Multivariate Linear Regression

Max Turgeon

STAT 4690–Applied Multivariate Analysis

Multivariate Linear Regression model

- We are interested in the relationship between p outcomes $Y_1, \dots, Y_p$ and q covariates $X_1, \dots, X_q$.
  - We will write $\mathbf{Y} = (Y_1, \dots, Y_p)$ and $\mathbf{X} = (1, X_1, \dots, X_q)$.
- We will assume a **linear relationship**:
  - $E(\mathbf{Y} \mid \mathbf{X}) = B^T\mathbf{X}$, where B is a $(q+1) \times p$ matrix of *regression coefficients*.
- We will also assume **homoscedasticity**:
  - $\mathrm{Cov}(\mathbf{Y} \mid \mathbf{X}) = \Sigma$, where Σ is positive-definite.
  - In other words, the (conditional) covariance of $\mathbf{Y}$ does not depend on $\mathbf{X}$.

Relationship with Univariate regression i

- Let σ_i^2 be the i-th diagonal element of Σ.
- Let β_i be the i-th column of B.
- From the model above, we get p univariate regressions:
  - $E(Y_i \mid \mathbf{X}) = \mathbf{X}^T\beta_i$;
  - $\mathrm{Var}(Y_i \mid \mathbf{X}) = \sigma_i^2$.
- However, we will use the correlation between outcomes for hypothesis testing
- This follows from the assumption that each component Y_i is linearly associated with the *same* covariates $\mathbf{X}$.

Relationship with Univariate regression ii

- If we assumed a different set of covariates $\mathbf{X}_i$ for each outcome Y_i and still wanted to use the correlation between the outcomes, we would get the **Seemingly Unrelated Regressions** (SUR) model.
    - This model is sometimes used by econometricians.

Least-Squares Estimation i

- Let $\mathbf{Y}_1 \dots, \mathbf{Y}_n$ be a random sample of size n, and let $\mathbf{X}_1, \dots, \mathbf{X}_n$ be the corresponding sample of covariates.
- We will write $\mathbb{Y}$ and $\mathbb{X}$ for the matrices whose i-th row is $\mathbf{Y}_i$ and $\mathbf{X}_i$, respectively.
  - We can then write $E(\mathbb{Y} \mid \mathbb{X}) = \mathbb{X}B$.
- For Least-Squares Estimation, we will be looking for the estimator $\hat{B}$ of B that minimises a least-squares criterion:
  - $LS(B) = \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right]$
  - **Note**: This criterion is also known as the (squared) *Frobenius norm*; i.e. $LS(B) = \|\mathbb{Y} - \mathbb{X}B\|_F^2$.

Least-Squares Estimation ii

  - **Note 2**: If you expand the matrix product and look at the diagonal, you can see that the Frobenius norm is equivalent to the sum of the squared entries.
- To minimise $LS(B)$, we could use matrix derivatives...
- Or, we can expand the matrix product along the diagonal and compute the trace.
- Let $\mathbf{Y}_{(j)}$ be the j-th column of $\mathbb{Y}$.

Least-Squares Estimation iii

- In other words, $\mathbf{Y}_{(j)} = (Y_{1j}, \ldots, Y_{nj})$ contains the n values for the outcome Y_j. We then have

$$\begin{aligned} LS(B) &= \mathrm{tr}\left[(\mathbb{Y} - \mathbb{X}B)^T(\mathbb{Y} - \mathbb{X}B)\right] \\ &= \sum_{j=1}^p (\mathbf{Y}_{(j)} - \mathbb{X}\beta_j)^T(\mathbf{Y}_{(j)} - \mathbb{X}\beta_j) \\ &= \sum_{j=1}^p \sum_{i=1}^n (Y_{ij} - \beta_j^T\mathbf{X}_i)^2. \end{aligned}$$

Least-Squares Estimation iv

- For each j, the sum $\sum_{i=1}^n (Y_{ij} - \beta_j^T \mathbf{X}_i)^2$ is simply the least-squares criterion for the corresponding univariate linear regression.
- $\hat{\beta}_j = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}_{(j)}$
- But since $LS(B)$ is a sum of p positive terms, each minimised at $\hat{\beta}_j$, the whole is sum is minimised at

$$\hat{B} = \begin{pmatrix} \hat{\beta}_1 & \cdots & \hat{\beta}_p \end{pmatrix}.$$

- Or put another way:

$$\hat{B} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}.$$

Comments i

- We still have not made any distributional assumptions on $\mathbf{Y}$.
  - We do not need to assume normality to derive the least-squares estimator.
- The least-squares estimator is *unbiased*:

$$\begin{aligned} E(\hat{B} \mid \mathbb{X}) &= (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}E(\mathbb{Y} \mid \mathbb{X}) \\ &= (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{X}B \\ &= B. \end{aligned}$$

Comments ii

- We did not use the covariance matrix Σ anywhere in the estimation process. But note that:

$$\begin{aligned}
\mathrm{Cov}(\hat{\beta}_i, \hat{\beta}_j) &= \mathrm{Cov}\left((\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}_{(i)}, (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}_{(j)}\right)\\
&= (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathrm{Cov}\left(\mathbf{Y}_{(i)}, \mathbf{Y}_{(j)}\right)\left((\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\right)^T\\
&= (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\left(\sigma_{ij}I_n\right)\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\\
&= \sigma_{ij}(\mathbb{X}^T\mathbb{X})^{-1},
\end{aligned}$$

where σ_{ij} is the (i,j)-th entry of Σ.

Example i

```r
# Let's revisit the plastic film data
library(heplots)
library(tidyverse)

Y <- Plastic %>%
  select(tear, gloss, opacity) %>%
  as.matrix

X <- model.matrix(~ rate, data = Plastic)
head(X)
```

Example ii

```
##   (Intercept) rateHigh
## 1           1        0
## 2           1        0
## 3           1        0
## 4           1        0
## 5           1        0
## 6           1        0
```

```
(B_hat <- solve(crossprod(X)) %*% t(X) %*% Y)
```

Example iii

```
##             tear gloss opacity
## (Intercept) 6.49  9.57    3.79
## rateHigh    0.59 -0.51    0.29
```

```r
# Compare with lm output
fit <- lm(cbind(tear, gloss, opacity) ~ rate,
          data = Plastic)
coef(fit)
```

```
##             tear gloss opacity
## (Intercept) 6.49  9.57    3.79
## rateHigh    0.59 -0.51    0.29
```

Geometry of LS i

- Let $P = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$.
- P is symmetric and *idempotent*:

$$P^2 = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T = P.$$

- Let $\hat{\mathbb{Y}} = \mathbb{X}\hat{B}$ be the fitted values, and $\hat{\mathbb{E}} = \mathbb{Y} - \hat{\mathbb{Y}}$, the residuals.
    - We have $\hat{\mathbb{Y}} = P\mathbb{Y}$.
    - We also have $\hat{\mathbb{E}} = (I - P)\mathbb{Y}$.

Geometry of LS ii

- Putting all this together, we get

$$\begin{aligned}\hat{\mathbb{Y}}^T\hat{\mathbb{E}} &= (P\mathbb{Y})^T(I-P)\mathbb{Y}\\ &= \mathbb{Y}^TP(I-P)\mathbb{Y}\\ &= \mathbb{Y}^T(P-P^2)\mathbb{Y}\\ &= 0.\end{aligned}$$

- In other words, the fitted values and the residuals are **orthogonal**.
- Similarly, we can see that $\mathbb{X}^T\hat{\mathbb{E}} = 0$ and $P\mathbb{X} = \mathbb{X}$.

Geometry of LS iii

- **Interpretation**: $\hat{\mathbb{Y}}$ is the orthogonal projection of $\mathbb{Y}$ onto the column space of $\mathbb{X}$.

Example (cont’d) i

```r
Y_hat <- fitted(fit)
residuals <- residuals(fit)

crossprod(Y_hat, residuals)
```

```
##                  tear        gloss       opacity
## tear    -9.489298e-16 2.959810e-15 -4.720135e-15
## gloss   -1.424461e-15 1.109357e-15 -1.150262e-14
## opacity -7.268852e-16 1.211209e-15  1.648459e-16
```

Example (cont'd) ii

```r
crossprod(X, residuals)
```

```
##             tear        gloss       opacity
## (Intercept)    0 5.828671e-16 -4.440892e-16
## rateHigh       0 1.387779e-16  4.440892e-16
```

Example (cont'd) iii

```r
# Is this really zero?
isZero <- function(mat) {
  all.equal(mat, matrix(0, ncol = ncol(mat),
                        nrow = nrow(mat)),
            check.attributes = FALSE)
}

isZero(crossprod(Y_hat, residuals))
```

```
## [1] TRUE
```

Example (cont’d) iv

```r
isZero(crossprod(X, residuals))
```

```
## [1] TRUE
```

Bootstrapped Confidence Intervals i

- We still have not made any assumption about the distribution of $\mathbf{Y}$, beyond the conditional mean and covariance function.
  - Let's see how much further we can go.
- We will use **bootstrap** to derive confidence intervals for our quantities of interest.
- Bootstrap is a resampling technique for estimating the sampling distribution of an estimator of interest.
  - Particularly useful when we think the usual assumptions may not hold, or when the sampling distribution would be difficult to derive.

Bootstrapped Confidence Intervals ii

- Let’s say we want to estimate the sampling distribution of the correlation coefficient.
- We have a sample of pairs $(U_1, V_1), \ldots, (U_n, V_n)$, from which we estimated the correlation $\hat{\rho}$.
- The idea is to resample **with replacement** from our sample to mimic the process of “repeating the experiment”.

Bootstrapped Confidence Intervals iii

- For each bootstrap sample $(U_1^{(b)}, V_1^{(b)}), \ldots, (U_n^{(b)}, V_n^{(b)})$, we compute the sample correlation $\hat{\rho}^{(b)}$.
- We now have a whole sample of *correlation coefficients* $\hat{\rho}^{(1)}, \ldots, \hat{\rho}^{(B)}$.
- From its quantiles, we can derive a confidence interval for $\hat{\rho}$.

Example i

```r
library(candisc)

dataset <- HSB[,c("math", "sci")]

(corr_est <- cor(dataset)[1,2])
```

```
## [1] 0.6495261
```

Example ii

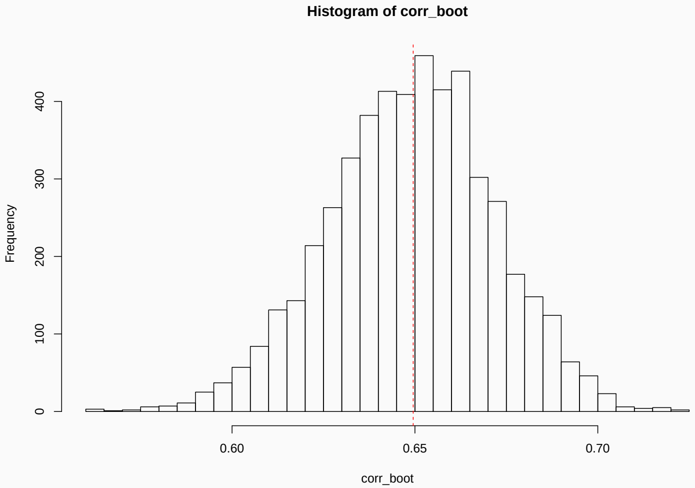
```r
# Choose a number of bootstrap samples
B <- 5000
corr_boot <- replicate(B, {
  samp_boot <- sample(nrow(dataset),
                      replace = TRUE)
  dataset_boot <- dataset[samp_boot,]
  cor(dataset_boot)[1,2]
})

quantile(corr_boot,
         probs = c(0.025, 0.975))
```

Example iii

```
##      2.5%     97.5%
## 0.6033765 0.6920060
```

```
hist(corr_boot, breaks = 50)
abline(v = corr_est, col = 'red',
       lty = 2)
```

Example iv



Histogram of corr_boot
Frequency
0
100
200
300
400
0.60
0.65
0.70
corr_boot

Bootstrapped Confidence Intervals (cont'd) i

- Going back to our multivariate linear regression setting, we can bootstrap our estimate of the matrix of regression coefficients!
- We will sample with replacement the rows of $\mathbb{Y}$ and $\mathbb{X}$
  - It's important to sample the **same** rows in both matrices. We want to keep the relationship between $\mathbf{Y}$ and $\mathbf{X}$ intact.
- For each bootstrap sample, we can compute the estimate $\hat{B}^{(b)}$.
- From these samples, we can compute confidence intervals for each entry in B.

Bootstrapped Confidence Intervals (cont'd) ii

- We can also technically compute confidence regions for multiple entries in B
    - E.g. a whole column or a whole row
    - But multivariate quantiles are tricky...

Example (cont'd) i

```
B_boot <- replicate(B, {
  samp_boot <- sample(nrow(Y),
                      replace = TRUE)
  X_boot <- X[samp_boot,]
  Y_boot <- Y[samp_boot,]

  solve(crossprod(X_boot)) %*% t(X_boot) %*% Y_boot
})

# The output is a 3-dim array
dim(B_boot)
```

Example (cont'd) ii

```
## [1]    2    3 5000
```

```
B_boot[,,1]
```

```
##                tear   gloss   opacity
## (Intercept) 6.1125  9.5375 3.3750000
## rateHigh    0.9375 -0.5375 0.8083333
```

```
# CI for effect of rate on tear
quantile(B_boot["rateHigh", "tear",],
         probs = c(0.025, 0.975))
```

Example (cont'd) iii

```
##      2.5%     97.5%
## 0.2615152 0.9101010
```

```r
# CI for effect of rate on gloss
quantile(B_boot["rateHigh", "gloss",],
         probs = c(0.025, 0.975))
```

```
##       2.5%      97.5%
## -0.9000000 -0.1110859
```

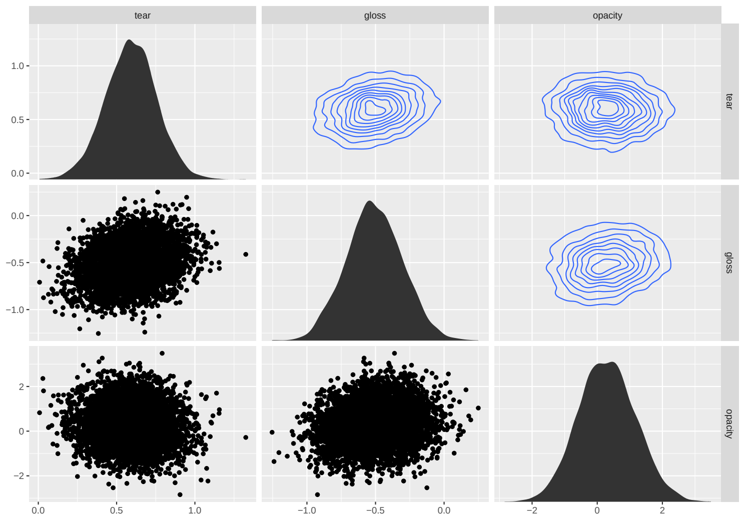
Example (cont'd) iv

```r
# CI for effect of rate on opacity
quantile(B_boot["rateHigh", "opacity",],
         probs = c(0.025, 0.975))
```

```
##      2.5%     97.5%
## -1.380083  2.041935
```

Example (cont'd) v

```r
library(ggforce)

B_boot["rateHigh",,] %>%
  t() %>%
  as.data.frame() %>%
  ggplot(aes(x = .panel_x, y = .panel_y)) +
  geom_point() +
  geom_autodensity() +
  geom_density2d() +
  facet_matrix(vars(everything()),
               layer.diag = 2,
               layer.upper = 3)
```


tear
gloss
opacity
tear
gloss
opacity
1.0
0.5
0.0
0.0
−0.5
−1.0
2
0
−2
0.0
0.5
1.0
−1.0
−0.5
0.0
−2
0
2

```r
# There is some correlation, but not much
B_boot["rateHigh",,] %>%
  t() %>%
  cor()
```

```
##                 tear     gloss     opacity
## tear      1.00000000 0.2463271 -0.07083196
## gloss     0.24632709 1.0000000  0.16697108
## opacity  -0.07083196 0.1669711  1.00000000
```

Maximum Likelihood Estimation i

- We now introduce distributional assumptions on $\mathbf{Y}$:

$$\mathbf{Y} \mid \mathbf{X} \sim N_p(B^T\mathbf{X}, \Sigma).$$

- This is the same conditions on the mean and covariance as above. The only difference is that we now assume the residuals are normally distributed.
- **Note**: The distribution above is conditional on $\mathbf{X}$. It could happen that the marginal distribution of $\mathbf{Y}$ is not normal.

Maximum Likelihood Estimation ii

- **Theorem**: Suppose $\mathbb{X}$ has full rank $q+1$, and assume that $n \geq q+p+1$. Then the least-squares estimator $\hat{B} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbb{Y}$ of B is also the *maximum likelihood estimator*. Moreover, we have
    1. $\hat{B}$ is normally distributed.
    2. The maximum likelihood estimator for Σ is $\hat{\Sigma} = \frac{1}{n}\hat{\mathbb{E}}^T\hat{\mathbb{E}}$.
    3. $n\hat{\Sigma}$ follows a Wishart distribution $W_{n-q-1}(\Sigma)$ on $n-q-1$ degrees of freedom.
    4. The maximised likelihood is $L(\hat{B}, \hat{\Sigma}) = (2\pi)^{-np/2}|\hat{\Sigma}|^{-n/2}\exp(-pn/2)$.

Maximum Likelihood Estimation iii

- **Note**: Looking at the degrees of freedom of the Wishart distribution, we can infer that $\hat{\Sigma}$ is a biased estimator of Σ. An *unbiased* estimator is

$$S = \frac{1}{n-q-1}\hat{\mathbb{E}}^T\hat{\mathbb{E}}.$$

Confidence and Prediction Regions i

- Suppose we have a new observation $\mathbf{X}_0$. We are interested in making predictions and inference about the corresponding outcome vector $\mathbf{Y}_0$.
- First, since $\hat{B}$ is an unbiased estimator of B, we see that

$$E(\mathbf{X}_0^T\hat{B}) = \mathbf{X}_0^T E(\hat{B}) = \mathbf{X}_0^T B = E(\mathbf{Y}_0).$$

  Therefore, it makes sense to estimate $\mathbf{Y}_0$ using $\mathbf{X}_0^T\hat{B}$.

Confidence and Prediction Regions ii

- *What is the estimation error?* Let's look at the covariance of $\mathbf{X}_0^T\hat{\beta}_i$ and $\mathbf{X}_0^T\hat{\beta}_j$

$$\begin{aligned}\mathrm{Cov}\left(\mathbf{X}_0^T\hat{\beta}_i, \mathbf{X}_0^T\hat{\beta}_j\right) &= \mathbf{X}_0^T\mathrm{Cov}\left(\hat{\beta}_i, \hat{\beta}_j\right)\mathbf{X}_0\\ &= \sigma_{ij}\mathbf{X}_0^T(\mathbb{X}^T\mathbb{X})^{-1}\mathbf{X}_0.\end{aligned}$$

- *What is the forecasting error?* In that case, we also need to take into account the extra variation coming from the residuals.
- In other words, we also need to sample a new "error" term $\mathbf{E}_0 = (E_{01}, \ldots, E_{0p})$ independently of $\mathbf{X}_0$.

Confidence and Prediction Regions iii

  - Let $\tilde{\mathbf{Y}}_0 = \mathbf{X}_0^T B + \mathbf{E}_0$ be the new value.

- The **forecast error** is given by

$$\tilde{\mathbf{Y}}_0 - \mathbf{X}_0^T \hat{B} = \mathbf{E}_0 - \mathbf{X}_0^T (\hat{B} - B).$$

- Since $E(\tilde{\mathbf{Y}}_0 - \mathbf{X}_0^T \hat{B}) = 0$, we can still deduce that $\mathbf{X}_0^T \hat{B}$ is an unbiased predictor of $\mathbf{Y}_0$.

Confidence and Prediction Regions iv

- Now let's look at the covariance of the forecast errors in each component:

$$
\begin{aligned}
&E\left[\left(\tilde{Y}_{0i} - \mathbf{X}_0^T\hat{\beta}_i\right)\left(\tilde{Y}_{0j} - \mathbf{X}_0^T\hat{\beta}_j\right)\right] \\
&= E\left[\left(E_{0i} - \mathbf{X}_0^T(\hat{\beta}_i - \beta_i)\right)\left(E_{0j} - \mathbf{X}_0^T(\hat{\beta}_j - \beta_j)\right)\right] \\
&= E(E_{0i}E_{0j}) + \mathbf{X}_0^T E\left[(\hat{\beta}_i - \beta_i)(\hat{\beta}_j - \beta_j)\right]\mathbf{X}_0 \\
&= \sigma_{ij} + \sigma_{ij}\mathbf{X}_0^T(\mathbb{X}^T\mathbb{X})^{-1}\mathbf{X}_0 \\
&= \sigma_{ij}\left(1 + \mathbf{X}_0^T(\mathbb{X}^T\mathbb{X})^{-1}\mathbf{X}_0\right).
\end{aligned}
$$

- Therefore, we can see that the difference between the *estimation* error and the *forecasting* error is σ_{ij}.

Example i

```
# Recall our model
fit <- lm(cbind(tear, gloss, opacity) ~ rate,
          data = Plastic)

new_x <- data.frame(rate = factor("High",
                                  levels = c("Low",
                                             "High")))
(prediction <- predict(fit, newdata = new_x))
```

```
##   tear gloss opacity
## 1 7.08  9.06    4.08
```

Example ii

```r
X <- model.matrix(fit)
S <- crossprod(resid(fit))/(nrow(Plastic) - ncol(X))
new_x <- model.matrix(~rate, new_x)

quad_form <- drop(new_x %*% solve(crossprod(X)) %*%
                    t(new_x))

# Estimation covariance
(est_cov <- S * quad_form)
```

Example iii

```
##                 tear       gloss      opacity
## tear     0.014027778 0.003994444 -0.006083333
## gloss    0.003994444 0.021027778  0.014716667
## opacity -0.006083333 0.014716667  0.409916667
```

```
# Forecasting covariance
(fct_cov <- S *(1 + quad_form))
```

```
##                tear      gloss     opacity
## tear     0.15430556 0.04393889 -0.06691667
## gloss    0.04393889 0.23130556  0.16188333
## opacity -0.06691667 0.16188333  4.50908333
```

Example iv

```
# Estimation CIs
cbind(drop(prediction) - 1.96*sqrt(diag(est_cov)),
      drop(prediction) + 1.96*sqrt(diag(est_cov)))
```

```
##              [,1]     [,2]
## tear     6.847860 7.312140
## gloss    8.775781 9.344219
## opacity 2.825115 5.334885
```

Example v

```r
# Forecasting CIs
cbind(drop(prediction) - 1.96*sqrt(diag(fct_cov)),
      drop(prediction) + 1.96*sqrt(diag(fct_cov)))
```

```
##                   [,1]      [,2]
## tear      6.31007778  7.849922
## gloss     8.11735297 10.002647
## opacity -0.08198204  8.241982
```

Likelihood Ratio Tests i

- We can use a Likelihood Ratio test to assess the evidence in support of two nested models.
- Write
  $$B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}, \qquad \mathbb{X} = \begin{pmatrix} \mathbb{X}_1 & \mathbb{X}_2 \end{pmatrix},$$
  where B_1 is $(r+1) \times p$, B_2 is $(q-r) \times p$, $\mathbb{X}_1$ is $n \times (r+1)$, $\mathbb{X}_2$ is $n \times (q-r)$, and $r \geq 0$ is a non-negative integer.

Likelihood Ratio Tests ii

- We want to compare the following models:

$$\begin{aligned} \text{Full model} &: E(\mathbf{Y} \mid \mathbf{X}) = B^T\mathbf{X} \\ \text{Nested model} &: E(\mathbf{Y} \mid \mathbf{X}_1) = B_1^T\mathbf{X}_1 \end{aligned}$$

- According to our previous theorem, the corresponding maximised likelihoods are

Likelihood Ratio Tests iii

$$\begin{aligned} \text{Full model} : L(\hat{B}, \hat{\Sigma}) &= (2\pi)^{-np/2} |\hat{\Sigma}|^{-n/2} \exp(-pn/2) \\ \text{Nested model} : L(\hat{B}_1, \hat{\Sigma}_1) &= (2\pi)^{-np/2} |\hat{\Sigma}_1|^{-n/2} \exp(-pn/2) \end{aligned}$$

- Therefore, taking the ratio of the likelihoods of the nested model to the full model, we get

$$\Lambda = \frac{L(\hat{B}_1, \hat{\Sigma}_1)}{L(\hat{B}, \hat{\Sigma})} = \left(\frac{|\hat{\Sigma}|}{|\hat{\Sigma}_1|} \right)^{n/2}.$$

Likelihood Ratio Tests iv

- Or equivalently, we get *Wilks' lambda statistic*:

$$\Lambda^{2/n} = \frac{|\hat{\Sigma}|}{|\hat{\Sigma}_1|}.$$

- As discussed in the lecture on MANOVA, there is no closed-form solution for the distribution of this statistic under the null hypothesis $H_0 : B_2 = 0$, but there are many approximations.
- **Two important special cases**:
    - When $r = 0$, we are testing the full model against the empty model (i.e. only the intercept).

Likelihood Ratio Tests v

- When $\mathbb{X}_2$ only contains one covariate, we are testing the full model against a simpler model without that covariate. In other words, we are testing for the *significance* of that covariate.

Other Multivariate Test Statistics i

- The Wilks' lambda statistic can actually be expressed in terms of the (generalized) eigenvalues of a pair of matrices (H, E):
  - $E = n\hat{\Sigma}$ is the **error** matrix.
  - $H = n(\hat{\Sigma}_1 - \hat{\Sigma})$ is the **hypothesis** matrix.
- Under our assumptions about the rank of $\mathbb{X}$ and the sample size, E is (almost surely) invertible, and therefore we can look at the nonzero eigenvalues of HE^{-1}:
  - Let $\eta_1 \geq \cdots \geq \eta_s$ be those nonzero eigenvalues, where $s = \min(p, q - r)$.

Other Multivariate Test Statistics ii

  - Equivalently, these eigenvalues are the nonzero roots of the determinantal equation $\det\left((\hat{\Sigma}_1 - \hat{\Sigma}) - \eta\hat{\Sigma}\right) = 0$.
- The four classical multivariate test statistics are:

$$\begin{aligned}
\text{Wilks' lambda} &: \prod_{i=1}^{s} \frac{1}{1+\eta_i} = \frac{|E|}{|E+H|} \\
\text{Pillai's trace} &: \sum_{i=1}^{s} \frac{\eta_i}{1+\eta_i} = \operatorname{tr}\left(H(H+E)^{-1}\right) \\
\text{Hotelling-Lawley trace} &: \sum_{i=1}^{s} \eta_i = \operatorname{tr}\left(HE^{-1}\right) \\
\text{Roy's largest root} &: \frac{\eta_1}{1+\eta_1}
\end{aligned}$$

Other Multivariate Test Statistics iii

- Under the null hypothesis $H_0 : B_2 = 0$, all four statistics can be well-approximated using the F distribution.
- **Note**: When $r = q - 1$, all four tests are equivalent.
- In general, as the sample size increases, all four tests give similar results. For finite sample size, Roy's largest root has good power only if there the leading eigenvalue η_1 is significantly larger than the other ones.

Example i

```r
# Going back to our example
full_model <- lm(cbind(tear, gloss,
                       opacity) ~ rate*additive,
                 data = Plastic)

anova(full_model, test = "Wilks") %>%
  broom::tidy()  %>%
  knitr::kable(digits = 3)
```

Example ii

term	df	Wilks	approx.F	num.Df	den.Df	p.value
(Intercept)	1	0.001	5950.906	3	14	0.000
rate	1	0.382	7.554	3	14	0.003
additive	1	0.523	4.256	3	14	0.025
rate:additive	1	0.777	1.339	3	14	0.302
Residuals	16	-	-	-	-	-

Example iii

```r
anova(full_model, test = "Roy") %>%
  broom::tidy()  %>%
  knitr::kable(digits = 3)
```

term	df	Roy	approx.F	num.Df	den.Df	p.value
(Intercept)	1	1275.194	5950.906	3	14	0.000
rate	1	1.619	7.554	3	14	0.003
additive	1	0.912	4.256	3	14	0.025
rate:additive	1	0.287	1.339	3	14	0.302
Residuals	16	-	-	-	-	-

Example iv

```r
# Fit a model with only rate
rate_model <- lm(cbind(tear, gloss,
                       opacity) ~ rate,
                 data = Plastic)

# Removing the dfs from approx
anova(full_model, rate_model,
      test = "Wilks") %>%
  broom::tidy()  %>%
  dplyr::select(-num.Df, -den.Df) %>%
  knitr::kable(digits = 3)
```

Example v

res.df	df	Gen.var.	Wilks	approx.F	p.value
16	-	0.407	-	-	-
18	2	0.479	0.43	2.447	0.05

Example vi

```
anova(full_model, rate_model,
      test = "Roy") %>%
  broom::tidy()  %>%
  dplyr::select(-num.Df, -den.Df) %>%
  knitr::kable(digits = 3)
```

res.df	df	Gen.var.	Roy	approx.F	p.value
16	-	0.407	-	-	-
18	2	0.479	1.084	5.418	0.01

Example vii

```r
# Let's look at the eigenvalues
E <- crossprod(residuals(full_model))
H <- crossprod(residuals(rate_model)) - E

result <- eigen(H %*% solve(E),
                only.values = TRUE)
result$values[seq_len(2)]
```

```
## [1] 1.083657 0.115087
```

Information Criteria i

- We can use hypothesis testing for model building:
  - Add covariates that significantly improve the model (*forward selection*);
  - Remove non-significant covariates (*backward elimination*).
- Another approach is to use *Information Criteria*.
- The general form of Akaike's information criterion:

$$-2\log L(\hat{B}, \hat{\Sigma}) + 2d,$$

where d is the number of parameters to estimate.

Information Criteria ii

    - In multivariate regression, this would be $d = (q+1)p + p(p+1)/2$.
- Therefore, we get (up to a constant):

$$AIC = n \log|\hat{\Sigma}| + 2(q+1)p + p(p+1).$$

- The intuition behind AIC is that it estimates the Kullback-Leibler divergence between the posited model and the true data-generating mechanism.
    - So smaller is better.
- Model selection using information criteria proceeds as follows:

Information Criteria iii

1. Select models of interest $\{M_1, \ldots, M_K\}$. They do not need to be nested, and they do not need to involve the same variables.
2. Compute the AIC for each model.
3. Select the model with the smallest AIC.

- The set of interesting models should be selected using domain-specific knowledge when possible.
    - If it is not feasible, you can look at all possible models between the empty model and the full model.
- There are many variants of AIC, each with their own trade-offs.
    - For more details, see Timm (2002) Section 4.2.d.

Example (cont'd) i

```
## AIC(full_model)
# Error in logLik.lm(full_model) :
#   'logLik.lm' does not support multiple responses
class(full_model)
```

```
## [1] "mlm" "lm"
```

Example (cont’d) ii

```r
logLik.mlm <- function(object, ...) {
  resids <- residuals(object)
  Sigma_ML <- crossprod(resids)/nrow(resids)
  ans <- sum(mvtnorm::dmvnorm(resids,
                              sigma = Sigma_ML,
                              log = TRUE))

  df <- prod(dim(coef(object))) +
    choose(ncol(Sigma_ML) + 1, 2)
  attr(ans, "df") <- df
  class(ans) <- "logLik"
  return(ans)
}
```

```r
logLik(full_model)
```

```
## 'log Lik.' -51.45783 (df=18)
```

```r
AIC(full_model)
```

```
## [1] 138.9157
```

```r
AIC(rate_model)
```

```
## [1] 143.7768
```

Multivariate Influence Measures i

- Earlier we introduced the projection matrix

$$P = \mathbb{X}(\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T$$

  and we noted that $\hat{\mathbb{Y}} = P\mathbb{Y}$.
- Looking at one row at a time, we can see that

$$\begin{aligned} \mathbf{Y}_i &= \sum_{j=1}^n P_{ij}\mathbf{Y}_j \\ &= P_{ii}\mathbf{Y}_i + \sum_{j\neq i} P_{ij}\mathbf{Y}_i, \end{aligned}$$

  where P_{ij} is the (i,j)-th entry of P.

Multivariate Influence Measures ii

- In other words, the diagonal element P_{ii} represents the *leverage* (or influence) of observation $\mathbf{Y}_i$ on the fitted value $\hat{\mathbf{Y}}_i$.
  - Observation $\mathbf{Y}_i$ is said to have a **high leverage** if P_{ii} is large compared to the other element on the diagonal.
- Let $S = \frac{1}{n-q-1}\hat{\mathbb{E}}^T\hat{\mathbb{E}}$ be the unbiased estimator of Σ, and let $\hat{\mathbf{E}}_i$ be the i-th row of $\hat{\mathbb{E}}$.
- We define the multivariate **internally Studentized residuals** as follows:

$$r_i = \frac{\hat{\mathbf{E}}_i^T S^{-1}\hat{\mathbf{E}}_i}{1 - P_{ii}}.$$

Multivariate Influence Measures iii

- If we let $S_{(i)}$ be the estimator of Σ where we have removed row i from the residual matrix $\hat{\mathbb{E}}$, we define the multivariate **externally Studentized residuals** as follows:

$$T_i^2 = \frac{\hat{\mathbf{E}}_i^T S_{(i)}^{-1} \hat{\mathbf{E}}_i}{1 - P_{ii}}.$$

- An observation $\mathbf{Y}_i$ may be considered a potential outlier if

$$\left(\frac{n-q-p-1}{p(n-q-2)}\right) T_i^2 > F_\alpha(p, n-q-2).$$

Multivariate Influence Measures iv

- Yet another measure of influence is the multivariate **Cook's distance**.

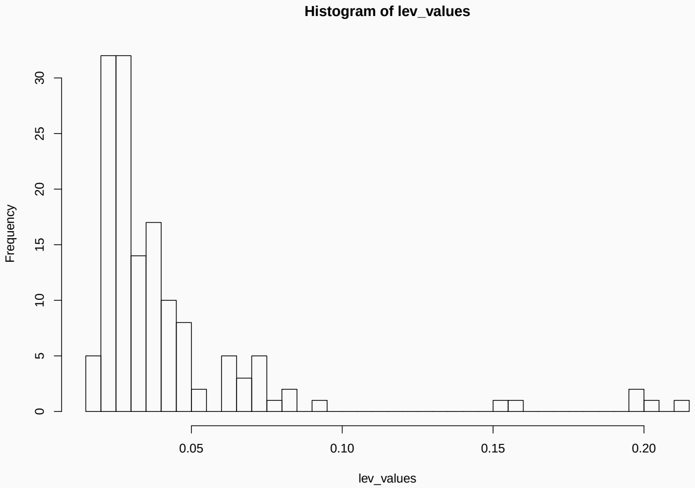
$$C_i = \frac{P_{ii}}{(1 - P_{ii})^2} \hat{\mathbf{E}}_i^T S^{-1} \hat{\mathbf{E}}_i / (q + 1).$$

- An observation $\mathbf{Y}_i$ may be considered a potential outlier if C_i is larger than the median of a chi square distribution with $\nu = p(n - q - 1)$ degrees of freedom.

Example i

```
library(openintro)
model <- lm(cbind(startPr, totalPr) ~
              nBids + cond + sellerRate +
              wheels + stockPhoto,
            data = marioKart)

X <- model.matrix(model)
P <- X %*% solve(crossprod(X)) %*% t(X)
lev_values <- diag(P)

hist(lev_values, 50)
```

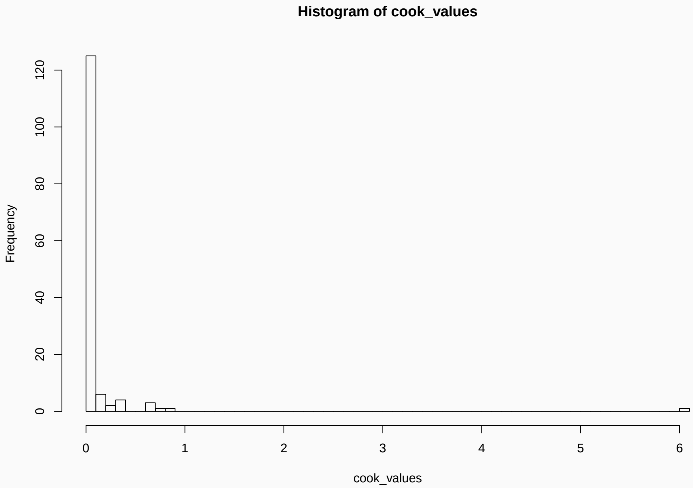
Example ii


Histogram of lev_values
Frequency
0
5
10
15
20
25
30
0.05
0.10
0.15
0.20
lev_values

Example iii

```
n <- nrow(HSB)
resids <- residuals(model)
S <- crossprod(resids)/(n - ncol(X))

S_inv <- solve(S)

const <- lev_values/((1 - lev_values)^2*ncol(X))
cook_values <- const * diag(resids %*% S_inv
                            %*% t(resids))

hist(cook_values, 50)
```

Example iv


Histogram of cook_values
Frequency
0
20
40
60
80
100
120
0
1
2
3
4
5
6
cook_values

Example v

```
# Cut-off value
(cutoff <- qchisq(0.5, ncol(S)*(n - ncol(X))))
```

```
## [1] 1187.333
```

```
which(cook_values > cutoff)
```

```
## named integer(0)
```

Strategy for Multivariate Model Building

1. Try to identify outliers.
    - This should be done graphically at first.
    - Once the model is fitted, you can also look at influence measures.
2. Perform a multivariate test of hypothesis.
3. If there is evidence of a multivariate difference, calculate Bonferroni confidence intervals and investigate component-wise differences.
    - The projection of the confidence region onto each variable generally leads to confidence intervals that are too large.