

Derivation of a test for equality of means with unequal variances

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Contents

Hypotheses	2
Definitions	2
Derivation of the maximum likelihood under the null	2
Numerical approximation of MLEs	4
Derivation of the unrestricted maximum likelihood	7
Likelihood ratio	9

Hypotheses

Let Y_{ij} denote the j th observation of the i th treatment group. Where $i = 1, 2, 3, \dots, m$ and $j = 1, 2, 3, \dots, n_i$. Under the null hypothesis: $Y_{ij} \sim N(\mu, \sigma_i^2)$. Under the alternative hypothesis: $Y_{ij} \sim N(\mu_i, \sigma_i^2)$, where $\mu_i \neq \mu_k$ for at least one pair of i and k values.

Definitions

$$\begin{aligned} n &= \sum_{i=1}^m n_i \\ \bar{Y} &= \frac{1}{n} \sum_{i=1}^m \sum_{j=1}^{n_i} Y_{ij} \\ \bar{Y}_i &= \frac{1}{n_i} \sum_{j=1}^{n_i} Y_{ij} \end{aligned}$$

We will later use δ_{ik} , which is the Kronecker delta symbol. It equals 0 if $i \neq k$ and 1 otherwise.

Derivation of the maximum likelihood under the null

In this section we will use $L(H_0)$ to denote the likelihood under the null.

$$\begin{aligned} L(H_0) &= \prod_{i=1}^m \prod_{j=1}^{n_i} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{1}{2\sigma_i^2}(Y_{ij} - \mu)^2\right) \\ &= (2\pi)^{-n/2} \left(\prod_{i=1}^m \sigma_i^{-n_i}\right) \exp\left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\sigma_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \mu)^2\right). \end{aligned} \tag{1}$$

Taking the natural logarithm yields:

$$\ln L(H_0) = -\frac{n}{2} \ln 2\pi - \frac{1}{2} \sum_{i=1}^m n_i \ln \sigma_i^2 - \frac{1}{2} \sum_{i=1}^m \frac{1}{\sigma_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \mu)^2.$$

Differentiating the log-likelihood with respect to μ and setting to zero to maximize the likelihood:

$$\begin{aligned}
\frac{\partial \ln L(H_0)}{\partial \mu} \Big|_{\mu=\hat{\mu}, \sigma_i^2=\hat{\sigma}_i^2} &= -\frac{1}{2} \sum_{i=1}^m \frac{1}{\hat{\sigma}_i^2} \sum_{j=1}^{n_i} 2(-1)(Y_{ij} - \hat{\mu}) \\
&= 0 \\
\sum_{i=1}^m \frac{1}{\hat{\sigma}_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \hat{\mu}) &= 0 \\
\sum_{i=1}^m \frac{1}{\hat{\sigma}_i^2} (n_i \bar{Y}_i - n_i \hat{\mu}) &= 0 \\
\left(\sum_{i=1}^m \frac{n_i \bar{Y}_i}{\hat{\sigma}_i^2} \right) - \left(\sum_{i=1}^m \frac{n_i}{\hat{\sigma}_i^2} \right) \hat{\mu} &= 0 \\
\hat{\mu} &= \frac{\sum_{i=1}^m \frac{n_i \bar{Y}_i}{\hat{\sigma}_i^2}}{\sum_{i=1}^m \frac{n_i}{\hat{\sigma}_i^2}}. \tag{2}
\end{aligned}$$

Differentiating the log-likelihood with respect to σ_k^2 and setting to zero to maximize the likelihood:

$$\begin{aligned}
\frac{\partial \ln L(H_0)}{\partial \sigma_k^2} \Big|_{\mu=\hat{\mu}, \sigma_i^2=\hat{\sigma}_i^2} &= -\frac{1}{2} \sum_{i=1}^m \frac{n_i}{\hat{\sigma}_i^2} \delta_{ik} - \frac{1}{2} \sum_{i=1}^m -\frac{1}{\hat{\sigma}_i^4} \delta_{ik} \sum_{j=1}^{n_i} (Y_{ij} - \hat{\mu})^2 \\
&= -\frac{1}{2} \frac{n_k}{\hat{\sigma}_k^2} + \frac{1}{2\hat{\sigma}_k^4} \sum_{j=1}^{n_k} (Y_{kj} - \hat{\mu})^2 \\
&= 0.
\end{aligned}$$

Multiplying by $2\hat{\sigma}_k^4$ yields:

$$\begin{aligned}
-n_k \hat{\sigma}_k^2 + \sum_{j=1}^{n_k} (Y_{kj} - \hat{\mu})^2 &= 0 \\
\hat{\sigma}_k^2 &= \frac{1}{n_k} \sum_{j=1}^{n_k} (Y_{kj} - \hat{\mu})^2. \tag{3}
\end{aligned}$$

Some simplification of our likelihood can be done now using our MLEs, although unfortunately Equations 2 and 3 cannot be analytically solved, they must be numerically solved to yield values for $\hat{\mu}$ and $\hat{\sigma}_k^2$.

$$\begin{aligned}
L(H_0) &= (2\pi)^{-n/2} \left(\prod_{i=1}^m \widehat{\sigma}_i^2^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\widehat{\sigma}_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m n_i \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2} \right) \exp \left(-\frac{n}{2} \right) \\
&= (2\pi e)^{-n/2} \prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2}.
\end{aligned}$$

Numerical approximation of MLEs

So here we must numerically approximate $\widehat{\mu}$ and $\widehat{\sigma}_i^2$ using a technique like Newton's method and substitute this into our expression for $L(H_0)$ to get the maximum likelihood under the null. If we use Newton's method, we must have functions we are finding the zeros of. Let:

$$\begin{aligned}
f(\widehat{\mu}, \widehat{\sigma}_k^2) &= \widehat{\mu} - \frac{\sum_{k=1}^m \frac{n_k \bar{Y}_k}{\widehat{\sigma}_k^2}}{\sum_{k=1}^m \frac{n_k}{\widehat{\sigma}_k^2}} \\
g_i(\widehat{\mu}, \widehat{\sigma}_k^2) &= \widehat{\sigma}_i^2 - \frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2.
\end{aligned}$$

Therefore:

$$\begin{aligned}
\frac{\partial f}{\partial \hat{\mu}} &= 1 \\
\frac{\partial f}{\partial \hat{\sigma}_i^2} &= -\frac{\sum_{k=1}^m -\frac{n_k \bar{Y}_k}{\hat{\sigma}_k^4} \delta_{ik}}{\sum_{k=1}^m \frac{n_k}{\hat{\sigma}_k^2}} - \frac{\sum_{k=1}^m \frac{n_k \bar{Y}_k}{\hat{\sigma}_k^2}}{\left(\sum_{k=1}^m \frac{n_k}{\hat{\sigma}_k^2} \right)^2} \sum_{k=1}^m -\frac{n_k}{\hat{\sigma}_k^4} \delta_{ik} \\
&= \frac{\frac{n_i \bar{Y}_i}{\hat{\sigma}_i^4}}{\sum_{k=1}^m \frac{n_k}{\hat{\sigma}_k^2}} - \frac{\sum_{k=1}^m \frac{n_k \bar{Y}_k}{\hat{\sigma}_k^2}}{\left(\sum_{k=1}^m \frac{n_k}{\hat{\sigma}_k^2} \right)^2} \frac{n_i}{\hat{\sigma}_i^4} \\
&= \frac{n_i}{\hat{\sigma}_i^4 \sum_{k=1}^m \frac{n_k}{\hat{\sigma}_k^2}} \left(\bar{Y}_i - \frac{\sum_{i=1}^m \frac{n_i \bar{Y}_i}{\hat{\sigma}_i^2}}{\sum_{i=1}^m \frac{n_i}{\hat{\sigma}_i^2}} \right).
\end{aligned}$$

As for the derivatives of $g_i(\hat{\mu}, \hat{\sigma}_k^2)$:

$$\begin{aligned}
\frac{\partial g_i(\hat{\mu}, \hat{\sigma}_k^2)}{\partial \hat{\mu}} &= -\frac{1}{n_i} \sum_{j=1}^{n_i} 2(-1)(Y_{ij} - \hat{\mu}) \\
&= \frac{2}{n_i} (n_i \bar{Y}_i - n_i \hat{\mu}) \\
&= 2(\bar{Y}_i - \hat{\mu}) \\
\frac{\partial g_i(\hat{\mu}, \hat{\sigma}_k^2)}{\partial \hat{\sigma}_k^2} &= \delta_{ik}.
\end{aligned}$$

This thus gives us a Jacobian:

$$J = \begin{bmatrix} \frac{\partial f}{\partial \widehat{\mu}} & \frac{\partial f}{\partial \widehat{\sigma}_1^2} & \frac{\partial f}{\partial \widehat{\sigma}_2^2} & \frac{\partial f}{\partial \widehat{\sigma}_3^2} & \dots & \frac{\partial f}{\partial \widehat{\sigma}_m^2} \\ \frac{\partial g_1}{\partial \widehat{\mu}} & \frac{\partial g_1}{\partial \widehat{\sigma}_1^2} & \frac{\partial g_1}{\partial \widehat{\sigma}_2^2} & \frac{\partial g_1}{\partial \widehat{\sigma}_3^2} & \dots & \frac{\partial g_1}{\partial \widehat{\sigma}_m^2} \\ \frac{\partial g_2}{\partial \widehat{\mu}} & \frac{\partial g_2}{\partial \widehat{\sigma}_1^2} & \frac{\partial g_2}{\partial \widehat{\sigma}_2^2} & \frac{\partial g_2}{\partial \widehat{\sigma}_3^2} & \dots & \frac{\partial g_2}{\partial \widehat{\sigma}_m^2} \\ \frac{\partial g_3}{\partial \widehat{\mu}} & \frac{\partial g_3}{\partial \widehat{\sigma}_1^2} & \frac{\partial g_3}{\partial \widehat{\sigma}_2^2} & \frac{\partial g_3}{\partial \widehat{\sigma}_3^2} & \dots & \frac{\partial g_3}{\partial \widehat{\sigma}_m^2} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \frac{\partial g_m}{\partial \widehat{\mu}} & \frac{\partial g_m}{\partial \widehat{\sigma}_1^2} & \frac{\partial g_m}{\partial \widehat{\sigma}_2^2} & \frac{\partial g_m}{\partial \widehat{\sigma}_3^2} & \dots & \frac{\partial g_m}{\partial \widehat{\sigma}_m^2} \end{bmatrix}.$$

Interestingly, this Jacobian's main diagonal (left to right, top to bottom) consists entirely of 1s. The only off-diagonal elements that are non-zero are in the first row or first column. We also have this function vector:

$$\mathbf{F} = \begin{bmatrix} f(\widehat{\mu}, \widehat{\sigma}_k^2) \\ g_1(\widehat{\mu}, \widehat{\sigma}_k^2) \\ g_2(\widehat{\mu}, \widehat{\sigma}_k^2) \\ g_3(\widehat{\mu}, \widehat{\sigma}_k^2) \\ \dots \\ g_m(\widehat{\mu}, \widehat{\sigma}_k^2) \end{bmatrix}.$$

And we use the algorithm:

$$\begin{bmatrix} \widehat{\mu} \\ \widehat{\sigma}_1^2 \\ \widehat{\sigma}_2^2 \\ \widehat{\sigma}_3^2 \\ \dots \\ \widehat{\sigma}_m^2 \end{bmatrix}_{\text{New}} = \begin{bmatrix} \widehat{\mu} \\ \widehat{\sigma}_1^2 \\ \widehat{\sigma}_2^2 \\ \widehat{\sigma}_3^2 \\ \dots \\ \widehat{\sigma}_m^2 \end{bmatrix}_{\text{Old}} - J^{-1}\mathbf{F}$$

$$\begin{bmatrix} \hat{\mu} \\ \hat{\sigma}_1^2 \\ \hat{\sigma}_2^2 \\ \hat{\sigma}_3^2 \\ \dots \\ \hat{\sigma}_m^2 \end{bmatrix}$$

to numerically approximate our MLEs under the null. What should we use as our initial guess for ? Well,

how about the overall mean for $\hat{\mu}$ and the k th sample variance for $\hat{\sigma}_k^2$.

Derivation of the unrestricted maximum likelihood

We will use L_u to denote the unrestricted likelihood function.

$$\begin{aligned} L_u &= \prod_{i=1}^m \prod_{j=1}^{n_i} \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{1}{2\sigma_i^2}(Y_{ij} - \mu_i)^2\right) \\ &= (2\pi)^{-n/2} \left(\prod_{i=1}^m \sigma_i^{-n_i}\right) \exp\left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\sigma_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \mu_i)^2\right). \end{aligned}$$

Hence the unrestricted log-likelihood is:

$$\ln L_u = -\frac{n}{2} \ln 2\pi - \frac{1}{2} \sum_{i=1}^m n_i \ln \sigma_i^2 - \frac{1}{2} \sum_{i=1}^m \frac{1}{\sigma_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \mu_i)^2.$$

Setting the derivative with respect to μ_l to zero to find the MLE for μ_l :

$$\begin{aligned}
\frac{\partial \ln L_u}{\partial \mu_l} \Big|_{\mu_l = \hat{\mu}_l, \sigma_k^2 = \hat{\sigma}_k^2} &= -\frac{1}{2} \sum_{i=1}^m \frac{1}{\hat{\sigma}_i^2} \sum_{j=1}^{n_i} 2(-1)(Y_{ij} - \hat{\mu}_i) \delta_{il} \\
&= \frac{1}{\hat{\sigma}_l^2} \sum_{j=1}^{n_l} (Y_{lj} - \hat{\mu}_l) \\
&= \frac{1}{\hat{\sigma}_l^2} (n_l \bar{Y}_l - n_l \hat{\mu}_l) \\
&= 0. \\
\implies \hat{\mu}_l &= \bar{Y}_l.
\end{aligned}$$

Setting the derivative with respect to σ_k^2 to zero to find the MLE for σ_k^2 :

$$\begin{aligned}
\frac{\partial \ln L_u}{\partial \hat{\sigma}_k^2} \Big|_{\mu_l = \hat{\mu}_l, \sigma_k^2 = \hat{\sigma}_k^2} &= -\frac{1}{2} \sum_{i=1}^m \frac{n_i}{\hat{\sigma}_i^2} \delta_{ik} - \frac{1}{2} \sum_{i=1}^m -\frac{1}{\hat{\sigma}_i^4} \delta_{ik} \sum_{j=1}^{n_i} (Y_{ij} - \hat{\mu}_i)^2 \\
&= -\frac{n_k}{2\hat{\sigma}_k^2} + \frac{1}{2\hat{\sigma}_k^4} \sum_{j=1}^{n_k} (Y_{kj} - \hat{\mu}_k)^2 \\
&= 0. \\
\implies \hat{\sigma}_k^2 &= \frac{1}{n_k} \sum_{j=1}^{n_k} (Y_{kj} - \hat{\mu}_k)^2 \\
&= \frac{1}{n_k} \sum_{j=1}^{n_k} (Y_{kj} - \bar{Y}_k)^2.
\end{aligned}$$

Substituting these MLEs into our expression for L_u to get the unrestricted maximum likelihood:

$$\begin{aligned}
L_u &= (2\pi)^{-n/2} \left(\prod_{i=1}^m (\widehat{\sigma}_i^2)^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\widehat{\sigma}_i^2} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu}_i)^2 \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m \frac{1}{\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2} \right) \exp \left(-\frac{1}{2} \sum_{i=1}^m n_i \right) \\
&= (2\pi)^{-n/2} \left(\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2} \right) \exp \left(-\frac{n}{2} \right) \\
&= (2\pi e)^{-n/2} \prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2}.
\end{aligned}$$

Likelihood ratio

Hence our likelihood ratio is:

$$\begin{aligned}
\lambda &= \frac{(2\pi e)^{-n/2} \prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2}}{(2\pi e)^{-n/2} \prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2}} \\
&= \frac{\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2 \right)^{-n_i/2}}{\prod_{i=1}^m \left(\frac{1}{n_i} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 \right)^{-n_i/2}} \\
&= \prod_{i=1}^m \left(\frac{\sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2}{\sum_{j=1}^{n_i} (Y_{ij} - \widehat{\mu})^2} \right)^{n_i/2}.
\end{aligned}$$

And our test statistic is:

$$-2 \ln \lambda \sim \chi_{m-1}^2.$$

As the unrestricted maximum likelihood has $m - 1$ more parameters than the maximum likelihood under the null.