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Section 1

The Big Picture

The Big Picture: Univariate vs Multivariate

- Review: A random sample, denoted by X_1, \dots, X_n , from a (univariate) normal distribution $N(\mu, \sigma^2)$
 - What are the distributions of \bar{X} , s^2 ? What useful statistics can be constructed?
- New material: A random sample, denoted by $\mathbf{X}_1, \dots, \mathbf{X}_n$, from a multivariate normal distribution $N(\mu, \Sigma)$
 - What are the distributions of $\bar{\mathbf{X}}, \mathbf{S}$? What useful statistics can be constructed?

- A random sample, denoted by X_1, \dots, X_n , from a (univariate) normal distribution $N(\mu, \sigma^2)$
- Let $\mathbf{X}_{n\times 1} = (X_1, \dots, X_n)^T$. It is random vector with a multivarite normal distribution, i.e.,

$$\mathbf{X}_{n\times 1} = (X_1, \cdots, X_n)^T \sim \mathbf{N}(\mu \mathbf{1}, \sigma^2 \mathbf{I})$$

- $\bullet \quad \bar{X} \sim N(\mu, \sigma^2/n)$
- $\frac{(n-1)s^2}{\sigma^2} \sim \chi_{n-1}^2$
- 3 Independence between \bar{X} and s^2 .
- a t-statistic is

$$\frac{\frac{\bar{X}-\mu}{\sqrt{\sigma^2/n}}}{\sqrt{\frac{(n-1)s^2/\sigma^2}{n-1}}} = \frac{\sqrt{n}(\bar{X}-\mu)}{s}$$

It follows the t-distribution with n-1 degrees of freedom, denoted by t_{n-1} .

The Big Picture: Multivariate

- A random sample X_1, \dots, X_n from a multivariate normal distribution $N(\mu, \Sigma)$.
- Let

$$\mathbf{X}_{n \times p} = \begin{pmatrix} \mathbf{X}_1^T \\ \vdots \\ \mathbf{X}_n^T \end{pmatrix}$$

X follows a matrix normal distribution.

- Sample mean vector follows a multivariate normal, i.e., $\bar{\mathbf{X}} \sim \mathbf{N}(\mu, \mathbf{\Sigma}/n)$
- ② Sample covariance matrix (n-1)**S** follows a Wishart distribution, i.e., (n-1)**S** \sim Wishart $_p(n-1,\Sigma)$
- **1** Independence between $\bar{\mathbf{X}}$ and S.
- Hoetelling's T^2 : $T^2 = (\bar{\mathbf{X}} \mu)^T \left(\frac{\mathbf{S}}{n}\right)^{-1} (\bar{\mathbf{X}} \mu)$

The Big Picture: outline

The Big Picture

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- Sample variance and chi-squared distribution
- Sample covariance matrix and Wishart distribution
- Hotelling's T²
- Maximum likelihood estimate

Section 2

Sample Variance

Sample Variance and Chi-squared Distribution

- Let $\mathbf{X} = (X_1, \dots, X_n)$ denote a random sample from $N(\mu, \sigma^2)$.
- Equivalently, $\mathbf{X} \sim N(\mu \mathbf{1}, \sigma^2 \mathbf{I})$.
- Let $s^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i \bar{X})^2$ denote the sample variance.
- We would like to show that

$$\frac{(n-1)s^2}{\sigma^2} \sim \chi_{n-1}^2$$

- Outline of proof
 - Projection matrices
 - Chi-squared distribution
 - **3** Rewrite $(n-1)s^2/\sigma^2$ as the sum of squared N(0,1) random variables

Projection Matrices

• A projection matrix is a square matrix that is both idempotent and symmetric

$$\mathbf{P}^2 = \mathbf{P}, \ \mathbf{P} = \mathbf{P}^T$$

Projection Matrices

The Big Picture

- Suppose **P** is a projection matrix. We have
 - The eigenvalues of **P** has eigenvalues are either 0 or 1, and the number of 1's is the same as the rank of the projection matrix.
 - $tr(\mathbf{P}) = rank(\mathbf{P})$
 - The spectral decomposition of **P** is

$$\mathbf{P} = \sum_{i=j}^{r} \gamma_j \gamma_j^T$$

where $r = rank(\mathbf{P})$, and $(\gamma_1, \dots, \gamma_r)$ are orthogonal vectors of norm 1. i.e..

$$\gamma_i^T \gamma_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

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- The centering matrix $\mathbb{C} = \mathbf{I} \frac{1}{n}\mathbf{1}\mathbf{1}^T$ is a very special matrix.
- It is a projection matrix, which is defined as both symmetric and idempotent:
 - $\mathbb{C}^T = \mathbb{C}$ (symmetric)
 - $\mathbb{C}^2 = \mathbb{C}$ (idempotent)
- One important result about a projection matrix is that its eigenvalues are either zero or one.
- By properties of projection matrices, we have
 - $rank(\mathbb{C}) = tr(\mathbb{C}) = n-1$
 - $\bullet \ \mathbb{C} = \sum_{j=1}^{n-1} \gamma_j \gamma_j^T$

A Special Projection Matrix: the Centering Matrix

- The centering matrix centers data
- Univariate: Let $\mathbf{X}_{n\times 1}$ be a random sample from $N(\mu, \sigma^2)$, i.e.,

$$\mathbf{X}_{n\times 1} \sim N(\mu \mathbf{1}, \sigma^2 \mathbf{I})$$

 $\mathbb{C} X$ is a linear function of X and it can be verified that $\mathbb{C} 1 = 0$, we have

$$E[\mathbb{C}\mathbf{X}] = \mu \mathbb{C}\mathbf{1} = \mathbf{0}$$

- Multivariate: Let $\mathbf{X}_{n \times p}$ be a random sample from $N(\mu, \mathbf{\Sigma})$ Similarly, it can be shown that $\mathbb{C}\mathbf{X}$ has mean $\mathbf{0}_{n \times p}$. We have verified this numerically.
- In either situation, we have $\mathbb{C}\mathbf{X} = \mathbb{C}(\mathbf{X} E[\mathbf{X}])$ This fact will be used later.

Chi-squared distribution

The Big Picture

- Definition. Let $Z_1, Z_2, ..., Z_k$ be independent standard normal random variables. Then, the sum of squares $Q = Z_1^2 + Z_2^2 + ... + Z_k^2$ has a chi-squared distribution with k degrees of freedom, denoted by χ_k^2 .
- Alternative definition. Let $\mathbf{Z}_{k\times 1} \sim N(\mathbf{0}, \mathbf{I})$. We say $||\mathbf{Z}||^2 = \mathbf{Z}^T \mathbf{Z}$ follows χ_k^2 .
- The PDF of a chi-squared random variable with k degrees of freedom is given by:

$$f(x) = \frac{1}{2^{k/2}\Gamma(k/2)} x^{k/2-1} e^{-x/2}, x > 0$$

where $\Gamma(\cdot)$ is the gamma function.

Chi-squared distribution

The Big Picture

- The chi-squared distribution is a special case of the gamma distribution, where the shape parameter is k/2 and the rate parameter is 1/2.
- The MGF of a chi-squared random variable with k degrees of freedom is:

$$M_X(t) = (1-2t)^{-k/2}$$

• The mean and variance of a chi-squared random variable with k degrees of freedom are:

$$\mathsf{E}[X] = k, \, \mathsf{Var}[X] = 2k$$

Construct Chi-squared R.V.s using Normal R.V.s and **Projection Matrices**

• Let $P_{n\times n}$ be a projection matrix with rank r and let $\mathbf{Z}_{n\times 1} \sim N(\mathbf{0}, \mathbf{I})$

$$\mathbf{Z}^{T}\mathbf{P}\mathbf{Z} = \mathbf{Z}^{T} \sum_{i=1}^{r} \gamma_{i} \gamma_{i}^{T} \mathbf{Z} = \sum_{i=1}^{r} \mathbf{Z}^{T} \gamma_{i} \gamma_{i}^{T} \mathbf{Z}$$
$$= \sum_{i=1}^{r} (\gamma_{i}^{T} \mathbf{Z})^{T} (\gamma_{i}^{T} \mathbf{Z})$$

Let $Y_i = \gamma_i^T \mathbf{Z}$. Note that Y_i is univariate and it is a linear combination of **Z**, from which we can show that $Y_i \sim N(0,1)$.

• Note that $\mathbf{Z}^T \mathbf{P} \mathbf{Z} = \sum_{i=1}^r Y_i^2$. By the definition of chi-squared distribution, we have $\mathbf{Z}^T \mathbf{PZ} \sim \chi^2_r$

The Sample Variance

- We have shown that
 - $\mathbb{C} = I \frac{1}{2} \mathbf{1} \mathbf{1}^T$
 - $\bullet \mathbb{C}^T = \mathbb{C} \cdot \mathbb{C}^2 = \mathbb{C}$.
 - It is a projection matrix with rank n-1 and

$$\mathbb{C} = \sum_{j=1}^{n-1} \gamma_i \gamma_i^T$$

-The he centering matrix does center data, i.e.,

$$\mathbb{C}\mathbf{X} = \mathbb{C}(\mathbf{X} - E[\mathbf{X}])$$

• $(n-1)s^2 = \mathbf{X}^T \mathbb{C} \mathbf{X}$, where

The Sample Variance

• Therefore.

$$\frac{(n-1)s^2}{\sigma^2} = \frac{(\mathbf{X} - E[\mathbf{X}])^T}{\sigma} \mathbb{C}^T \mathbb{C} \mathbb{C} \frac{(\mathbf{X} - E[\mathbf{X}])}{\sigma}$$
$$= \frac{(\mathbf{X} - E[\mathbf{X}])^T}{\sigma} \mathbb{C} \frac{(\mathbf{X} - E[\mathbf{X}])}{\sigma}$$

Let

The Big Picture

$$\mathbf{Z} = \frac{(\mathbf{X} - E[\mathbf{X}])}{\sigma}$$

• Easy to see that $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$. Thus,

$$\frac{(n-1)s^2}{\sigma^2} = \mathbf{Z}^T \mathbb{C} \mathbf{Z}$$

• Use the result in previous slides, we have

$$\frac{(n-1)s^2}{\sigma^2} = \mathbf{Z}^T \mathbb{C} \mathbf{Z} \sim \chi_{n-1}^2$$

Section 3

Sample Covariance

Sample Covariance

The Sample Covriance from A MVN Random Sample

- Let $X_1, \dots, X_n \stackrel{iid}{\sim} N(\mu, \Sigma)$.
- Recall that the sample covariance matrix is defined as

$$\mathbf{S} = \frac{1}{n-1} \sum_{i=1}^{n} (\mathbf{X}_i - \bar{\mathbf{X}}) (\mathbf{X}_i - \bar{\mathbf{X}})^T$$

We have shown that

$$(n-1)\mathbf{S} = \mathbf{X}^T \mathbb{C} \mathbf{X}$$

where **X** is the $n \times p$ random matrix.

The Sample Covriance from A MVN Random Sample

• The goal is to show that (n-1)**S** follows a Wishart distribution. More specifically, we would like to show that

$$(n-1)$$
S $\sim Wishart_p(n-1,\Sigma)$

- Outline of proof
 - Wishart-distribution
 - 2 Rewrite (n-1)**S**
 - Apply properties of a projection matrix
 - Use the definition of Wishart distribution

Wishart Distribution

The Big Picture

 The Wishart distribution is named after the British statistician John Wishart, who introduced it in his 1928 paper published in Biometrika

Sample Covariance 00000000000000

- Wishart was interested in the problem of estimating the covariance matrix of a multivariate normal distribution.
- Wishart showed that the sample covariance matrix follows a particular probability distribution that we now call the Wishart distribution.
- The Wishart distribution has become a fundamental tool in multivariate statistical analysis

Definition of Wishart Distribution

The Big Picture

A Wishart distribution can be defined in the following way

Sample Covariance 00000000000000

- Let **W** be a $p \times p$ random matrix. We say **W** follows Wishart_p (k, Σ) if **W** can be written as **W** = $\mathbf{X}^T \mathbf{X}$ where **X** denotes the random matrix formed by a random sample of size k from MVN $N(\mathbf{0}, \mathbf{\Sigma})$.
- The definition indicates that if we have a random sample $X_1, \cdots X_k$ from $N(0, \Sigma)$, then $\mathbf{X}^T\mathbf{X} = \sum_{i=1}^k \mathbf{X}_i \mathbf{X}_i^T \sim Wishart_n(k, \mathbf{\Sigma}).$
- Remark: $E[\mathbf{W}] = k\Sigma$.

• Wishart: If $X_1, \dots X_k \stackrel{iid}{\sim} N(0, \Sigma)$, then

$$\mathbf{X}^T\mathbf{X} = \sum_{i=1}^k \mathbf{X}_i \mathbf{X}_i^T \sim Wishart_p(k, \mathbf{\Sigma}), \text{ where } \mathbf{X}_{k \times p} = \begin{pmatrix} X_1' \\ \vdots \\ X_k^T \end{pmatrix}$$

• Chi-squared: If $X_1, \dots, X_k \stackrel{iid}{\sim} N(0,1)$, then

$$\mathbf{X}^T\mathbf{X} = \sum_{i=1}^k X_i^2 \sim \chi_k^2$$
, where $\mathbf{X}_{k \times 1} = \begin{pmatrix} X_1 \\ \vdots \\ X_k \end{pmatrix}$

Wishart vs Chi-squared (continued)

• When p=1,

$$W = \sum_{i=1}^{k} X_i^2 = \sigma^2 \sum_{i=1}^{k} \left(\frac{X_i}{\sigma}\right)^2 \sim \sigma^2 \chi_k^2$$

The Big Picture

• Let $X_1, \dots X_n$ be a random sample from $N(\mu, \Sigma)$. The $X_{n \times n}$ follows a matrix normal distribution:

$$X \sim N(\mathbf{1}_n \otimes \boldsymbol{\mu}^T, \boldsymbol{\Sigma}, \mathbf{I}_n)$$

Sample Covariance

- The sample covariance $(n-1)\mathbf{S} = \mathbf{X}^T \mathbb{C} \mathbf{X}$ is based on the centered data. The definition of Wishart distribution is not applicable immediately.
- Next we show that (n-1)**S** follows Wishart_n $(n-1, \Sigma)$.

• Rewrite (n-1)**S**:

The Big Picture

$$(n-1)\mathbf{S} = \mathbf{X}^T \mathbb{C}^T \mathbb{C} \mathbb{C} \mathbf{X} = (\mathbb{C} \mathbf{X})^T (\mathbb{C} \mathbf{X})$$

$$= (\mathbb{C} \mathbf{X})^T \mathbb{C} (\mathbb{C} \mathbf{X})$$

$$= (\mathbb{C} \mathbf{X})^T \sum_{j=1}^{n-1} \gamma_i \gamma_i^T (\mathbb{C} \mathbf{X})$$

$$= \sum_{i=1}^{n-1} (\gamma_i^T \mathbb{C} \mathbf{X})^T (\gamma_i^T \mathbb{C} \mathbf{X})$$

The Big Picture

- Let $Y_i = (\gamma_i^T \mathbb{C} \mathbf{X})^T$, we have
 - $E[Y_i] = 0$ because \mathbb{C} is the centering matrix
 - In the following, we show that Y_i and Y_j are uncorrelated for $i \neq j$:

$$Cov[Y_i, Y_j] = E[(Y_i - \mathbf{0})(Y_j - \mathbf{0})^T]$$

$$= E[Y_i Y_j^T]$$

$$= E[(\gamma_i^T \mathbb{C} \mathbf{X})^T (\gamma_j^T \mathbb{C} \mathbf{X})]$$

$$= E[\mathbf{X}^T \mathbb{C} \gamma_i \gamma_j^T \mathbb{C} \mathbf{X}]$$

$$= \mathbf{0}$$

The last step is true because for $i \neq j$, $\gamma_i \gamma_i^T = 0$

The Big Picture

Since Y_i and Y_j are two linear combinations of the same MVN distributed random matrix (or its vectorized version), we have Y_i and Y_j are independent for $i \neq j$.

- It can also be shown that $Y_i \sim N(\mathbf{0}, \Sigma)$.
- By the definition of Wishart, we can conclude that

$$(n-1)$$
S $\sim Wishart_p(n-1, \Sigma)$

Some Interesting Results

The Big Picture

• Consider a random sample from MVN $N(\mu, \Sigma)$. Let **S** denote the sample covariance matrix.

Sample Covariance 00000000000000

- We have already shown that $(n-1)\mathbf{S} \sim Wishart_{p}(n-1, \mathbf{\Sigma})$
- What is the distribution of a diagonal element of (n-1)**S**?
- What is the distribution of the sum of elements of (n-1)**S**?
- What is the distribution of $(n-1)BSB^T$ where B is a fixed $q \times p$ matrix?
- If time permits, we will run some simulations

Some Interesting Results (continued)

- If you cannot get the answer to the last question, let's use the definition of Wishart distribution.
- Let $\mathbf{W} = (n-1)S$. Because it follows $Wishart_p(n-1, \mathbf{\Sigma})$, we know that $\mathbf{W} = \sum_{j=1}^{n-1} \mathbf{Z}_j \mathbf{Z}_j^T$ where \mathbf{Z}_j 's are iid frm $N(\mathbf{0}, \mathbf{\Sigma})$.
- Then

The Big Picture

$$(n-1)\mathsf{BSB}^T = \mathsf{B}\sum_{j=1}^{n-1} \mathsf{Z}_j \mathsf{Z}_j^T \mathsf{B} = \sum_{j=1}^{n-1} \mathsf{B} \mathsf{Z}_j \mathsf{Z}_j^T \mathsf{B}^T$$

$$= \sum_{j=1}^{n-1} (\mathsf{B} \mathsf{Z}_j) (\mathsf{B} \mathsf{Z}_j)^T$$

Some Interesting Results (continued)

Let $\mathbf{Y}_i = \mathbf{BZ}_i$. Note that it is a linear function of \mathbf{Z}_i ; therefore

$$\mathbf{Y}_{j} \sim \mathcal{N}(\mathbf{0}, \mathbf{B}\mathbf{\Sigma}\mathbf{B}^{T})$$

and the \mathbf{Y}_i 's are iid (becaue ...).

By the definition of Wishart distribution, we have

$$(n-1)\mathsf{BSB}^{\mathsf{T}} \sim \mathit{Wishart}_q(n-1,\mathsf{B}\boldsymbol{\Sigma}\mathsf{B}^{\mathsf{T}})$$

Section 4

Hotelling's T^2

Hotelling's T^2

- Finally we are ready to introduce Hotelling's
- The student's t is used for making inference of mean(s) of normal distribution(s)
- Hotelling generalized the student's t, which is for univarite, to Hotelling's T2, which the multivariate version

- Definition. We say a random variable follows Hotelling's T^2 $T_{p,
 u}^2$ if the random variable can be written as $\mathbf{Z}^T \left(rac{W}{
 u}
 ight)^{-1} \mathbf{Z}$ where
 - $\mathbf{0} \ \mathsf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$
 - **2** $\mathbf{W} \sim W_p(\nu, \boldsymbol{\sigma})$
 - Z ⊥ W

One-Sample Hotelling T^2

The Big Picture

- Let $X_1, X_2, ..., X_n$ be a random sample from a multivariate normal distribution with mean vector μ and covariance matrix Σ
- The sample mean vector and sample covariance matrix are denoted by **X** and **S**, respectively.
- The null hypothesis of interest H_0 : $\mu = \mu_0$
- The one-sample Hotelling T^2 is defined as

$$T^2 = (\hat{\mu} - \mu_0)^T (Cov(\hat{\mu}))^{-1} (\hat{\mu} - \mu_0)$$

One-Sample Hotelling T^2 (continued)

• To see that T^2 does follow Hotelling's T^2 , we rewrite it

$$T^{2} = (\hat{\mu} - \mu_{0})^{T} (Cov(\hat{\mu}))^{-1} (\hat{\mu} - \mu_{0})$$

$$= (\bar{\mathbf{X}} - \mu_{0})^{T} (Cov(\bar{\mathbf{X}}))^{-1} (\bar{\mathbf{X}} - \mu_{0})$$

$$= (\bar{\mathbf{X}} - \mu_{0})^{T} (\frac{S}{n})^{-1} (\bar{\mathbf{X}} - \mu_{0})$$

$$= [\sqrt{n}(\bar{\mathbf{X}} - \mu_{0})]^{T} (\frac{(n-1)S}{n-1})^{-1} [\sqrt{n}(\bar{\mathbf{X}} - \mu_{0})]$$

- We have shown that all the three conditions for constructing a Hotelling's T^2 are satisfied
- As a result, $T^2 \sim T_{n,n-1}^2$.

Hotelling's T^2 Distribution vs F Distribution

Hotelling's T^2

Claim:
$$T_{p,\nu}^2 \sim \frac{\nu p}{\nu+1-p} F_{p,\nu+1-p}$$
.

For the T^2 statistic, we have $T^2 \stackrel{H_0}{\sim} \frac{(n-1)p}{n-p} F_{p,n-p}$. We reject H_0 at significance level α when $T^2 > \frac{(n-1)p}{n-p} F_{p,n-p,1-\alpha}$.

Corollary.

The Big Picture

$$\frac{n-p}{p}(\bar{X}-\mu_0)^T(\hat{\Sigma})^{-1}(\bar{X}-\mu_0) \stackrel{H_0}{\sim} F_{p,n-p}$$

where
$$\hat{\Sigma} = \frac{1}{n}X^T H X = \frac{1}{n}\sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^T = \frac{(n-1)S}{n}$$
.

Section 5

MLE

MLE: Introduction

- The maximum likelihood estimate (MLE) is a widely used method for estimating the parameters of a statistical model.
- In this presentation, we will focus on the MLE for a multivariate normal distribution.

MLF: Multivariate Normal Distribution

• A random vector **X** follows a p-dimensional multivariate normal distribution with mean vector μ and covariance matrix Σ , denoted by $X \sim \mathcal{N}_p(\mu, \Sigma)$, if its probability density function is given by:

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{1}{(2\pi)^{p/2} |\mathbf{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

where $|\Sigma|$ denotes the determinant of Σ .

MLE:Maximum Likelihood Estimate

- Let $\pmb{X}_1, \pmb{X}_2, ..., \pmb{X}_n$ be a random sample from a multivariate normal distribution with mean vector $\pmb{\mu}$ and covariance matrix $\pmb{\Sigma}$.
- The log-likelihood function for the sample is given by:

$$\ell(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log|\boldsymbol{\Sigma}| - \frac{1}{2} \sum_{i=1}^{n} (\boldsymbol{X}_i - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{X}_i - \boldsymbol{\mu})$$

• The MLE of μ is the sample mean $\bar{\boldsymbol{X}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{X}_{i}$.

MLE:Maximum Likelihood Estimate (continued)

• To derive the MLE of Σ , we first take the derivative of the log-likelihood function with respect to Σ and set it equal to zero:

$$\frac{\partial \ell}{\partial \mathbf{\Sigma}} = -\frac{n}{2} \mathbf{\Sigma}^{-1} + \frac{1}{2} \sum_{i=1}^{n} (\mathbf{X}_i - \boldsymbol{\mu}) (\mathbf{X}_i - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-2} = 0$$

• Solving for Σ , we obtain the MLE as:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{i=1}^{n} (\boldsymbol{X}_i - \hat{\boldsymbol{\mu}}) (\boldsymbol{X}_i - \hat{\boldsymbol{\mu}})^T$$

• where $\hat{\mu}$ is the MLE of μ , as previously derived.