = x_{i2} - x_{i1}$ , i = 1,...,n does not appear to be normal, then **x** is probably not multivariate normal.

4. The distribution of

Q(
$$\mathbf{x} - \mathbf{\mu}$$
,  $\mathbf{\Sigma}$ ) =  $(\mathbf{x} - \mathbf{\mu})'\mathbf{\Sigma}^{-1}(\mathbf{x} - \mathbf{\mu})$  is  $\chi_p^2$ .

Except for a factor of 1/2,  $Q(x-\mu, \Sigma)$  is the exponent in the density.

5. Zero covariance or correlation implies independence

When 
$$\Sigma = \begin{bmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{bmatrix}$$
,

that is,  $\Sigma_{12} = \text{Cov}[\mathbf{x}_1, \mathbf{x}_2] = 0$ , then  $\mathbf{x}_1$  and  $\mathbf{x}_2$  are *independent*.

In particular, when  $\sigma_{ij}$  = 0,  $x_i$  and  $x_j$  are independent

Since  $\rho_{ij} = 0 \iff \sigma_{ij} = 0$ , uncorrelated  $x_i$  and  $x_i$  are independent.

17

Statistics 5401

Lecture 6

September 19, 2005

Statistics 5401

Lecture

September 19, 2005

#### Standardization

When Y is a *univariate* random variable, an important re-expression of Y is as a *standardized random variable* (**z-score**)

$$Z = (Y - \mu_{Y})/\sigma_{Y}$$

Z has mean O and standard deviation 1:

$$\mu_z = 0$$
,  $\sigma_z = 1$ 

## Example:

When  $Y = \underline{\text{test statistic}}$  or  $\underline{\text{estimator}}$  (e.g.  $\overline{x}$ ) with *hypothesized* mean  $\mu_{Y} = \mu_{D}$ , often 0, and *standard error*  $\sigma_{Y}$ .

Then Z =  $(Y - \mu_0)/\sigma_y$  is a Z-statistic for testing  $H_0$ :  $\mu_y = \mu_0$ 

You can often replace an  $\underline{unknown}$   $\sigma_{_Y}$  by an estimator  $\hat{\sigma}_{_Y}$  and standardize to get the test statistic

$$t = (Y - \mu_0)/\hat{\sigma}_{v}$$

- When Y is (approximately)  $N(\mu_{Y}, \sigma_{Y}^{2})$ , Z is (approximately)  $N(0,1^{2})$  and  $Z^{2} = (Y \mu_{Y})^{2}/\sigma_{Y}^{2}$  or  $t^{2} = (Y \mu_{Y})^{2}/\hat{\sigma}_{Y}^{2}$  is (approximately)  $\chi_{1}^{2}$  ( $\chi^{2}$  on 1 d.f.).
- When Y is exactly  $N(\mu_{Y}, \sigma_{Y}^{2})$  and  $\hat{\sigma}_{Y}^{2}$  is an <u>independent</u> estimate of  $\sigma_{Y}^{2}$  such that  $\hat{\sigma}_{Y}^{2}/\sigma_{Y}^{2} = \chi_{f_{e}}^{2}/f_{e}$ , then t is distributed as  $t_{f_{e}} =$ **Student's** t on  $f_{e}$  degrees of freedom and

 $t^2 = (Y - \mu_Y)^2 / \hat{\sigma}_Y^2$  is distributed as  $F_{1,f_0}$ .

**Note**:  $E[\chi_{\ell}^2] = f$ , so  $E[\chi_{\ell}^2/f] = 1$ 

Notation: I consistently use the notation

 $f_{\rm e}$  = error degrees of freedom

Later I will use the notation

f, = hypothesis degrees of freedom

These notations are not used in the text.

## Familiar example

Y = X and you are testing  $H_0$ :  $\mu = \mu_0$ .

Then  $\sigma_{Y} = \sigma_{\overline{X}} = \sigma_{X} / \sqrt{n}$  and  $\hat{\sigma}_{Y} = \hat{\sigma}_{\overline{X}} = s / \sqrt{n}$ and

Lecture 6

$$Z = (\overline{X} - \mu_0)/(\sigma/\sqrt{n})$$

$$t = (\overline{X} - \mu_0)/(s/\sqrt{n})$$

When  $\overline{x}$  is computed from a random sample:

- In large samples,  $Z \sim N(0, 1^2)$  and  $Z^2 \sim$
- When X is normal t  $\sim$  t<sub>n-1</sub> and t<sup>2</sup>  $\sim$  F<sub>1 n-1</sub>

Multivariate standardization

A multivariate vector **Z** is *standardized* when

•  $\mu_{7} = 0$ 

with mean 0.

•  $V[Z] = I_n = diag[1,1,...,1].$ 

When Y is an multivariate random vector, then for any pxp matrix  $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n]$ ,  $E[A'(Y - \mu_{Y})] = A'E[Y - \mu_{Y}] = A'0 = 0.$ 

So it's easy to transform Y to a form

21

Statistics 5401

Lecture 6

September 19, 2005

Statistics 5401

Lecture 6

22

September 19, 2005

It's harder to find a matrix **A** such that

$$Z = A'(Y - \mu_{\downarrow})$$

has variance matrix I.

However, when you have such an A,

$$Z = A'(Y - \mu_{\downarrow})$$

is a standardized version of Y.

Or, if 
$$C = A^{-1}$$
,

$$Z = (C')^{-1}(Y - \mu_{Y})$$

is a standardized version of Y.

## Matrix Square Roots

## Vocabulary:

Let **B** be a *positive semi-definite* p×p symmetric matrix. Then, when the p×p matrix C satisfies C'C = B, we say C is a *matrix square root* of B.

• C is not unique; you can choose C to be

symmetric, triangular



or none of these.

Cmd> b # previously entered matrix 12

Cmd> upper <- cholesky(b); upper # Upper triangular

Cmd> upper' %\*% upper # Check: upper' upper = b 16 12 1.0

Cmd> matsqrt(b) # does same as cholesky() (2,1)

Cmd> lower <- matsqrt(b,lower:T); lower # lower triangular sqrt (1,1) 1.2649 0 4/sqrt(10) 0 3.1623

Cmd> lower' %\*% lower # Check: lower' lower = b 12

# You can get still other square roots by swapping the rows:

Cmd> asym <- sym[vector(2,1),]; asym #not symmetric, triangular (1,1) 2.058 2.401 (2,1) 3.43 2.058 Cmd> asym' \*\*\* asym (1,1) 16 12 (2,1) 12 10

#### Vocabulary

When C is upper triangular, C'C = B is the Cholesky Decomposition of B.

#### MacAnova

When b is a symmetric matrix,

Cmd> c <- cholesky(b)

computes the upper triangular square root of b