GEP BOX'S M-TEST FOR EQUALITY OF POPULATION COVARIANCE MATRICES

FINAL PROJECT: UIC STAT522 (SPRING 2023)

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1. Executive Summary

When each of independent observations has several components, we are in the situation of multivariate statistics. When those responses are organized into finitely many known groups and we would like to test for similarity of the subpopulations (typically, of their intragroup mean vectors and intragroup covariance matrices), we would then like to apply multivariate analysis of variance (MANOVA). Typically the model is set up with a grand mean, then a fixed treatment-effect offset to each group's mean, possibly more offsets if studying multiway (multifactor) effects, and idiosyncratic errors. However, the mechanism of MANOVA has three assumptions (see textbook's two models [JW07, 6-38, 6-59]):

- (1) the errors have intergroup independence (the subpopulations don't influence each other) as well as intragroup independence,
- (2) per group the errors are identically multinormally distributed with population mean zero, and
- (3) population covariance matrices between groups are identical.

The purpose of GEP Box's *M*-test is to check whether the latter condition (3) is satisfied, given that the former two conditions are satisfied. Thus, it is a critical tool for the correct setup of any MANOVA model.

Box's M-test works well when both the dimension of observations and the number of groups are each less than five, and the number of observations per group is more than twenty. Besides limited ranges, it is known to be sensitive to the normality assumption (2), whereas Wilks' Λ^* for testing equality of means is more robust to nonnormality.

In Sections 2–3, we consider the rigorous mathematics behind the statistical test, especially its weighting coefficient. In subsequent sections, we discuss the appendices in which R programs are run on various multivariate datasets. There is a prebuilt function boxM() in the CRAN library heplots. This library of Michael Friendly handles sum-of-squares-and-cross-products (SSP) matrices for linear hypotheses (H) and errors (E) using intervals/ellipses; graphics are drawn via plot().

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2. HISTORICAL CONTEXT AND SCIENTIFIC STATEMENT

The main source of this exposition is Box's original paper [Box49]. We use the same notation, except we write g for the number of population groups rather than k, which we reserve for a summation index.

Consider g mutually independent groups (1) of random multivariate samples $x_{lj} \in \mathbb{R}^p$. Suppose that they are multinormally (2) distributed:

$$X_{l1}, \ldots, X_{ln_l} \stackrel{\text{iid}}{\sim} \mathcal{N}_p(\mu_l, A_l)$$
 for all $1 \leq l \leq g$.

Here, the *l*-th group nonuniformly has n_l samples, $\mu_l \in \mathbb{R}^p$ is unknown population mean, and $A_l \in \mathbb{R}^{p \times p}$ is the unknown population covariance.

Write $\nu_l := n_l - 1$ for the l-th degree of freedom, $N := \nu_1 + \cdots + \nu_g$ for total number of degrees of freedom, and $\nu := N/g$ for average number of degrees of freedom. The (unbiased) sample covariance matrix is

$$S_l := \nu_l^{-1} \sum_{j=1}^{n_l} (x_{lj} - \overline{x}_l) (x_{lj} - \overline{x}_l)' \in \mathbb{R}^{p \times p}$$

where $\overline{x}_l := n_l^{-1} \sum_{j=1}^{n_l} x_{lj} \in \mathbb{R}^p$ is the *l*-th sample mean. Abbreviate $n := N + g = \sum_{l=1}^g n_l$. The **pooled sample covariance matrix** is

$$S_0 := N^{-1} \sum_{l=1}^g \nu_l S_l \in \mathbb{R}^{p \times p}.$$

Consider the null hypothesis that population covariances are equal

$$H_0: A_1 = \ldots = A_q =: A.$$

The likelihood ratio (LR) statistic is introduced in [NP28, xix]. Our 3rd textbook [And03, 10.2:8] and Homework5#3 (g = 2) both calculate the maximum likelihood estimate (MLE) and LR in general and under H_0 .

Result 2.1. The likelihood ratio test (LRT) statistic of H_0 is

$$\Lambda_0 = \prod_{l=1}^g \left(\frac{|\widehat{A}_l|}{|\widehat{A}_0|} \right)^{n_l/2} \in [0, 1]$$

where $\widehat{A}_l = \frac{\nu_l}{n_l} S_l$ is MLE of A_l and $\widehat{A}_0 = \frac{N}{n} S_0$ is MLE of A under H_0 .

The ratio of likelihoods of null hypothesis over none is in [NP33, 12].

Theorem 2.2 (Neyman–Pearson 1933). For any significance level $0 < \alpha < 1$, most powerful (MP) is the hypothesis test that is defined by rejection of H_0 if LRT statistic $\Lambda_0 < \lambda_{\alpha}$, for appropriate constant λ_{α} .

In the univariate case (p=1), the above Λ_0 reduces to the so-called L_1 -statistic of Neyman–Pearson (1931), which was proven an unbiased test by Brown [Bro39]. Here, a hypothesis test at level α with binary loss is **unbiased** if the **power function** $\beta(\theta) := \mathbb{P}[\text{reject } H_0|\theta]$ satisfies $\beta \leqslant \alpha$ under assumption H_0 is true and $\beta > \alpha$ assuming H_0 is false.

The constant λ_{α} can be determined asymptotically also, as follows. The following statement and a sketch is in [Wil38]; with appropriate hypotheses, a simple rigorous proof is provided by R M Dudley [Dud03].

Theorem 2.3 (Wilks 1938). Under suitable regularity hypotheses (such as for existence and uniqueness of an interior-point MLE), the statistic $M_0 := -2 \log \Lambda_0$ is asymptotically distributed as $\chi^2((p+1)(g-1)p/2)$.

A correction to the univariate case (p = 1) of Result 2.1 was offered in [Bar37, 15]. We state it for multivariate observations via determinants.

Definition 2.4 (Bartlett 1937). Consider the non-MLE based statistic

$$\Lambda = \prod_{l=1}^{g} \left(\frac{|S_l|}{|S_0|} \right)^{\nu_l/2} \in [0, 1].$$

Write $M := -2 \log \Lambda$. The univariate M was used and studied by HO Hartley [Har40]. The unbiasedness of the multivariate Bartlett's Λ -test was eventually proven rigorously by MD Perlman [Per80, 2.1].

GEP Box is responsible for the development of multivariate M, so the test is named after him, and proposed a further correction [Box49].

Definition 2.5 (Box 1949, "Box's M-test"). Consider the constant

$$1 - \rho := \frac{2p^2 + 3p - 1}{6(p+1)(g-1)} \left(\sum_{l=1}^{g} \nu_l^{-1} - N^{-1} \right).$$

Reject the above H_0 if $\rho M > \chi_{\alpha}^2((p+1)(g-1)p/2)$, for a given level α .

Remark 2.6. In practice it seems to work well if p, g < 5 and all $n_l > 20$.

3. Partly Deriving the ρ -factor

The purpose of this section is to begin to reveal some of the mystery of the formula for ρ in Definition 2.5. The full derivation is extremely complicated because of asymptotic analysis of special functions, so we refer the reader to [Box49] for the details of the full tour-de-force story.

For motivation, consider the univariate case (p=1). If $Z \sim \mathcal{N}(0,1)$ which has density $(2\pi)^{-1/2} \exp(-z^2/2)$ for all $z \in \mathbb{R}$, by change-of-variables its square Z^2 has density $\frac{(1/2)^{1/2}}{\Gamma(1/2)}x^{-1/2}e^{-x/2}$ for all x > 0, which is Gamma $(1/2, 1/2) = \chi^2(1)$ with rate parameterization, hence

 Z^2 has moment generating function $(1-2t)^{-1/2}$ for all t<1/2. So if $Z_1,\ldots,Z_d\stackrel{\mathrm{iid}}{\sim}\mathcal{N}(0,1)$, then their squares are also independent and identitically distributed, so the sum $Z_1^2+\cdots+Z_d^2$ has moment generating function the product $[(1-2t)^{-1/2}]^d=(1-2t)^{-d/2}$, hence the sum has distribution $\mathrm{Gamma}(d/2,1/2)=\chi^2(d)$. Therefore, if $Y_1,\ldots,Y_{d+1}\stackrel{\mathrm{iid}}{\sim}\mathcal{N}(\mu,\sigma^2)$, then the scaled sample variance $s^2/\sigma^2:=\sum_{j=1}^{d+1}\left((Y_j-\overline{Y})/\sigma\right)^2$ has a $\chi^2(d)$ distribution, since we lose one degree of freedom due to \overline{Y} . The probability density function of x>0 is $\frac{(1/2)^{d/2}}{\Gamma(d/2)}x^{d/2-1}e^{-x/2}$. Notice therein the occurence of the special function of Daniel Bernoulli (1729):

$$\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} dt \text{ for all } s > 0,$$

where $\Gamma(n+1) = n!$. The special numbers B_n of Jacob Bernoulli (1713), where $B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/6$, $B_3 = 0$, now occur because Stirling's approximation $n! \approx \sqrt{2\pi n} (n/e)^n$ has this generalization [Bar00].

Theorem 3.1 (Barnes 1900). For all complex $s \in \mathbb{C}$ and small $h \in \mathbb{C}$,

$$\log \frac{\Gamma(s+h)}{\sqrt{2\pi}} = (s+h-\frac{1}{2})\log s - s - \sum_{r=1}^{n} (-1)^r \frac{B_{r+1}(h)}{r(r+1)s^r} + \mathcal{O}(s^{-n-1})$$

where the Bernoulli function is $B_n(h) := (B+h)^n = \sum_{k=0}^n \binom{n}{k} B_{n-k} h^k$.

Now consider the multivariate case $(p \ge 1)$. If $Z_1, \ldots, Z_d \stackrel{\text{iid}}{\sim} \mathcal{N}_p(0, A)$, then the sum $\sum_{j=1}^d Z_j Z_j'$ is a $p \times p$ random matrix that by definition has the Wishart distribution $\mathcal{W}_d(A)$ where $d \ge p$ is the degrees of freedom. For example, our setting has $\nu_l S_l \sim \mathcal{W}_{\nu_l}(A_l)$. Its density is in [Wis28].

Theorem 3.2 (Wishart 1928). The matrix-valued distribution $W_d(A)$ has probability density function of positive definite $W \in \mathbb{R}^{p \times p}$ given by

$$\frac{|W|^{(d-p-1)/2} \exp\left(-\operatorname{tr} A^{-1} W/2\right)}{2^{dp/2} |A|^{d/2} \cdot \pi^{p(p-1)/4} \prod_{k=0}^{p-1} \Gamma\left(\frac{d-k}{2}\right)}.$$

Box uses these two theorems as a starting point for intricate analysis of the characteristic exponent. We only jump in to show notation of his resulting algebra. He selects the multiplier ρ so that $\alpha_1 = 0$. Here, it lies in a family of constants with a particular definition [Box49, (43)]

$$\alpha_1 := -\frac{g}{3}(3D_1\beta + 2D_2)$$

where ρ occurs in $\beta := (1 - \rho)\nu$, and $D_r := \delta_r \gamma_r$ with [Box49, (39–40)]

$$\delta_r := B_{r+1} \left(-\frac{B+p}{2} \right) - B_{r+1} \left(-\frac{B}{2} \right)$$

$$\gamma_r := g^{-1} \sum_{l=1}^g \left(\frac{\nu}{\nu_l} \right)^{r-1} - g^{-r}.$$

Note $\alpha_1=0$ iff $1-\rho=-\frac{2D_2}{3D_1}/\nu=-\frac{2\delta_2}{3\delta_1}\frac{\gamma_2/\nu}{\gamma_1}$. Next, since $\nu=N/g$, note

$$\gamma_1 = 1 - g^{-1}$$

$$\gamma_2 = g^{-1} \sum_{l=1}^g \frac{\nu}{\nu_l} - g^{-2} = \nu g^{-1} \left(\sum_{l=1}^g \nu_l^{-1} - N^{-1} \right).$$

Now, using the aforementioned special values of the Bernoulli numbers,

$$B_2(h) = (B+h)^2 = B_2 + 2B_1h + B_0h^2 = \frac{1}{6} - h + h^2$$

$$B_3(h) = (B+h)^3 = B_3 + 3B_2h + 3B_1h^2 + B_0h^3 = \frac{1}{2}h - \frac{3}{2}h^2 + h^3.$$

Then the formal variable "B" can be expanded to yield $[Box 49, (42)]^1$

$$\delta_1 = 4^{-1} [(B-p)^2 - B^2] = 4^{-1} [-(-p) + (-p)^2] = 4^{-1} p(p+1)$$

$$\delta_2 = 8^{-1} [(B-p)^3 - B^3] = 8^{-1} \left[\frac{1}{2} (-p) - \frac{3}{2} (-p)^2 + (-p)^3 \right]$$

$$= -16^{-1} p(2p^2 + 3p - 1).$$

Thus
$$-\frac{2\delta_2}{3\delta_1} = \frac{2p^2 + 3p - 1}{6(p+1)}$$
 and $\frac{\gamma_2/\nu}{\gamma_1} = \frac{1}{g-1} \left(\sum_{l=1}^g \nu_l^{-1} - N^{-1} \right)$, as desired.

4. Example: Weight gain in rats

In Figure 4, three treatment groups of rats' weight gains are measured in Weeks 1–4 (i.e. once-differenced timeseries) [Box50, Table D]. The Appendix has the output of an R notebook that runs boxM() from Michael Friendly's library heplots, containing a version of the rat data.

Here p=4 and g=3. The plot of confidence intervals of $\log |S_l|$ and $\log |S_0|$ shows large overlaps between the sample covariances of all three groups and the pooled one. The total degrees of freedom is (p+1)(g-1)p/2=20 and Box's $\chi^2(20)$ -statistic is $\rho M \doteq 12.14$. The associated (right-tailed) p-value is 91.12%. Therefore, at 5% significance level, we fail to reject the null hypothesis that all three treatments have the same covariance that describes the evolution of rat weight gains.

¹Our last equality of δ_2 actually yields "+1" instead of "-1", so $2p^2 + 3p + 1 = (2p+1)(p+1)$. Is this a typo carried forward in the literature and computer code?

We can proceed with MANOVA for this dataset. Despite p, g < 5, note that $n_1 = 10, n_2 = 7, n_3 = 10$ are all ≤ 20 (Remark 2.6). We did not check the assumption of multivariate normality per group.

Group 1. Control							Group 2. Thyroxin					Group 3. Thiouracil					
Rat	<i>y</i> ₀	y_1	y_2	уз	<i>y</i> ₄	Rat	y 0	<i>y</i> 1	<i>y</i> ₂	<i>y</i> ₃	y ₄	Rat	<i>y</i> ₀	y_1	y_2	<i>y</i> ₃	y
1	57	29	28	25	33	11	59	26	36	35	35	18	61	25	23	11	
2	60	33	30	23	31	12	54	17	19	20	28	19	59	21	21	10	1
3	52	25	34	33	41	13	56	19	33	43	38	20	53	26	21	6	2
4	49	18	33	29	35	14	59	26	31	32	29	21	59	29	12	11	1
5	56	25	23	17	30	15	57	15	25	23	24	22	51	24	26	22	1
6	46	24	32	29	22	16	52	21	24	19	24	23	51	24	17	8	1
7	51	20	23	16	31	17	52	18	35	33	33	24	56	22	17	8	
8	63	28	21	18	24							25	58	11	24	21	2
9	49	18	23	22	28							26	46	15	17	12	1
10	57	25	28	29	30							27	53	19	17	15	1
	repres gain i				tht of	rat		y ₃ ga	in in	2nd v 3rd v 4th v	veek				,,,,,		

FIGURE 4.1. weight gains of rats per treatment group

5. Example : Egyptian skulls

Five epochs of ancient human skulls in Egypt were obtained, and according to Figure 5 the following four measurements were made.

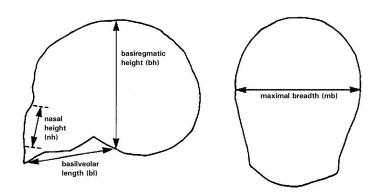


Figure 5.1. four types of skull measurements

Here p=4 and g=5. The plot of confidence intervals of $\log |S_l|$ and $\log |S_0|$ shows large overlaps between the the latter three sample covariances, with extremal shifts of the earliest two epochs, and the pooled one still overlaps the five epochs but has a much smaller range. The total degrees of freedom is (p+1)(g-1)p/2=40 and Box's $\chi^2(40)$ -statistic is $\rho M \doteq 45.67$. The associated (right-tailed) p-value is 24.83%.

Therefore, at 5% significance level, we fail to reject the null hypothesis that all five epochs have the same covariance that describes shifts in cranial measurements over time. We can proceed with MANOVA for this dataset. Despite p < 5 and $n_1 = n_2 = n_3 = n_4 = n_5 = 30 > 20$, note that $g \ge 5$ (Remark 2.6). We did not check the assumption of multivariate normality per group.

6. Example: Wine cultivars

Wine from three cultivars in the same region in Italy were obtained, and thirteen measurements of chemical composition were made.

Here p=13 and g=3. The plot of confidence intervals of $\log |S_l|$ and $\log |S_0|$ shows large overlaps between the cultivars barbera and barolo, whereas grignolino was completely separate, which has a minor overlap with the small range of the the pooled one. The total degrees of freedom is (p+1)(g-1)p/2=182 and Box's $\chi^2(182)$ -statistic is $\rho M \doteq 684$. The associated (right-tailed) p-value is 2.2×10^{-16} . Therefore, at 5% significance level, we do reject the null hypothesis that all three cultivars have the same covariance that describes chemical composition of their wines. We cannot proceed with MANOVA for this dataset. Despite g < 5 and $n_1 = 48, n_2 = 59, n_3 = 71$ all > 20, note that $p \geqslant 5$ (Remark 2.6). We did not check the assumption of multivariate normality per group.

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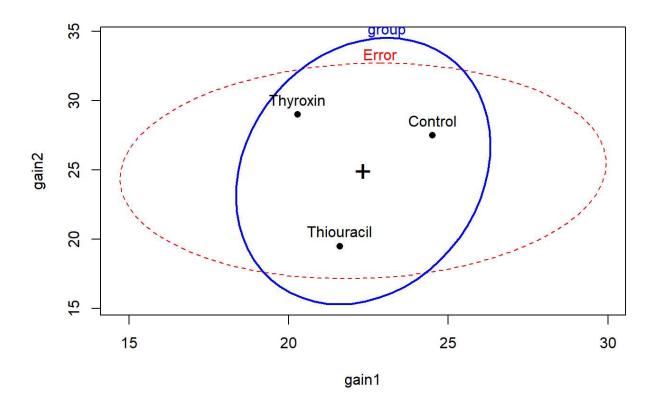
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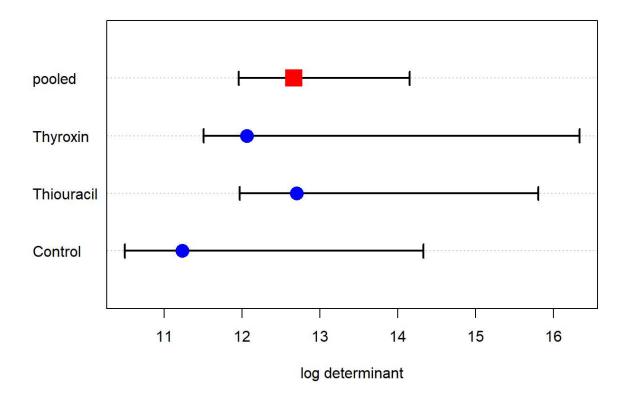
APPENDIX: Examples of Application of Box's M-test

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Example 1 : Rat Weights - a once-differenced timeseries Figure D of Box's 1950 article is already a datafile.



```
RatTest <- boxM( RatFormula, data=RatGain )
plot( RatTest ) # 95% confidence intervals, determined by Cai--Liang--Zhou (2015)
```



```
summary( RatTest, cov=F )
```

```
## Summary for Box's M-test of Equality of Covariance Matrices
## Chi-Sq: 12.1383
## df: 20
## p-value: 0.9112
##
## log of Covariance determinants:
     Control Thiouracil Thyroxin
                                      pooled
##
     11.22898 12.70088 12.05800
                                    12.66151
## Eigenvalues:
      Control Thiouracil Thyroxin
                                      pooled
## 1 63.392798 63.824832 121.423002 72.468683
## 2 23.940349 31.837288 26.826905 25.210030
## 3 19.244905 17.826403 7.931672 22.118624
## 4 2.577504 9.055921 6.675563 7.804448
##
## Statistics based on eigenvalues:
##
                 Control Thiouracil
                                         Thyroxin
## product 75281.014845 3.280364e+05 1.724742e+05 3.153727e+05
              109.155556 1.225444e+02 1.628571e+02 1.276018e+02
## precision
              2.010134 4.681667e+00 3.111498e+00 4.409003e+00
## max
               63.392798 6.382483e+01 1.214230e+02 7.246868e+01
```

Example 2: Skull Measurements

30

c4000BC c3300BC c1850BC c200BC cAD150

30

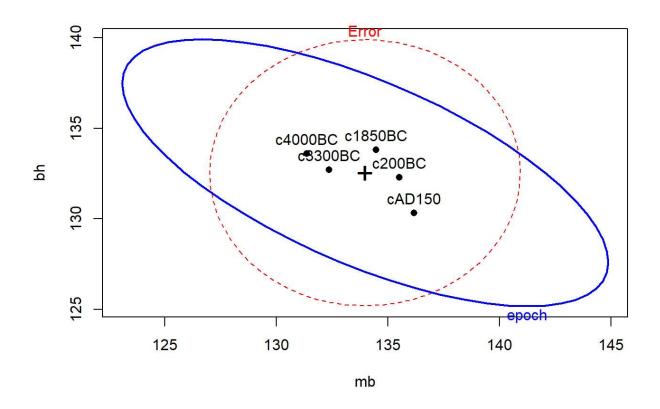
30

##

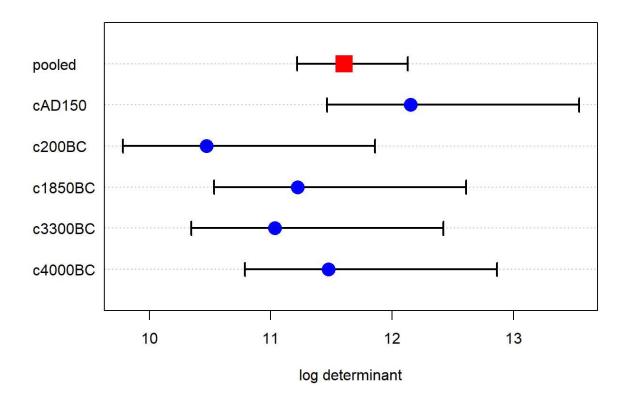
30

```
data( Skulls )
table( Skulls$epoch )
```

```
 SkullFormula <- as.formula( cbind(mb,bh,bl,nh) \sim epoch ) \\ SkullModel <- lm( SkullFormula, data=Skulls ) \\ heplot( SkullModel )
```



SkullTest <- boxM(SkullFormula, data=Skulls)
plot(SkullTest) # 95% confidence intervals, determined by Cai--Liang--Zhou (2015)



```
summary( SkullTest, cov=F )
```

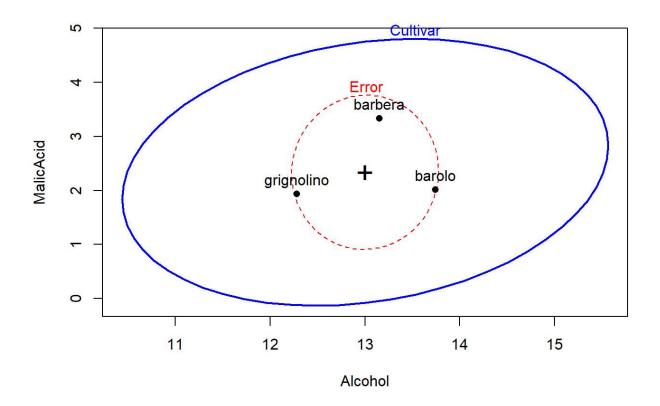
```
## Summary for Box's M-test of Equality of Covariance Matrices
## Chi-Sq: 45.66723
## df: 40
## p-value: 0.2483
## log of Covariance determinants:
    c4000BC c3300BC c1850BC c200BC cAD150 pooled
## 11.47659 11.03211 11.22162 10.46913 12.15302 11.60530
## Eigenvalues:
      c4000BC c3300BC c1850BC
                                  c200BC cAD150
## 1 34.823361 28.39920 26.93111 35.906372 37.33170 29.461507
## 2 30.333915 22.03058 19.07469 16.955955 28.59993 21.440705
## 3 18.435832 15.59589 13.20735 13.675102 14.79973 18.778959
## 4 4.951721 6.33640 11.01443 4.229238 12.00313 9.245956
## Statistics based on eigenvalues:
                             c3300BC
##
                 c4000BC
                                          c1850BC
                                                       c200BC
                                                                    cAD150
## product 96431.295985 61827.946165 74729.072524 35211.657580 1.896666e+05
               88.544828 72.362069 70.227586 70.766667 9.273448e+01
## precision
               3.145891
                            3.305332
                                        3.905294
                                                     2.522696 4.702951e+00
               34.823361
                           28.399195
                                       26.931111 35.906372 3.733170e+01
## max
                  pooled
          1.096775e+05
            7.892713e+01
## sum
## precision 4.132414e+00
## max
            2.946151e+01
```

Example 3: Chemical Composition of Wine

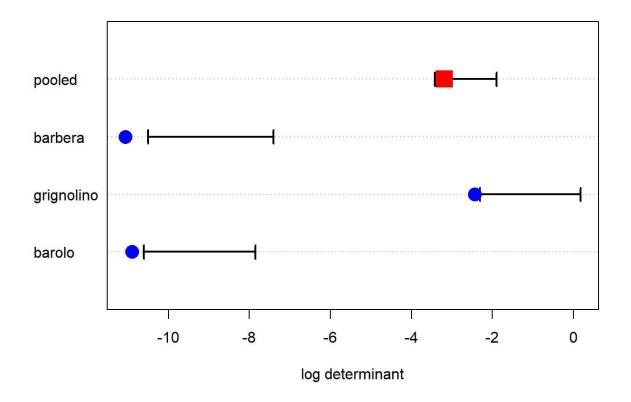
```
data( Wine )
table( Wine$Cultivar )
```

```
## barolo grignolino barbera
## 59 71 48
```

```
WineFormula <- as.formula( cbind(Alcohol, MalicAcid, Ash, AlcAsh, Mg, Phenols, Flav, NonFlavPhenols, Proa, Color, Hue, OD, P roline) ~ Cultivar )
WineModel <- lm( WineFormula, data=Wine )
heplot( WineModel )
```



WineTest <- boxM(WineFormula, data=Wine)
plot(WineTest) # 95% confidence intervals, determined by Cai--Liang--Zhou (2015)



```
summary( WineTest, cov=F )
```

```
## Summary for Box's M-test of Equality of Covariance Matrices
## Chi-Sq: 684.2031
## df: 182
## p-value: < 2.2e-16
##
## log of Covariance determinants:
##
      barolo grignolino
                          barbera
## -10.902255 -2.443270 -11.055300 -3.189442
##
## Eigenvalues:
##
            barolo grignolino
                                    barbera
## 1 4.907464e+04 2.478610e+04 1.325179e+04 2.971561e+04
## 2 1.083042e+02 2.100615e+02 1.145923e+02 1.730817e+02
## 3 6.199478e+00 1.143357e+01 6.052432e+00 7.951330e+00
## 4 9.329764e-01 1.130294e+00 4.306843e+00 2.257991e+00
## 5 4.120210e-01 9.589978e-01 1.091765e+00 8.197491e-01
## 6 1.816698e-01 6.395512e-01 2.362204e-01 4.260405e-01
## 7 1.117702e-01 2.543443e-01 1.278753e-01 2.295385e-01
## 8 9.972618e-02 1.814558e-01 8.229714e-02 1.451121e-01
## 9 7.915028e-02 1.155837e-01 3.304591e-02 1.117280e-01
## 10 3.052211e-02 5.564865e-02 2.379950e-02 6.357011e-02
## 11 2.033566e-02 3.259644e-02 9.232194e-03 3.446343e-02
## 12 6.754625e-03 2.952448e-02 6.517815e-03 1.961628e-02
## 13 2.163809e-03 7.368581e-03 3.108240e-03 7.986643e-03
##
## Statistics based on eigenvalues:
##
                  barolo grignolino
            1.841667e-05 8.687630e-02 1.580318e-05 4.119487e-02
            4.919102e+04 2.501101e+04 1.337835e+04 2.990076e+04
## precision 1.364415e-03 4.168275e-03 1.467840e-03 4.077078e-03
            4.907464e+04 2.478610e+04 1.325179e+04 2.971561e+04
```