

Polynomial contrasts with carbon wire data (continued)

Displays for Statistics 5303

Lecture 21

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Class Web Page

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```

Cmd> anova("y=(temp+time+degas)^3", pvals:T)
Model used is y=(temp+time+degas)^3

```

	DF	SS	MS	P-value
CONSTANT	1	36154	36154	< 1e-08
temp	2	410.69	205.35	< 1e-08
time	2	80.541	40.27	< 1e-08
degas	1	0.46722	0.46722	0.21249
temp.time	4	14.814	3.7035	2.5659e-07
temp.degas	2	0.31361	0.15681	0.58919
time.degas	2	0.70194	0.35097	0.31036
temp.time.degas	4	0.87472	0.21868	0.56559
ERROR1	54	15.85	0.29352	

```

Cmd> c_lin <- vector(-1,0,1); c_quad <- vector(-1,2,-1)
Cmd> contrast(temp,c_lin) #temp main effect line
component: estimate
(1) 5.85 t = 5.85/.1564 = 37.4
component: ss
(1) 410.67
component: se
(1) 0.1564
Cmd> contrast(temp,c_quad) #temp main effect quadratic
component: estimate
(1) 0.075 t = 0.075/0.27089 = -0.277
component: ss
(1) 0.0225
component: se
(1) 0.27089

```

There is a strong linear effect of temperature ($t = 37.4$) but no quadratic effect ($t = 0.277$).

2

Note $SS_{lin} + SS_{quad} = 410.67 + 0.0225 = 410.69 = SS_{temp}$, in the ANOVA table.

```

Cmd> contrast(time,c_lin) #time main effect linear
component: estimate
(1) 2.4417 t = 2.4417/.1564 = 15.61
component: ss
(1) 71.541
component: se
(1) 0.1564
Cmd> contrast(time,c_quad) #time main effect quadratic
component: estimate
(1) 1.5 t = 1.5/.27089 = 5.537
component: ss
(1) 9
component: se
(1) 0.27089

```

Both linear and quadratic main effect contrasts in time are significant, but the quadratic effect is much smaller. Again $SS_{lin} + SS_{quad} = 71.541 + 9 = 80.541 = SS_{time}$

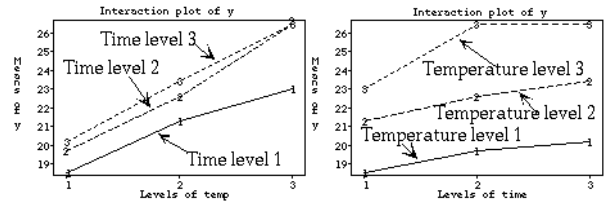
3

Look at time by temperature interaction effects.

```

Cmd> interactplot(y,temp,time)
Cmd> interactplot(y,time,temp)

```



The lines are not very parallel, suggesting interaction of time and temp.

The main effect linear contrasts are isolating the **average** of linear contrasts for each level of the other factor (along each line) separately. That can be near zero when slopes are of opposite signs or curvatures in opposite directions.

It should be fairly clear why we found significant linear main effect contrasts, and why there was some quadratic dependence on time and none on temperature.

4

Interaction contrasts allow you to extract various features of the interaction. First I calculate the \bar{y}_{ij} .

```
Cmd> ybar_ijdot <- tabs(y,temp,time,means:T); ybar_ijdot
(1,1) 18.538 19.675 20.2
(2,1) 21.275 22.575 23.45
(3,1) 23 26.475 26.488
```

Now I compute linear contrasts comparing temp levels in each column (level of time) and comparing time levels in each row (level of temp)

```
Cmd> lins_temp <- vector(sum(c_lin*ybar_ijdot)); lins_temp
(1) 4.4625 6.8 6.2875
Cmd> lins_time <- vector(sum(c_lin*ybar_ijdot')); lins_time
(1) 1.6625 2.175 3.4875
```

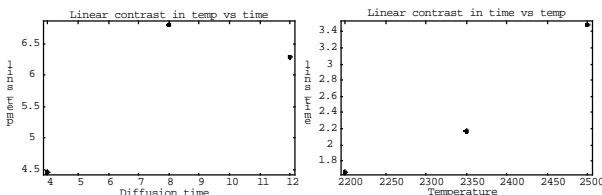
Note the use of the transpose operator ' to swap rows and columns so sum() would sum accross a row rather than a column.

The averages of these are the same as the main effect linear contrasts computed previously.

```
Cmd> vector(sum(lins_temp)/3, sum(lins_time)/3)
(1) 5.85 2.4417
```

Let's see how these contrasts vary over levels of the other factor.

```
Cmd> actualtemp <- run(2200,2500,150)
Cmd> actualtime <- run(4,12,4)
Cmd> plot(actualtime,lins_temp,xlab:"Diffusion time",\
title:"Linear contrast in temp vs time")
Cmd> plot(actualtemp,lins_time,xlab:"Temperature",\
title:"Linear contrast in time vs temp")
```



The pattern of linear contrasts on the left looks like a curved dependence on time, while the pattern on the right is fairly close to linear on temperature, with only a hint of curvature.

Since a linear contrast is proportional to a least squares slope, it appears the slope on temp may depend quadratically on time, while the slope on time depends linearly on temperature.

A more "black box" way to find these separate contrasts is using contrast() with a third argument.

```
Cmd> contrast(temp,c_lin,time)
component: estimate
(1) 4.4625 6.8 6.2875
component: ss
(1) 79.656 184.96 158.13
component: se
(1) 0.27089 0.27089 0.27089
```

The estimate component contains the separate contrasts for each level of time.

```
Cmd> contrast(time,c_lin,temp)
component: estimate
(1) 1.6625 2.175 3.4875
component: ss
(1) 11.056 18.923 48.651
component: se
(1) 0.27089 0.27089 0.27089
```

Now the estimate component contains the separate contrasts for each level of temp.

This also provides standard errors and SS.

Linear contrast coefficients are good for extracting information about a linear trend, so we can apply them to the separate linear contrast values to extract information about their linear dependence on the other factor.

```
Cmd> sum(c_lin*lins_temp)
(1) 1.825
```

You can do this in one step using an interaction contrast created from the separate contrasts using outer().

Linear by Linear

```
Cmd> outer(c_lin,c_lin) # same thing
(1,1) 1 0 -1
(2,1) 0 0 0
(3,1) -1 0 1

Cmd> contrast("temp.time",outer(c_lin,c_lin))
component: estimate
(1) 1.825
component: ss
(1) 6.6612
component: se
(1) 0.38309
```

This is the linear by linear interaction contrast computed above. It is highly significant ($t = 1.8254/.38309 = 4.76$).

The SS = 6.6612 is much less than the overall interaction SS_{time,temp} = 14.814, so there is a lot more interaction to "explain".

Linear in temp by quadratic in time

```
Cmd> outer(c_lin,c_quad) # linear by quadratic
(1,1)      1      -2      1
(2,1)      0      0      0
(3,1)     -1      2     -1

Cmd> contrast("temp.time",outer(c_lin,c_quad))
component: estimate
(1)      2.85
component: ss
(1)      5.415
component: se
(1)      0.66353
```

t = 2.85/0.66353 = 4.30 is significant

Quadratic in temp by linear in time

```
Cmd> contrast("temp.time",outer(c_quad,c_lin))
component: estimate
(1)     -0.8
component: ss
(1)      0.42667
component: se
(1)      0.66353
```

t = 0.8/0.66353 = 1.21 is not significant

What sort of a model underlies the use of these contrasts?

Suppose you have a two factor model where the two factors are defined by values x_{Ai} , $i = 1, \dots, a$ and x_{Bj} , $j = 1, \dots, b$ of quantitative variables x_A and x_B so that $\mu_{ij} = f(x_{Ai}, x_{Bj})$ for some function $f(x_A, x_B)$.

Suppose for each fixed value x_B , the dependence of $f(x_A, x_B)$ on x_A is quadratic.

$f(x_A, x_B) = \beta_0(x_B) + \beta_1(x_B)x_A + \beta_2(x_B)x_A^2$, where $\beta_k(x_B)$ are the coefficients for that level of x_B .

Quadratic by quadratic

```
Cmd> contrast("temp.time",outer(c_quad,c_quad))
component: estimate
(1)     -3.225
component: ss
(1)      2.3112
component: se
(1)      1.1493
```

t = -3.225/1.1493 = -2.81, significant at the 1% level.

Conclusion:

For each level of time, the response on temp is curved, but the curvature varies from level to level.

For each level of temp, the response on time is curved, but the curvature varies from level to level.

The 4 interaction contrasts SS add up to the overall 4 degree of freedom SS_{temp,time}

$$6.6612 + 5.415 + 0.42667 + 2.3112 = 14.814.$$

Now suppose the dependence of each coefficient $\beta_k(x_B)$ on x_B is also quadratic

$$\begin{aligned} \beta_0(x_B) &= \delta_{00} + \delta_{01}x_B + \delta_{02}x_B^2 \\ \beta_1(x_B) &= \delta_{10} + \delta_{11}x_B + \delta_{12}x_B^2 \\ \beta_2(x_B) &= \delta_{20} + \delta_{21}x_B + \delta_{22}x_B^2 \end{aligned}$$

$$\begin{aligned} \text{Then } f(x_A, x_B) &= \delta_{00} + \delta_{10}x_A + \delta_{01}x_B \\ &\quad + \delta_{20}x_A^2 + \delta_{11}x_Ax_B + \delta_{02}x_B^2 \\ &\quad + \delta_{21}x_A^2x_B + \delta_{12}x_Ax_B^2 + \delta_{22}x_A^2x_B^2 \end{aligned}$$

In the context of this model, when $\delta_{11} = \delta_{12} = \delta_{21} = \delta_{22} = 0$, all $\alpha\beta_{ij} = 0$ and

- the A_{quad} by B_{quad} F or t tests $H_0: \delta_{22} = 0$.
- Provided $\delta_{22} = 0$, the A_{lin} by B_{quad} F or t tests $H_0: \delta_{12} = 0$
- Provided $\delta_{22} = 0$, the A_{quad} by B_{lin} F or t tests $H_0: \delta_{21} = 0$
- Provided $\delta_{12} = \delta_{21} = \delta_{22} = 0$, the A_{lin} by B_{lin} F or t tests $H_0: \delta_{11} = 0$

One degree of freedom for non-additivity

Part of the purpose of using interaction contrasts is the hope they will help you describe the pattern of interaction.

Another approach, which is particularly useful in experiments with no replication, goes under the name of **Tukey's one degree of freedom for non-additivity**.

Tukey was looking for the simplest sort of model beyond an additive model. He asked the question,

What sort of a model would I get if the data were derived by some transformation of an additive model?

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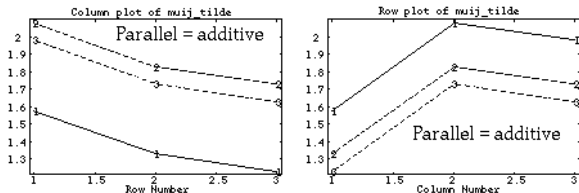
Although it won't be exact, in many cases the means will be similarly related.

That is $\mu_{ij} = E(y_{ij}) = g(\tilde{\mu}_{ij})$

Here is a 3 by 3 additive table of $\tilde{\mu}_{ij}$

```
Cmd> muij_tilde
(1,1) 1.58 2.08 1.98
(2,1) 1.33 1.83 1.73
(3,1) 1.23 1.73 1.63
```

```
Cmd> colplot(muij_tilde,title:"Column plot of muij_tilde")
Cmd> rowplot(muij_tilde,title:"Row plot of muij_tilde")
```



In this scale the factors act additively, with no interaction.

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That is, in the two factor case, suppose there is an **additive model** for a response \tilde{y}_{ij} which is related to y by $\tilde{y}_{ij} = f(y_{ij})$ for some function f . For example, you might have $\tilde{y}_{ij} = \log_{10} y_{ij}$ or $\tilde{y}_{ij} = y_{ij}^p$.

To say that \tilde{y}_{ij} has an additive model means that the mean $\tilde{\mu}_{ij}$ of \tilde{y}_{ij} for levels i and j of factors A and B has the form

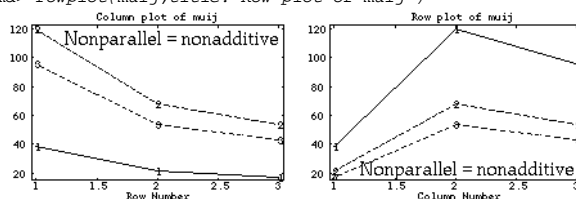
$$\tilde{\mu}_{ij} = \tilde{\mu} + \tilde{\alpha}_i + \tilde{\beta}_j.$$

Suppose $y = g(\tilde{y})$ is the inverse transformation to f . For example, when $\tilde{y}_{ij} = \log_{10} y_{ij}$, $y_{ij} = g(\tilde{y}_{ij}) = 10^{\tilde{y}_{ij}}$ and when $\tilde{y}_{ij} = y_{ij}^p$, $y_{ij} = g(\tilde{y}_{ij}) = \tilde{y}_{ij}^{1/p}$.

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Now transform to $\mu = 10^\mu$ and make interaction plots.

```
Cmd> muij <- 10^muij_tilde # muji <- g(muij_tilde)
Cmd> colplot(muij,title:"Column plot of muij")
Cmd> rowplot(muij,title:"Row plot of muij")
```



The lines are no longer parallel. The model is no longer additive.

When $\mu_{ij} = g(\tilde{\mu} + \tilde{\alpha}_i + \tilde{\beta}_j)$, and the $(\tilde{\alpha}_i + \tilde{\beta}_j)/\tilde{\mu}$ are not too big, approximately,

$$\begin{aligned} \mu_{ij} &\approx g(\tilde{\mu}_{ij}) = g(\tilde{\mu} + \tilde{\alpha}_i + \tilde{\beta}_j) \\ &\approx g(\tilde{\mu}) + c(\tilde{\alpha}_i + \tilde{\beta}_j) + d(\tilde{\alpha}_i + \tilde{\beta}_j)^2 \end{aligned}$$

where $c = g'(\tilde{\mu})$ and $d = g''(\tilde{\mu})/2$ (derivatives of $g(\tilde{\mu})$)

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After some simplification, leaving out terms of 3rd or 4th degree in $\tilde{\alpha}_i$ and $\tilde{\beta}_j$, you can find effects $\{\alpha_i\}$ and $\{\beta_j\}$ such that

$$\mu_{ij} \approx \mu + \alpha_i + \beta_j + \gamma\alpha_i\beta_j$$

where $\gamma = 2d/c^2 = g''(\tilde{\mu})/g'(\tilde{\mu})^2$. This is a model with interaction with a simple model for the interaction effects:

$$\alpha\beta_{ij} = \gamma\alpha_i\beta_j, i = 1, \dots, a, j = 1, \dots, b$$

requiring just 1 additional parameter γ .

In the particular case when $f(\mu) = \mu^p$ and $g(\tilde{\mu}) = \tilde{\mu}^{1/p}$,

$$\gamma = g''(\tilde{\mu})/g'(\tilde{\mu})^2 = (1 - p)/\tilde{\mu}^{1/p} \approx (1 - p)/\mu$$

Then $p = 1 - \mu\gamma$. From estimates $\hat{\mu}$ and $\hat{\gamma}$ of μ and γ you can get a handle on a possible transformation, $y \rightarrow y^{1-\hat{\mu}\hat{\gamma}}$.

Here is an example from Snedecor and Cochran Table 15.9.1. The response is the number of insects caught in a trap over night. There were 5 nights and three traps.

```

Cmd> sned15_9 <- vector(19.1,23.4,29.5,23.4,16.6,\
50.1,166.1,223.9,58.9,64.6, 123,407.4,398.1,229.1,251.2)
Cmd> print(matrix(sned15_9,5,\
labels:structure("Trap ","Night ")),format:"11.1f")
MATRIX:
      Night 1   Night 2   Night 3
Trap 1    19.1     50.1    123.0
Trap 2    23.4    166.1    407.4
Trap 3    29.5    223.9    398.1
Trap 4    23.4     58.9    229.1
Trap 5    16.6     64.6    251.2

Cmd> period <- factor(rep(run(5),3))
Cmd> trap <- factor(rep(run(3),rep(5,3)))
Cmd> anova("sned15_9=period + trap", fstat:T)
Model used is sned15_9=period + trap
      DF   SS      MS      F      P-value
CONSTANT 1 2.8965e+05 2.8965e+05 75.70780 2.3739e-05
period   4 52066      13016  3.40223 0.06611
trap     2 1.7333e+05 86667    22.65276 0.00050731
ERROR1   8 30607      3825.9

Cmd> fitted <- sned15_9 - RESIDUALS # muij_hat
    
```

fitted contains the additive fit because
RESIDUALS = sned15_9 - fitted.

The model

$$y_{ij} = \mu + \alpha_i + \beta_j + \gamma\alpha_i\beta_j + \epsilon_{ij}$$

might be called the **1-dofna two-factor model**. If it is appropriate, then the null hypothesis $H_0: \alpha\beta_{ij} = 0$ all i and j is equivalent to $H_0: \gamma = 0$

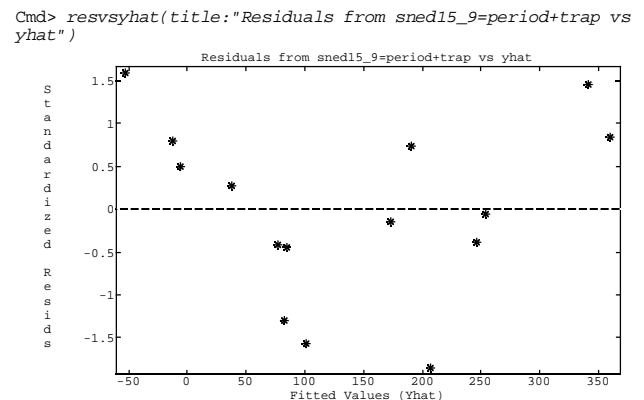
How can you fit the 1-dofna model?

You can do it in two stages:

1. Fit the additive model $\mu_{ij} = \mu + \alpha_i + \beta_j$ and from it find the fitted values $\hat{\mu}_{ij} = \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j$.
2. Compute $z_{ij} = (\hat{\mu}_{ij} - \hat{\mu})^2/2 = (\hat{\alpha}_i + \hat{\beta}_j)^2/2$
3. Fit the model with an additional term

$$y_{ij} = \mu + \alpha_i + \beta_j + \gamma z_{ij} + \epsilon_{ij}$$

The F- or t-statistic for z is a test of $H_0: \gamma = 0$, that is H_0 : model is additive.



There seems to be some sort of quadratic dependence of residuals on fitted values.

```

Cmd> grandmean <- describe(sned15_9,mean:T)
Cmd> z <- (fitted - grandmean)^2/2
Cmd> anova("sned15_9=period + trap + z", fstat:T)
Model used is sned15_9=period + trap + z
WARNING: summaries are sequential
      DF   SS      MS      F      P-value
CONSTANT 1 2.8965e+05 2.8965e+05 322.45184 4.1032e-07
period   4 52066      13016  14.49064 0.0016932
trap     2 1.7333e+05 86667    96.48180 8.0263e-06
z        1 24319      24319  27.07330 0.0012486
ERROR1   7 6287.9      898.27
    
```

The original $SS_{\text{error}} = 30607$ was effectively the period by trap interaction SS. The 1 degree of freedom SS = 24319 associated with z - **1 degree of freedom for non-additivity** or **1-dofna** - has "explained" about 80% of that. $F_{1,7} = 27.07$ is highly significant.

The error MS has been reduced from 3825.9 to 898.27 and both main effects are significant.