

STAT 3690 Lecture Note

Week Four (Jan 30, Feb 1, & 3, 2023)

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Multivariate normal (MVN) distribution (con'd, J&W Sec 4.2)

Definition

- Standard MVN
 - $\mathbf{Z} = [Z_1, \dots, Z_p]^\top \sim \text{MVN}_p(\mathbf{0}, \mathbf{I}) \Leftrightarrow Z_1, \dots, Z_p \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$
 - pdf
$$f_{\mathbf{Z}}(\mathbf{z}) = (2\pi)^{-p/2} \exp(-\mathbf{z}^\top \mathbf{z} / 2) \cdot \mathbf{1}_{\mathbb{R}^p}(\mathbf{z})$$
- General MVN
 - $\mathbf{X} = [X_1, \dots, X_p]^\top \sim \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \Leftrightarrow$ there exists $\boldsymbol{\mu} \in \mathbb{R}^p$, $\mathbf{A} \in \mathbb{R}^{p \times p}$ and $\mathbf{Z} \sim \text{MVN}_p(\mathbf{0}, \mathbf{I})$ such that $\mathbf{X} = \mathbf{AZ} + \boldsymbol{\mu}$ and $\boldsymbol{\Sigma} = \mathbf{AA}^\top$
 - * Limited to non-degenerate cases, i.e., invertible \mathbf{A} ($\Leftrightarrow \boldsymbol{\Sigma} > 0$)
 - pdf
$$f_{\mathbf{X}}(\mathbf{x}) = (2\pi)^{-p/2} (\det \boldsymbol{\Sigma})^{-1/2} \exp\{-(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) / 2\} \cdot \mathbf{1}_{\mathbb{R}^p}(\mathbf{x})$$

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- Exercise: Density of $\text{MVN}_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ evaluated at $(4, 7)$, where

$$\boldsymbol{\mu} = [3, 6]^\top, \quad \boldsymbol{\Sigma} = \begin{bmatrix} 10 & 2 \\ 2 & 5 \end{bmatrix}.$$

Properties of MVN

- \mathbf{X} is of MVN $\Leftrightarrow a^\top \mathbf{X}$ is normally distributed for ALL non-zero $a \in \mathbb{R}^p$.
 - Warning: marginal normals do not imply the joint normal.
- If $\mathbf{X} \sim \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $\mathbf{AX} + \mathbf{b} \sim \text{MVN}_q(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top)$ for $\mathbf{A} \in \mathbb{R}^{q \times p}$ of full-row-rank. Hence,
 - (Stochastic representation of MVN) if $\mathbf{X} \sim \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then there is $\mathbf{Z} \sim \text{MVN}_p(\mathbf{0}, \mathbf{I})$ such that $\mathbf{X} = \boldsymbol{\Sigma}^{1/2} \mathbf{Z} + \boldsymbol{\mu}$. Actually, $\mathbf{Z} = \boldsymbol{\Sigma}^{-1/2} (\mathbf{X} - \boldsymbol{\mu})$.
- $(\mathbf{X} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{X} - \boldsymbol{\mu}) \sim \chi^2(p)$ if $\mathbf{X} \sim \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.

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- Exercise: Generate six iid samples following bivariate normal $\text{MVN}_2(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with

$$\boldsymbol{\mu} = [3, 6]^\top, \quad \boldsymbol{\Sigma} = \begin{bmatrix} 10 & 2 \\ 2 & 5 \end{bmatrix}.$$

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- Exercise: Suppose $X_1 \sim \mathcal{N}(0, 1)$. In the following two cases, verify that $X_2 \sim \mathcal{N}(0, 1)$ as well. Does $\mathbf{X} = [X_1, X_2]^\top$ follow an MVN in both cases?
 - a. $X_2 = -X_1$;
 - b. $X_2 = (2Y - 1)X_1$, where $Y \sim \text{Ber}(p)$ and $Y \perp\!\!\!\perp \mathbf{X}$. (Hint: $\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \Leftrightarrow f_{\mathbf{Z}}(\mathbf{z}) = f_{\mathbf{X}}(\mathbf{x})f_{\mathbf{Y}}(\mathbf{y})$, where $\mathbf{Z} = [\mathbf{X}^\top, \mathbf{Y}^\top]^\top$.)
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Marginal and conditional MVN

- If $\mathbf{X} \sim \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{bmatrix}, \quad \boldsymbol{\mu} = \begin{bmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{bmatrix}$$

with

- random p_i -vector \mathbf{X}_i , $i = 1, 2$,
 - p_i -vector $\boldsymbol{\mu}_i$, $i = 1, 2$,
 - $p_i \times p_i$ matrix $\boldsymbol{\Sigma}_{ii} > 0$, $i = 1, 2$,
 - then
 - (Marginals of MVN are still MVN) $\mathbf{X}_i \sim \text{MVN}_{p_i}(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_{ii})$
 - $\mathbf{X}_i \mid \mathbf{X}_j = \mathbf{x}_j \sim \text{MVN}_{p_i}(\boldsymbol{\mu}_{i|j}, \boldsymbol{\Sigma}_{i|j})$
 - * $\boldsymbol{\mu}_{i|j} = \boldsymbol{\mu}_i + \boldsymbol{\Sigma}_{ij}\boldsymbol{\Sigma}_{jj}^{-1}(\mathbf{x}_j - \boldsymbol{\mu}_j)$
 - * $\boldsymbol{\Sigma}_{i|j} = \boldsymbol{\Sigma}_{ii} - \boldsymbol{\Sigma}_{ij}\boldsymbol{\Sigma}_{jj}^{-1}\boldsymbol{\Sigma}_{ji}$
 - $\mathbf{X}_1 \perp\!\!\!\perp \mathbf{X}_2 \Leftrightarrow \boldsymbol{\Sigma}_{12} = \mathbf{0}$
 - * Warning: the prerequisite for this equivalence is the joint normal of \mathbf{X}_1 and \mathbf{X}_2 .
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- Exercise: The argument $\mathbf{X}_1 \perp\!\!\!\perp \mathbf{X}_2 \Leftrightarrow \boldsymbol{\Sigma}_{12} = \mathbf{0}$ is based on $[\mathbf{X}_1^\top, \mathbf{X}_2^\top]^\top \sim \text{MVN}$. That is, if \mathbf{X}_1 and \mathbf{X}_2 are both MVN BUT they are not jointly normal, the zero $\boldsymbol{\Sigma}_{12}$ doesn't suffice for the independence between \mathbf{X}_1 and \mathbf{X}_2 . Recall the instance in the previous exercise: $X_1 \sim \mathcal{N}(0, 1)$ and $X_2 = (2Y - 1)X_1$. Verify that X_1 and X_2 are not independent of each other.

Checking normality (J&W Sec 4.6)

- Checking the univariate marginal distributions
 - Normal Q-Q plot
 - * `qqnorm()`; `car::qqPlot()`
 - Univariate normality test
 - * `shapiro.test()`; `nortest::ad.test()`
 - Testing the multivariate normality
 - `MVN::mvn()`
 - Checking the quadratic form
 - χ^2 Q-Q plot
 - * $D_i^2 = (\mathbf{X}_i - \bar{\mathbf{X}})^\top \mathbf{S}^{-1}(\mathbf{X}_i - \bar{\mathbf{X}}) \approx \chi^2(p)$ if $\mathbf{X}_i \stackrel{\text{iid}}{\sim} \text{MVN}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
 - * `qqplot()`; `car::qqPlot()`
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Detecting outliers (J&W Sec 4.7)

- Scatter plot of standardized values
- Check the points farthest from the origin in χ^2 Q-Q plot

Improving normality (J&W Sec 4.8)

- (Original) Box-Cox (power) transformation: transform positive x into

$$x^* = \begin{cases} (x^\lambda - 1)/\lambda & \lambda \neq 0 \\ \ln(x) & \lambda = 0 \end{cases}$$

with λ selected with certain criterion

- If $x \leq 0$, change it to be positive first.
- See J. Tukey (1977). *Exploratory Data Analysis*. Boston: Addison-Wesley.
- Multivariate Box-Cox transformation

Maximum likelihood (ML) estimation of μ and Σ (J&W Sec 4.3)

- Sample: $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} \text{MVN}_p(\mu, \Sigma)$, $n > p$
- Parameter space: $\Theta = \{(\mu, \Sigma) \mid \mu \in \mathbb{R}^p, \Sigma \in \mathbb{R}^{p \times p}, \Sigma > 0\}$
- Likelihood function

$$\begin{aligned} L(\mu, \Sigma) &= \prod_{i=1}^n \left[\frac{1}{\sqrt{(2\pi)^p \det(\Sigma)}} \exp \left\{ -\frac{1}{2} (\mathbf{X}_i - \mu)^\top \Sigma^{-1} (\mathbf{X}_i - \mu) \right\} \right] \\ &= \frac{1}{\sqrt{(2\pi)^{np} \{\det(\Sigma)\}^n}} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n (\mathbf{X}_i - \mu)^\top \Sigma^{-1} (\mathbf{X}_i - \mu) \right\} \end{aligned}$$

- Log likelihood

$$\ell(\mu, \Sigma) = \ln\{L(\mu, \Sigma)\} = -\frac{np}{2} \ln(2\pi) - \frac{n}{2} \ln\{\det(\Sigma)\} - \frac{1}{2} \sum_{i=1}^n (\mathbf{X}_i - \mu)^\top \Sigma^{-1} (\mathbf{X}_i - \mu)$$

- ML estimator

$$(\hat{\mu}_{\text{ML}}, \hat{\Sigma}_{\text{ML}}) = \arg \max_{(\mu, \Sigma) \in \Theta} \ell(\mu, \Sigma) = (\bar{\mathbf{X}}, \frac{n-1}{n} \mathbf{S})$$

- Consistency: $(\hat{\mu}_{\text{ML}}, \hat{\Sigma}_{\text{ML}})$ approaches (μ, Σ) (in certain sense) as $n \rightarrow \infty$
- Efficiency: the covariance matrix of $(\hat{\mu}_{\text{ML}}, \hat{\Sigma}_{\text{ML}})$ is approximately optimal (in certain sense) as $n \rightarrow \infty$
- Invariance: For any function g , the ML estimator of $g(\mu, \Sigma)$ is $g(\hat{\mu}_{\text{ML}}, \hat{\Sigma}_{\text{ML}})$.

Sampling distributions of $\bar{\mathbf{X}}$ and \mathbf{S} (J&W Sec 4.4)

- Recall the univariate case
 - $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$
 - $S^2 \perp\!\!\!\perp \bar{X}$
 - * Sample variance $S^2 = (n-1)^{-1} \sum_{i=1}^n (X_i - \bar{X})^2$
 - $\sqrt{n}(\bar{X} - \mu)/\sigma \sim \mathcal{N}(0, 1)$
 - $(n-1)S^2/\sigma^2 \sim \chi^2(n-1)$
 - $\sqrt{n}(\bar{X} - \mu)/S \sim t(n-1)$
- The multivariate case
 - $\mathbf{X}_1, \dots, \mathbf{X}_n \stackrel{\text{iid}}{\sim} \text{MVN}_p(\mu, \Sigma)$, $n > p$
 - $\mathbf{S} \perp\!\!\!\perp \bar{\mathbf{X}}$, i.e., $\hat{\Sigma}_{\text{ML}} \perp\!\!\!\perp \hat{\mu}_{\text{ML}}$
 - $\sqrt{n}\Sigma^{-1/2}(\bar{\mathbf{X}} - \mu) \sim \text{MVN}_p(\mathbf{0}, \mathbf{I})$

- $(n-1)\mathbf{S} = n\widehat{\boldsymbol{\Sigma}}_{\text{ML}} \sim W_p(\boldsymbol{\Sigma}, n-1)$
 - $n(\bar{\mathbf{X}} - \boldsymbol{\mu})^\top \mathbf{S}^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu}) \sim \text{Hotelling's } T^2(p, n-1)$
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- Wishart distribution

- Def: $W_p(\boldsymbol{\Sigma}, n)$ is the distribution of $\sum_{i=1}^n \mathbf{Y}_i \mathbf{Y}_i^\top$ with $\mathbf{Y}_1, \dots, \mathbf{Y}_n \stackrel{\text{iid}}{\sim} \text{MVN}_p(\mathbf{0}, \boldsymbol{\Sigma})$
 - * A generalization of χ^2 -distribution: $W_p(\boldsymbol{\Sigma}, n) = \chi^2(n)$ if $p = \boldsymbol{\Sigma} = 1$
- Properties
 - * $\mathbf{A}\mathbf{A}^\top > 0$ and $\mathbf{W} \sim W_p(\boldsymbol{\Sigma}, n) \Rightarrow \mathbf{A}\mathbf{W}\mathbf{A}^\top \sim W_p(\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^\top, n)$
 - * $\mathbf{W}_i \stackrel{\text{iid}}{\sim} W_p(\boldsymbol{\Sigma}, n_i) \Rightarrow \mathbf{W}_1 + \mathbf{W}_2 \sim W_p(\boldsymbol{\Sigma}, n_1 + n_2)$
 - * $\mathbf{W}_1 \perp\!\!\!\perp \mathbf{W}_2$, $\mathbf{W}_1 + \mathbf{W}_2 \sim W_p(\boldsymbol{\Sigma}, n)$ and $\mathbf{W}_1 \sim W_p(\boldsymbol{\Sigma}, n_1) \Rightarrow \mathbf{W}_2 \sim W_p(\boldsymbol{\Sigma}, n - n_1)$
 - * $\mathbf{W} \sim W_p(\boldsymbol{\Sigma}, n)$ and $\mathbf{a} \in \mathbb{R}^p \Rightarrow$

$$\frac{\mathbf{a}^\top \mathbf{W} \mathbf{a}}{\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a}} \sim \chi^2(n)$$

- * $\mathbf{W} \sim W_p(\boldsymbol{\Sigma}, n)$, $\mathbf{a} \in \mathbb{R}^p$ and $n \geq p \Rightarrow$

$$\frac{\mathbf{a}^\top \boldsymbol{\Sigma}^{-1} \mathbf{a}}{\mathbf{a}^\top \mathbf{W}^{-1} \mathbf{a}} \sim \chi^2(n - p + 1)$$

- * $\mathbf{W} \sim W_p(\boldsymbol{\Sigma}, n) \Rightarrow$

$$\text{tr}(\boldsymbol{\Sigma}^{-1} \mathbf{W}) \sim \chi^2(np)$$

- Hotelling's T^2 distribution

- A generalization of (Student's) t -distribution
- If $\mathbf{X} \sim \text{MVN}_p(\mathbf{0}, \mathbf{I})$ and $\mathbf{W} \sim W_p(\mathbf{I}, n)$, then

$$\mathbf{X}^\top \mathbf{W}^{-1} \mathbf{X} \sim T^2(p, n)$$

- $Y \sim T^2(p, n) \Leftrightarrow \frac{n-p+1}{np} Y \sim F(p, n-p+1)$
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- Wilk's lambda distribution

- Wilks's lambda is to Hotelling's T^2 as F distribution is to Student's t in univariate statistics.
- Given independent $\mathbf{W}_1 \sim W_p(\boldsymbol{\Sigma}, n_1)$ and $\mathbf{W}_2 \sim W_p(\boldsymbol{\Sigma}, n_2)$ with $n_1 \geq p$,

$$\Lambda = \frac{\det(\mathbf{W}_1)}{\det(\mathbf{W}_1 + \mathbf{W}_2)} = \frac{1}{\det(\mathbf{I} + \mathbf{W}_1^{-1} \mathbf{W}_2)} \sim \Lambda(p, n_1, n_2)$$

- * Resort to an approximation in computation: $\{(p - n_2 + 1)/2 - n_1\} \ln \Lambda(p, n_1, n_2) \approx \chi^2(n_2 p)$

Inference on $\boldsymbol{\mu}$

Hypothesis testing

- Is it a squirrel?



Figure 1: Squirrel (Photograph by the Lacoste Garden Centre)



Figure 2: Flying Squirrel (Photograph by Joel Sartore)



Figure 3: Flying Squirrel (Photograph by Alex Badyaev)

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- Model: $\mathbf{X} \sim f_{\boldsymbol{\theta}^*} \in \{f_{\boldsymbol{\theta}} : \boldsymbol{\theta} \in \boldsymbol{\Theta}\}$
 - $\boldsymbol{\theta}^*$: parameters of interest, fixed and unknown
 - $\boldsymbol{\Theta}$: the parameter space
 - Hypotheses $H_0 : \boldsymbol{\theta}^* \in \boldsymbol{\Theta}_0$ v.s. $H_1 : \boldsymbol{\theta}^* \in \boldsymbol{\Theta}_1$
 - $\boldsymbol{\Theta}_0 \cap \boldsymbol{\Theta}_1 = \emptyset$
 - $\boldsymbol{\Theta}_0 \cup \boldsymbol{\Theta}_1 = \boldsymbol{\Theta}$
 - Rejection/critical region R

- Reject H_0 if $\mathbf{X} \in R$
- Level α : $\sup_{\boldsymbol{\theta} \in \Theta_0} \beta(\boldsymbol{\theta}) \leq \alpha$
 - Power function: $\beta(\boldsymbol{\theta}) = \Pr_{\boldsymbol{\theta}}(\mathbf{X} \in R)$
 - When $\boldsymbol{\theta}^* \in \Theta_0$, $\Pr(\text{type I error}) = \beta(\boldsymbol{\theta}^*) \leq \sup_{\boldsymbol{\theta} \in \Theta_0} \beta(\boldsymbol{\theta}) \leq \alpha$
 - * Type I error: H_0 is incorrectly rejected
 - When $\boldsymbol{\theta}^* \in \Theta_1$, $\Pr(\text{type II error}) = 1 - \beta(\boldsymbol{\theta}^*)$
 - * Type II error: H_0 is incorrectly accepted
- p -value: alternative to rejection region
 - Impossible to be well-defined in some cases
 - $p = p(\mathbf{x})$ is defined such that $\sup_{\boldsymbol{\theta} \in \Theta_0} \Pr_{\boldsymbol{\theta}}\{p(\mathbf{x}) \in [0, \alpha]\} \leq \alpha$ for all $\alpha \in [0, 1]$
 - * $R = \{\mathbf{x} : p(\mathbf{x}) \in [0, \alpha]\}$
- Necessary components in reporting a testing result
 1. Hypotheses
 2. Name of approach
 3. Value of test statistic
 4. Rejection region/ p -value
 5. Conclusion: e.g., at the α level, we reject/do not reject H_0 , i.e., we believe...

Likelihood ratio test (LRT)

- Minimize the type II error rate subject to a capped type I error rate (under certain classical circumstances)
- Test statistic

$$\lambda(\mathbf{X}) = \frac{\sup_{\boldsymbol{\theta} \in \Theta_0} L(\boldsymbol{\theta}; \mathbf{X})}{\sup_{\boldsymbol{\theta} \in \Theta} L(\boldsymbol{\theta}; \mathbf{X})} = \frac{L(\hat{\boldsymbol{\theta}}_0; \mathbf{X})}{L(\hat{\boldsymbol{\theta}}; \mathbf{X})}$$

- $\hat{\boldsymbol{\theta}}_0$: ML estimator for $\boldsymbol{\theta} \in \Theta_0$
- $\hat{\boldsymbol{\theta}}$: ML estimator for $\boldsymbol{\theta} \in \Theta$
- Rejection region $R = \{\mathbf{x} : \lambda(\mathbf{x}) \leq c\}$
 - \mathbf{x} is the realization of \mathbf{X}
 - $c \in \mathbb{R}$ is chosen such that

$$\sup_{\boldsymbol{\theta} \in \Theta_0} \Pr_{\boldsymbol{\theta}}(\lambda(\mathbf{X}) \leq c) = \alpha.$$

- * Have to know the null distribution of $\lambda(\mathbf{X})$, i.e., the distribution of $\lambda(\mathbf{X})$ with $\boldsymbol{\theta} \in \Theta_0$

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- p -value

$$p(\mathbf{x}) = \sup_{\boldsymbol{\theta} \in \Theta_0} \Pr_{\boldsymbol{\theta}}\{\lambda(\mathbf{X}) \leq \lambda(\mathbf{x})\}$$

- Null distribution of $\lambda(\mathbf{X})$
 - Use the accurate distribution of $\lambda(\mathbf{X})$ if it is known; otherwise see below for an approximation.
 - As $n \rightarrow \infty$,

$$-2 \ln \lambda(\mathbf{X}) \sim \chi^2(\nu)$$

- * ν : the difference in numbers of free parameters between H_0 and H_1
- * Leading to an (asymptotic) rejection region $\{\mathbf{x} : -2 \ln \lambda(\mathbf{x}) \geq \chi_{\nu, 1-\alpha}^2\}$
 - $\chi_{\nu, 1-\alpha}^2$ is the $(1 - \alpha)$ -quantile of $\chi^2(\nu)$.