# Additional **multcomp** Examples

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It is assumed that the reader is familiar with the theory and applications described in the generalsiminf vignette.

## 1 Simple Examples

**Example: Simple Linear Model.** Consider a simple univariate linear model regressing the distance to stop on speed for 50 cars:

```
R> lm.cars <- lm(dist ~ speed, data = cars)
R> summary(lm.cars)
Call:
lm(formula = dist ~ speed, data = cars)
Residuals:
  Min
          1Q Median
                       3Q
-29.07 -9.53 -2.27 9.21 43.20
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) -17.579 6.758 -2.60 0.012 *
speed
                        0.416 9.46 1.5e-12 ***
              3.932
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
Residual standard error: 15.4 on 48 degrees of freedom
                            Adjusted R-squared: 0.644
Multiple R-squared: 0.651,
```

The estimates of the regression coefficients  $\beta$  and their covariance matrix can be extracted from the fitted model via:

F-statistic: 89.6 on 1 and 48 DF, p-value: 1.49e-12

```
R> betahat <- coef(lm.cars)
R> Vbetahat <- vcov(lm.cars)</pre>
```

At first, we are interested in the hypothesis  $\beta_1 = 0$  and  $\beta_2 = 0$ . This is equivalent to the linear hypothesis  $\mathbf{K}\beta = 0$  where  $\mathbf{K} = \text{diag}(2)$ , i.e.,

```
R> K <- diag(2)
R> Sigma <- diag(1/sqrt(diag(K %*% Vbetahat %*% t(K))))
R> z <- Sigma %*% K %*% betahat
R> Cor <- Sigma %*% (K %*% Vbetahat %*% t(K)) %*% t(Sigma)</pre>
```

Note that  $\mathbf{z} = (-2.6011, 9.464)$  is equal to the t statistics. The multiplicity-adjusted p values can now be computed by means of the multivariate t distribution utilizing the pmvt function available in package **mvtnorm**:

```
R> library("mvtnorm")
R> df.cars <- nrow(cars) - length(betahat)
R> sapply(abs(z), function(x) 1 - pmvt(-rep(x, 2), rep(x, + 2), corr = Cor, df = df.cars))
[1] 1.661e-02 2.458e-12
```

Note that the p value of the global test is the minimum p value of the partial tests.

The computations above can be performed much more conveniently using the functionality implemented in package **multcomp**. The function glht just takes a fitted model and a matrix defining the linear functions, and thus hypotheses, to be tested:

```
R> library("multcomp")
R> cars.ht <- glht(lm.cars, linfct = K)
R> summary(cars.ht)
```

Simultaneous Tests for General Linear Hypotheses

```
Fit: lm(formula = dist ~ speed, data = cars)
```

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)

(Intercept) == 0 -17.579 6.758 -2.60 0.017 *

speed == 0 3.932 0.416 9.46 <1e-10 ***
---

Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1

(Adjusted p values reported -- single-step method)
```

Simultaneous confidence intervals corresponding to this multiple testing procedure are available via

```
R> confint(cars.ht)
```

Simultaneous Confidence Intervals

```
Fit: lm(formula = dist ~ speed, data = cars)
```

```
Quantile = 2.13
95% family-wise confidence level
```

Linear Hypotheses:

```
Estimate lwr upr
(Intercept) == 0 -17.579 -31.977 -3.181
speed == 0 3.932 3.047 4.818
```

The application of the framework isn't limited to linear models, nonlinear least-squares estimates can be tested as well. Consider constructing simultaneous confidence intervals for the model parameters (example from the manual page of nls):

Simultaneous Confidence Intervals

```
Fit: nls(formula = density ~ SSlogis(log(conc), Asym, xmid, scal),
  data = DNase1, algorithm = "default", control = list(maxiter = 50,
      tol = 1e-05, minFactor = 0.0009765625, printEval = FALSE,
  warnOnly = FALSE), trace = FALSE)
```

Quantile = 2.135 95% family-wise confidence level

Linear Hypotheses:

```
Estimate lwr upr

Asym == 0 2.345 2.178 2.512

xmid == 0 1.483 1.309 1.657

scal == 0 1.041 0.973 1.110
```

which is not totally different from univariate confidence intervals

R> confint(fm1DNase1)

```
2.5% 97.5%
Asym 2.1935 2.539
xmid 1.3215 1.679
scal 0.9743 1.115
```

because the parameter estimates are highly correlated

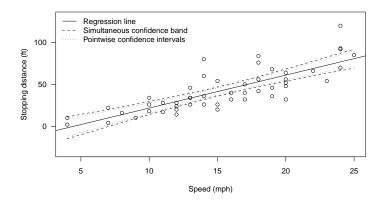


Figure 1: cars data: Regression line with confidence bands (dashed) and intervals (dotted).

R> cov2cor(vcov(fm1DNase1))

```
Asym xmid scal
Asym 1.0000 0.9868 0.9008
xmid 0.9868 1.0000 0.9063
scal 0.9008 0.9063 1.0000
```

Example: Confidence Bands for Regression Line. Suppose we want to plot the linear model fit to the cars data including an assessment of the variability of the model fit. This can be based on simultaneous confidence intervals for the regression line  $x_i^{\top}\hat{\beta}$ :

```
R> K <- model.matrix(lm.cars)[!duplicated(cars$speed),
+    ]
R> ci.cars <- confint(glht(lm.cars, linfct = K), abseps = 0.1)</pre>
```

Figure 1 depicts the regression fit together with the confidence band for the regression line and the pointwise confidence intervals as computed by predict(lm.cars).

# 2 Multiple Comparison Procedures

Multiple comparisons of means, i.e., regression coefficients for groups in AN(C)OVA models, are a special case of the general framework sketched in the previous section. The main difficulty is that the comparisons one is usually interested in, for example all-pairwise differences, can't be directly specified based on model

parameters of an AN(C)OVA regression model. We start with a simple one-way ANOVA example and generalize to ANCOVA models in the following.

Consider a one-way ANOVA model, i.e., the only covariate x is a factor at j levels. In the absence of an intercept term only, the elements of the parameter vector  $\beta \in \mathbb{R}^j$  correspond to the mean of the response in each of the j groups:

```
R> ex <- data.frame(y = rnorm(12), x = gl(3, 4, labels = LETTERS[1:3]))
R> aov.ex <- aov(y ~ x - 1, data = ex)
R> coef(aov.ex)
```

Thus, the hypotheses  $\beta_2 - \beta_1 = 0$  and  $\beta_3 - \beta_1 = 0$  can be written in form of a linear function  $\mathbf{K}\beta$  with

R> 
$$K \leftarrow rbind(c(-1, 1, 0), c(-1, 0, 1))$$
  
R>  $rownames(K) \leftarrow c("B - A", "C - A")$   
R>  $colnames(K) \leftarrow names(coef(aov.ex))$   
R>  $K$ 

Using the general linear hypothesis function glht, this so-called 'many-to-one comparison procedure' [Dunnett, 1955] can be performed via

```
R> summary(glht(aov.ex, linfct = K))
```

Simultaneous Tests for General Linear Hypotheses

```
Fit: aov(formula = y ~ x - 1, data = ex)
```

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)

B - A == 0 0.323 0.625 0.52 0.83

C - A == 0 0.695 0.625 1.11 0.46

(Adjusted p values reported -- single-step method)
```

Alternatively, a symbolic description of the general linear hypothesis of interest can be supplied to glht:

```
R> summary(glht(aov.ex, linfct = c("xB - xA = 0", "xC - xA = 0")))
```

Simultaneous Tests for General Linear Hypotheses

```
Fit: aov(formula = y ~ x - 1, data = ex)
```

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)

xB - xA == 0 0.323 0.625 0.52 0.83

xC - xA == 0 0.695 0.625 1.11 0.46

(Adjusted p values reported -- single-step method)
```

However, in the presence of an intercept term, the full parameter vector  $\theta = c(\mu, \beta_1, \dots, \beta_j)$  can't be estimated due to singularities in the corresponding design matrix. Therefore, a vector of *contrasts*  $\gamma^*$  of the original parameter vector  $\gamma$  is fitted. More technically, a contrast matrix  $\mathbf{C}$  is included into this model such that  $\beta = \mathbf{C}\gamma^*$  any we only obtain estimates for  $\gamma^*$ , but not for  $\gamma$ :

The default contrasts in R are so-called treatment contrasts, nothing but differences in means for one baseline group (compare the Dunnett contrasts and the estimated regression coefficients):

R> contr.treatment(table(ex\$x))

R> K %\*% contr.treatment(table(ex\$x)) %\*% coef(aov.ex2)[-1]

[,1] B - A 0.3235 C - A 0.6947

so that  $\mathbf{KC}\hat{\beta}^{\star} = \mathbf{K}\hat{\beta}$ .

When the mcp function is used to specify linear hypotheses, the glht function takes care of contrasts. Within mcp, the matrix of linear hypotheses  $\mathbf{K}$  can be written in terms of  $\gamma$ , not  $\gamma^*$ . Note that the matrix of linear hypotheses only applies to those elements of  $\hat{\gamma}^*$  attached to factor  $\mathbf{x}$  but not to the intercept term:

R> summary(glht(aov.ex2, linfct = mcp(x = K)))

Simultaneous Tests for General Linear Hypotheses

Multiple Comparisons of Means: User-defined Contrasts

```
Fit: aov(formula = y ~ x, data = ex)
```

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)

B - A == 0 0.323 0.625 0.52 0.83

C - A == 0 0.695 0.625 1.11 0.46

(Adjusted p values reported -- single-step method)
```

or, a little bit more convenient in this simple case:

```
R> summary(glht(aov.ex2, linfct = mcp(x = c("B - A = 0", + "C - A = 0")))
```

Simultaneous Tests for General Linear Hypotheses

Multiple Comparisons of Means: User-defined Contrasts

```
Fit: aov(formula = y ~ x, data = ex)
```

Linear Hypotheses:

```
Estimate Std. Error t value Pr(>|t|)
B - A == 0 0.323 0.625 0.52 0.83
C - A == 0 0.695 0.625 1.11 0.46
(Adjusted p values reported -- single-step method)
```

More generally, inference on linear functions of parameters which can be interpreted as 'means' are known as  $multiple\ comparison\ procedures\ (MCP)$ . For some of the more prominent special cases, the corresponding linear functions can be computed by convenience functions part of multcomp. For example, Tukey all-pair comparisons for the factor x can be set up using

General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts

Linear Hypotheses:

Estimate
B - A == 0 0.323
C - A == 0 0.695
C - B == 0 0.371

The initial parameterization of the model is automatically taken into account:

#### General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts

#### Linear Hypotheses:

					Estimate
В	-	Α	==	0	0.323
C	-	Α	==	0	0.695
C	-	В	==	0	0.371

### 3 Test Procedures

Several global and multiple test procedures are available from the summary method of glht objects and can be specified via its test argument:

- test = univariate() univariate p values based on either the t or normal distribution are reported. Controls the type I error for each partial hypothesis only.
- test = Ftest() global F test for  $H_0$ .
- test = Chisqtest() global  $\chi^2$  test for  $H_0$ .
- test = adjusted() multiple test procedures as specified by the type argument to adjusted: "single-step" denotes adjusted p values as computed from the joint normal or t distribution of the z statistics (default), "free" implements multiple testing procedures under free combinations, "Shaffer" implements Bonferroni-adjustments taking logical constraints into account Shaffer [1986] and "Westfall" takes both logical constraints and correlations among the z statistics into account Westfall [1997]. In addition, all adjustment methods implemented in p.adjust can be specified as well.

# 4 Quality Assurance

The analyses shown in Westfall et~al. [1999] can be reproduced using **multcomp** by running the R transcript file in inst/MCMT.

### References

Charles W. Dunnett. A multiple comparison procedure for comparing several treatments with a control. *Journal of the American Statistical Association*, 50(272):1096–1121, 1955.

- Juliet P. Shaffer. Modified sequentially rejective multiple test procedures. *Journal of the American Statistical Association*, 81:826–831, 1986.
- Peter H. Westfall. Multiple testing of general contrasts using logical constraints and correlations. *Journal of the American Statistical Association*, 92:299–306, 1997.
- Peter H. Westfall, Randall D. Tobias, Dror Rom, Russell D. Wolfinger, and Yosef Hochberg. *Multiple Comparisons and Multiple Tests Using the SAS System.* SAS Insitute, Cary, NC, 1999.