Multivariate Normal Theory

STA721 Linear Models Duke University

Merlise Clyde

September 2, 2019

Outline

- Expectations under Moments
- ► Spectral Theorem (Singular Value Decomposition)
- Multivariate Normal Distribution

Properties of OLS/MLEs

$$\hat{\mathbf{Y}}=\hat{\mu}=\mathbf{X}\hat{eta}$$
 is an unbiased estimate of $\mu=\mathbf{X}eta$
$$egin{array}{ll} \mathsf{E}[\hat{\mathbf{Y}}]&=&\mathsf{E}[\mathsf{P_XY}]\\ &=&\mathsf{P_XE[Y]}\\ &=&\mathsf{P_X}\mu\\ &=&\mu \end{array}$$

$$\mathsf{E}[\mathbf{e}] = \mathbf{0}$$
 if $\mu \in \mathit{C}(\mathbf{X})$ (Ex. 1.11 in Christensen)

Will not be $\mathbf{0}$ if $\mu \notin C(\mathbf{X})$ (useful for model checking)

Estimate of σ^2

MLE of σ^2 :

$$\hat{\sigma}^2 = \frac{\mathbf{e}^T \mathbf{e}}{n} = \frac{\mathbf{Y}^T (\mathbf{I} - \mathbf{P}_{\mathbf{X}}) \mathbf{Y}}{n}$$

- ▶ What is the expectation of $e^T e$?
- ▶ Is this an unbiased estimate of σ^2 ?

Need expectations of quadratic forms $\mathbf{Y}^T \mathbf{A} \mathbf{Y}$ for \mathbf{A} an $n \times n$ matrix \mathbf{Y} a random vector in \mathbb{R}^n

Quadratic Forms

Without loss of generality we can assume that $\mathbf{A} = \mathbf{A}^T$

- \triangleright **Y**^T**AY** is a scalar

$$\frac{\mathbf{Y}^{T}\mathbf{A}\mathbf{Y} + \mathbf{Y}^{T}\mathbf{A}^{T}\mathbf{Y}}{2} = \mathbf{Y}^{T}\mathbf{A}\mathbf{Y}$$
$$\mathbf{Y}^{T}\frac{(\mathbf{A} + \mathbf{A}^{T})}{2}\mathbf{Y} = \mathbf{Y}^{T}\mathbf{A}\mathbf{Y}$$

ightharpoonup may take $\mathbf{A} = \mathbf{A}^T$

Expectations of Quadratic Forms

Theorem

Let **Y** be a random vector in \mathbb{R}^n with $E[\mathbf{Y}] = \mu$ and $Cov(\mathbf{Y}) = \Sigma$. Then $E[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] = tr \mathbf{A} \Sigma + \mu^T \mathbf{A} \mu$.

Result useful for finding expected values of Mean Squares; no normality required! (See Christensen Thm 1.3.2)

Proof

Start with $(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\mu})$, expand and take expectations

$$\begin{split} \mathsf{E}[(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\mu})] &= \mathsf{E}[\mathbf{Y}^T \mathbf{A} \mathbf{Y} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \mathbf{Y} - \mathbf{Y}^T \mathbf{A} \boldsymbol{\mu}] \\ &= \mathsf{E}[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{E}[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \end{split}$$

Rearrange

$$\begin{split} \mathsf{E}[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] &= \mathsf{E}[(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\mu})] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{E}[\mathsf{tr}(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\mu})] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{E}[\mathsf{tr} \mathbf{A} (\mathbf{Y} - \boldsymbol{\mu}) (\mathbf{Y} - \boldsymbol{\mu})^T] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{tr} \mathsf{E}[\mathbf{A} (\mathbf{Y} - \boldsymbol{\mu}) (\mathbf{Y} - \boldsymbol{\mu})^T] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{tr} \mathbf{A} \mathsf{E}([(\mathbf{Y} - \boldsymbol{\mu}) (\mathbf{Y} - \boldsymbol{\mu})^T] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= \mathsf{tr} \mathbf{A} \mathbf{\Sigma} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \end{split}$$

$$tr \mathbf{A} \equiv \sum_{i=1}^{n} a_{ii}$$

Expectation of $\hat{\sigma}^2$

Use the theorem:

$$E[\mathbf{Y}^{T}(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{Y}] = tr(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\sigma^{2}\mathbf{I} + \mu^{T}(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mu$$

$$= \sigma^{2}tr(\mathbf{I} - \mathbf{P}_{\mathbf{X}})$$

$$= \sigma^{2}r(\mathbf{I} - \mathbf{P}_{\mathbf{X}})$$

$$= \sigma^{2}(n - r(\mathbf{X}))$$

Therefore an unbiased estimate of σ^2 is

$$\frac{\mathbf{e}^T\mathbf{e}}{n-r(\mathbf{X})}$$

If **X** is full rank $(r(\mathbf{X}) = p)$ and $\mathbf{P}_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ then the

$$tr(\mathbf{P}_{\mathbf{X}}) = tr(\mathbf{X}(\mathbf{X}^{T}\mathbf{X})^{-1}\mathbf{X}^{T})$$

$$= tr(\mathbf{X}^{T}\mathbf{X}(\mathbf{X}^{T}\mathbf{X})^{-1})$$

$$= tr(\mathbf{I}_{p}) = p$$

Spectral Theorem

Theorem

If \mathbf{A} $(n \times n)$ is a symmetric real matrix then there exists a \mathbf{U} $(n \times n)$ such that $\mathbf{U}^T \mathbf{U} = \mathbf{U} \mathbf{U}^T = \mathbf{I}_n$ and a diagonal matrix $\mathbf{\Lambda}$ with elements λ_i such that $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T$

- ▶ **U** is an orthogonal matrix; $\mathbf{U}^{-1} = \mathbf{U}^T$
- ▶ The columns of **U** from an Orthonormal Basis for \mathbb{R}^n
- lacktriangle rank of f A equals the number of non-zero eigenvalues λ_i
- Columns of U associated with non-zero eigenvalues form an ONB for C(A) (eigenvectors of A)
- $\blacktriangleright \ \mathbf{A}^p = \mathbf{U} \mathbf{\Lambda}^p \mathbf{U}^T \text{ (matrix powers)}$
- ▶ a square root of $\mathbf{A} > 0$ is $\mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{U}^T$

Projections

Projection Matrix

If **P** is an orthogonal projection matrix, then its eigenvalues λ_i are either zero or one with $\operatorname{tr}(\mathbf{P}) = \sum_i (\lambda_i) = r(\mathbf{P})$

- ightharpoonup $P = U\Lambda U^T$
- $P = P^2 \Rightarrow U \Lambda U^T U \Lambda U^T = U \Lambda^2 U^T$
- ▶ $\Lambda = \Lambda^2$ is true only for $\lambda_i = 1$ or $\lambda_i = 0$
- Since $r(\mathbf{P})$ is the number of non-zero eigenvalues, $r(\mathbf{P}) = \sum \lambda_i = \operatorname{tr}(\mathbf{P})$

$$\mathbf{P} = [\mathbf{U}_P \mathbf{U}_{P^{\perp}}] \left[\begin{array}{cc} \mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{n-r} \end{array} \right] \left[\begin{array}{c} \mathbf{U}_P^T \\ \mathbf{U}_{P^{\perp}}^T \end{array} \right] = \mathbf{U}_P \mathbf{U}_P^T$$

$$\mathbf{P} = \sum_{i=1}^{r} \mathbf{u}_{i} \mathbf{u}_{i}^{T}$$

sum of r rank 1 projections.

Univariate Normal

Definition

We say that Z has a standard Normal distribution

$$Z \sim N(0,1)$$

with mean 0 and variance 1 if it has density

$$f_Z(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z^2}$$

If $Y = \mu + \sigma Z$ then $Y \sim N(\mu, \sigma^2)$ with mean μ and variance σ^2

$$f_{\gamma}(y) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{z-\mu}{\sigma}\right)^2}$$

Standard Multivariate Normal

Let $z_i \stackrel{\text{iid}}{\sim} \mathsf{N}(0,1)$ for $i=1,\ldots,d$ and define

$$\mathbf{Z} \equiv \left[\begin{array}{c} z_1 \\ z_2 \\ \vdots \\ z_d \end{array} \right]$$

▶ Density of *Z*:

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{j=1}^{d} \frac{1}{\sqrt{2\pi}} e^{-z_i^2/2}$$

= $(2\pi)^{-d/2} e^{-\frac{1}{2}(\mathbf{Z}^T \mathbf{Z})}$

- ightharpoonup E[**Z**] = **0** and Cov[**Z**] = **I**_d
- ightharpoonup $m Z \sim N(\mathbf{0}_d, I_d)$

duke.ep:

Multivariate Normal

For a d dimensional multivariate normal random vector, we write $\mathbf{Y} \sim N_d(m{\mu}, m{\Sigma})$

- ightharpoonup $\mathrm{E}[\mathbf{Y}] = \mu$: d dimensional vector with means $E[Y_j]$
- ► Cov[**Y**] = Σ : $d \times d$ matrix with diagonal elements that are the variances of Y_j and off diagonal elements that are the covariances $E[(Y_j \mu_j)(Y_k \mu_k)]$

Density

If Σ is positive definite $(\mathbf{x}'\mathbf{\Sigma}\mathbf{x}>0$ for any $\mathbf{x}\neq 0$ in $\mathbb{R}^d)$ then \mathbf{Y} has a density 1

$$p(\mathbf{Y}) = (2\pi)^{-d/2} |\mathbf{\Sigma}|^{-1/2} \exp(-\frac{1}{2} (\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-1} (\mathbf{Y} - \boldsymbol{\mu}))$$

 $^{^1}$ with respect to Lebesgue measure on \mathbb{R}^d

Multivariate Normal Density

▶ Density of $Z \sim N(\mathbf{0}, \mathbf{I}_d)$:

$$f_{\mathbf{Z}}(\mathbf{z}) = \prod_{j=1}^{d} \frac{1}{\sqrt{2\pi}} e^{-z_{i}^{2}/2}$$
$$= (2\pi)^{-d/2} e^{-\frac{1}{2}(\mathbf{Z}^{T}\mathbf{Z})}$$

- ▶ Write $\mathbf{Y} = \boldsymbol{\mu} + \mathbf{AZ}$
- ► Solve for $\mathbf{Z} = g(\mathbf{Y})$
- ▶ Jacobian of the transformation $J(\mathbf{Z} o \mathbf{Y}) = |\frac{\partial g}{\partial \mathbf{Y}}|$
- ightharpoonup substitute $g(\mathbf{Y})$ for \mathbf{Z} in density and multiply by Jacobian

$$f_{\mathbf{Y}}(\mathbf{y}) = f_{\mathbf{Z}}(\mathbf{z})J(\mathbf{Z} \to \mathbf{Y})$$

Multivariate Normal Density

$$\mathbf{Y} = \boldsymbol{\mu} + \mathbf{AZ}$$
 for $\mathbf{Z} \sim \mathsf{N}(\mathbf{0}, \mathbf{I}_d)$ (1)

Proof.

- ▶ since $\Sigma > 0$, \exists by the spectral theorem an \mathbf{A} ($d \times d$) such that $\mathbf{A} > 0$ and $\mathbf{A}\mathbf{A}^T = \Sigma$ a (symmetric) square root of $\mathbf{A} > 0$ is $\mathbf{U}\mathbf{A}^{1/2}\mathbf{U}^T$
- ightharpoonup igh
- ► Multiply both sides (1) by \mathbf{A}^{-1} :

$$A^{-1}Y = A^{-1}\mu + A^{-1}AZ$$

- ightharpoonup Rearrange $\mathbf{A}^{-1}(\mathbf{Y} \boldsymbol{\mu}) = \mathbf{Z}$
- ▶ Jacobian of transformation $d\mathbf{Z} = |\mathbf{A}^{-1}| d\mathbf{Y}$
- Substitute and simplify algebra

$$f(\mathbf{Y}) = (2\pi)^{-d/2} |\mathbf{\Sigma}|^{-1/2} \exp(-\frac{1}{2}(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-1}(\mathbf{Y} - \boldsymbol{\mu}))$$



Singular Case

$$\mathbf{Y} = \boldsymbol{\mu} + \mathbf{AZ}$$
 with $\mathbf{Z} \in \mathbb{R}^d$ and \mathbf{A} is $n imes d$

- ightharpoonup $\mathsf{E}[\mathbf{Y}] = \mu$
- ightharpoonup Cov(m f Y) = $m f AA^T \geq 0$
- $ightharpoonup \mathbf{Y} \sim \mathsf{N}(oldsymbol{\mu}, oldsymbol{\Sigma}) ext{ where } oldsymbol{\Sigma} = oldsymbol{\mathsf{A}}oldsymbol{\mathsf{A}}^{T}$

If Σ is singular then there is no density (on \mathbb{R}^n), but claim that Y still has a multivariate normal distribution!

Definition

 $\mathbf{Y} \in \mathbb{R}^n$ has a multivariate normal distribution $N(\mu, \mathbf{\Sigma})$ if for any $\mathbf{v} \in \mathbb{R}^n$ $\mathbf{v}^T \mathbf{Y}$ has a univariate normal distribution with mean $\mathbf{v}^T \boldsymbol{\mu}$ and variance $\mathbf{v}^T \mathbf{\Sigma} \mathbf{v}$

see linked videos using characteristic functions:

$$Y \sim N(\mu, \sigma^2) \Leftrightarrow \varphi_y(t) \equiv E[e^{itY}] = e^{it\mu - t^2\sigma^2/2}$$

Linear Transformations are Normal

If
$$\mathbf{Y} \sim N_n(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$
 then for $\mathbf{A} \ m \times n$

$$\mathbf{AY} \sim \mathsf{N}_m(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}\mathbf{\Sigma}\mathbf{A}^T)$$

 $\mathbf{A} \mathbf{\Sigma} \mathbf{A}^T$ does not have to be positive definite! (Proof in book or linked video)

Use to prove that all marginal distributions of normals are normal!

Conditional Normals

Partition Y

$$\mathbf{Y} = \left[egin{array}{c} \mathbf{Y}_1 \ \mathbf{Y}_2 \end{array}
ight]$$

as well as the mean and covariance matrix. Then the joint distribution is:

$$\left[\begin{array}{c} \mathbf{Y}_1 \\ \mathbf{Y}_2 \end{array}\right] \sim \mathcal{N}\left(\left[\begin{array}{c} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{array}\right], \left[\begin{array}{cc} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{array}\right]\right)$$

The conditional distribution of \mathbf{Y}_1 given $\mathbf{Y}_2 = \mathbf{y}_2$

$$old Y_1 \mid old Y_2 \sim \mathcal{N} ig(oldsymbol{\mu}_1 + oldsymbol{\Sigma}_{12} oldsymbol{\Sigma}_{22}^{-1} oldsymbol{(y_2 - \mu_2)}, oldsymbol{\Sigma}_{11} - oldsymbol{\Sigma}_{12} oldsymbol{\Sigma}_{21}^{-1} oldsymbol{\Sigma}_{21} ig)$$

Brute Force or Linear Transformations!

Equal in Distribution

Multiple ways to define the same normal:

- ▶ $\mathbf{Z}_1 \sim \mathsf{N}(\mathbf{0}, \mathbf{I}_n)$, $\mathbf{Z}_1 \in \mathbb{R}^n$ and take $\mathbf{A} \ d \times n$
- $ightharpoonup egin{aligned} oldsymbol{\mathsf{Z}}_2 &\sim \mathsf{N}(oldsymbol{\mathsf{0}}, oldsymbol{\mathsf{I}}_p), \ oldsymbol{\mathsf{Z}}_2 \in \mathbb{R}^p \ ext{and take } oldsymbol{\mathsf{B}} \ d imes p \end{aligned}$
- ▶ Define $\mathbf{Y} = \boldsymbol{\mu} + \mathbf{A}\mathbf{Z}_1$
- ▶ Define $\mathbf{W} = \boldsymbol{\mu} + \mathbf{B}\mathbf{Z}_2$

Theorem

If
$$Y = \mu + AZ_1$$
 and $W = \mu + BZ_2$ then $Y \stackrel{\mathrm{D}}{=} W$ if and only if $AA^T = BB^T = \Sigma$

see linked video

Zero Correlation and Independence

Theorem

For a random vector $\mathbf{Y} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$ partitioned as

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \end{bmatrix} \sim N \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \mathbf{\Sigma}_{11} & \mathbf{\Sigma}_{12} \\ \mathbf{\Sigma}_{21} & \mathbf{\Sigma}_{22} \end{bmatrix} \right)$$

then $Cov(\mathbf{Y}_1, \mathbf{Y}_2) = \mathbf{\Sigma}_{12} = \mathbf{\Sigma}_{21}^T = \mathbf{0}$ if and only if \mathbf{Y}_1 and \mathbf{Y}_2 are independent.

Independence Implies Zero Covariance

Proof.

$$\mathsf{Cov}(\mathbf{Y}_1,\mathbf{Y}_2) = \mathsf{E}[(\mathbf{Y}_1 - \boldsymbol{\mu}_1)(\mathbf{Y}_2 - \boldsymbol{\mu}_2)^T]$$

If \mathbf{Y}_1 and \mathbf{Y}_2 are independent

$$\mathsf{E}[(\mathbf{Y}_1 - \mu_1)(\mathbf{Y}_2 - \mu_2)^T] = \mathsf{E}[(\mathbf{Y}_1 - \mu_1)\mathsf{E}(\mathbf{Y}_2 - \mu_2)^T] = \mathbf{00}^T = \mathbf{0}$$

therefore $\Sigma_{12} = \mathbf{0}$

Zero Covariance Implies Independence

Assume $\Sigma_{12} = 0$

Proof

Choose an

$$\mathbf{A} = \left[\begin{array}{cc} \mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_2 \end{array} \right]$$

such that $\mathbf{A}_1\mathbf{A}_1^{\mathcal{T}}=\mathbf{\Sigma}_{11},\,\mathbf{A}_2\mathbf{A}_2^{\mathcal{T}}=\mathbf{\Sigma}_{22}$

Partition

$$\mathbf{Z} = \left[egin{array}{c} \mathbf{Z}_1 \ \mathbf{Z}_2 \end{array}
ight] \sim \mathsf{N} \left(\left[egin{array}{cc} \mathbf{0}_1 \ \mathbf{0}_2 \end{array}
ight], \left[egin{array}{cc} \mathbf{I}_1 & \mathbf{0} \ \mathbf{0} & \mathbf{I}_2 \end{array}
ight]
ight) ext{ and } oldsymbol{\mu} = \left[egin{array}{c} oldsymbol{\mu}_1 \ oldsymbol{\mu}_2 \end{array}
ight]$$

lacksquare then $f Y \stackrel{
m D}{=} f AZ + m \mu \sim N(m \mu, m \Sigma)$

Continued

Proof.

$$\left[\begin{array}{c} \mathbf{Y}_1 \\ \mathbf{Y}_2 \end{array}\right] \stackrel{\mathrm{D}}{=} \left[\begin{array}{c} \mathbf{A}_1 \mathbf{Z}_1 + \boldsymbol{\mu}_1 \\ \mathbf{A}_2 \mathbf{Z}_2 + \boldsymbol{\mu}_2 \end{array}\right]$$

- ightharpoonup But $m {f Z}_1$ and $m {f Z}_2$ are independent
- ightharpoonup Functions of $m Z_1$ and $m Z_2$ are independent
- ightharpoonup Therefore $m Y_1$ and $m Y_2$ are independent

For Multivariate Normal Zero Covariance implies independence

duke.ep:

Corollary

Corollary

If $\mathbf{Y} \sim N(\boldsymbol{\mu}, \sigma^2 \mathbf{I}_n)$ and $\mathbf{A}\mathbf{B}^T = \mathbf{0}$ then $\mathbf{A}\mathbf{Y}$ and $\mathbf{B}\mathbf{Y}$ are independent.

Proof.

$$\left[\begin{array}{c} \mathbf{W}_1 \\ \mathbf{W}_2 \end{array}\right] = \left[\begin{array}{c} \mathbf{A} \\ \mathbf{B} \end{array}\right] \mathbf{Y} = \left[\begin{array}{c} \mathbf{AY} \\ \mathbf{BY} \end{array}\right]$$

- $ightharpoonup \operatorname{Cov}(\mathbf{W}_1,\mathbf{W}_2) = \operatorname{Cov}(\mathbf{AY},\mathbf{BY}) = \sigma^2 \mathbf{AB}^T$
- **AY** and **BY** are independent if $AB^T = 0$

duke.eps