Designs with two factors

Last time: Completely randomized designs

- Two equivalent parametrizations:

1. Group means parametrization:

$$Y_{ij} = \mu_i + \varepsilon_{ij}, \qquad \varepsilon_{ij} \overset{\text{iid}}{\sim} N(0, \sigma^2),$$

2. Sum-to-zero parametrization:

$$Y_{ij} = \mu + \tau_i + \varepsilon_{ij}, \qquad \sum_{i=1}^{a} \tau_i = 0, \qquad \varepsilon_{ij} \overset{\text{iid}}{\sim} N(0, \sigma^2),$$

- $i \in \{1, \dots a\}$ indexes group membership
- $j \in \{1, \dots, n_i\}$ indexes observations within a group

Today

Designs with two factors

- **One treatment and a block**
- **Two treatments**

One treatment and a block

One treatment and a block

- We want to quantify the effect of the treatment on the response
- In an experimental design, we can control the assignment mechanism of the treatment
- A block (or blocking variable) is a known source of variation we can control (assign). It affects the outcome but we are not interested in its effect

Example: Painting line

- An engineer working at a painting line wants to know if different types of paints have the same average drying times
- They will perform the experiments on four different days
- The engineers think that the weather may affect the outcome: that is, the day may affect the outcome
- The treatment is the type of paint, the block is the day

Balanced complete randomized block designs with replicates

- We assign experimental units randomly to blocks and treatments
- The block has b levels
- The treatment has a levels
- We collect r observations for each combination of block and treatment: there are r replicates
- Total sample size is $N = rba$

Terminology

- The design is *balanced* because each combination of block and treatment is observed the same number of times: r
- The design is *complete* because there are observations for each combination of block and treatment
- The term "balanced complete randomized block designs" usually refers to the case $r = 1$, which is the most common
- Designs with $r > 1$ are often referred to as "balanced complete randomized block designs with replicates"

Example: Painting line

- Day (block): $b = 4$ days
- Type of paint (treatment): $a = 3$ types
- $r = 1$ replicate
- $N = rba = 12$ observations

	Day 1	Day 2	Day 3	Day 4
Type A	2.60	2.10	3.5	2.65
Type B	3.25	2.65	3.8	3.50
Type C	2.60	2.05	3.1	2.62

Model

$$Y_{ijk} = \mu + \tau_i + \beta_j + \varepsilon_{ijk}, \qquad \sum_{i=1}^{a} \tau_i = \sum_{j=1}^{b} \beta_j = 0, \qquad \varepsilon_{ijk} \overset{\text{iid}}{\sim} N(0, \sigma^2)$$

- $i \in \{1, \ldots, a\}$ indexes treatments, $j \in \{1, \ldots, b\}$ indexes blocks, and $k \in \{1, \ldots, r\}$ indexes replicates
- As before, we assume that the errors are independent and normal, and that the variance σ^2 doesn't depend on the treatment or block
- We also assume an additive relationship between treatment and block

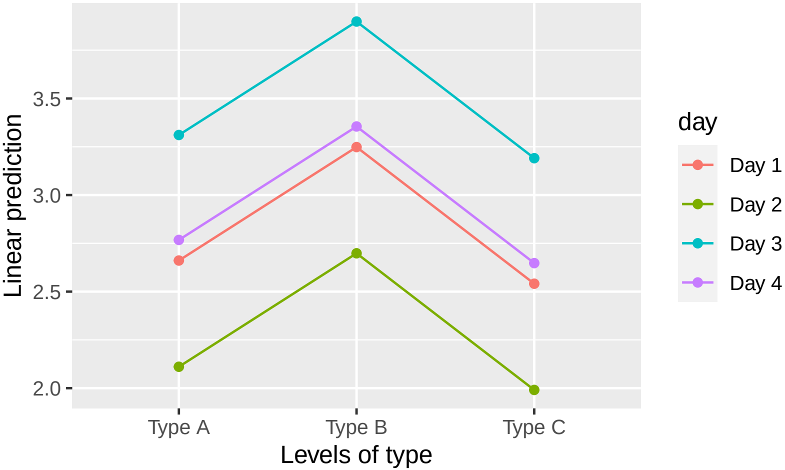
Additivity

- Treatment effect doesn't depend on blocks; block effect doesn't depend on treatment
- **Example:** $a = 2$ treatments and $b = 2$ blocks, table with expected values

	Block 1	Block 2
Treat 1	$\mu + \tau_1 + \beta_1$	$\mu + \tau_1 + \beta_1$
Treat 2	$\mu + \tau_2 + \beta_2$	$\mu + \tau_2 + \beta_2$

Average treatment effect in block 1: $\mathbb{E}(y_{11k} - y_{21k'}) = \tau_1 - \tau_2$
Average treatment effect in block 2: $\mathbb{E}(y_{12k} - y_{22k'}) = \tau_1 - \tau_2$
Average block effect in treat 1: $\mathbb{E}(y_{11k} - y_{12k'}) = \beta_1 - \beta_2$
Average block effect in treat 2: $\mathbb{E}(y_{21k} - y_{22k'}) = \beta_1 - \beta_2$

Example: estimated effects with additive model



Estimating parameters: Block design

- Let

$$\text{total mean} = \overline{Y} = \frac{1}{N}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r} Y_{ijk}$$

$$\text{treat } i \text{ mean } = \overline{Y}_{i.} = \frac{1}{br}\sum_{j=1}^{b}\sum_{k=1}^{r} Y_{ijk}$$

$$\text{block } j \text{ mean } = \overline{Y}_{.j} = \frac{1}{ar}\sum_{i=1}^{a}\sum_{k=1}^{r} Y_{ijk}$$

- Point estimates

$$\widehat{\mu} = \overline{Y}, \qquad \widehat{\tau}_i = \overline{Y}_{i.} - \overline{Y}, \qquad \widehat{\beta}_j = \overline{Y}_{.j} - \overline{Y},$$

and

$$\widehat{\sigma^2} = \frac{1}{N-1}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(Y_{ijk} - \widehat{\mu} - \widehat{\tau}_i - \widehat{\beta}_j)^2$$

Example: Reading in data

```
mat = matrix(c(2.60, 2.10, 3.50, 2.65,
              3.25, 2.65, 3.80, 3.5,
              2.60, 2.05, 3.10, 2.62),
       nrow = 3,
       ncol = 4,
       byrow = TRUE)
rownames(mat) = c("Type A", "Type B", "Type C")
colnames(mat) = c("Day 1", "Day 2", "Day 3", "Day 4")
```

Example: Converting into convenient (long) format

```
library(tidyverse)
df = as.data.frame(mat)
df$type = rownames(df)
df = df %>% pivot_longer(!type,
                         names_to = "day",
                         values_to = "outcome")
df$type = factor(df$type); df$day = factor(df$day)
```

Example: model with sum-to-zero constraint

```r
# sum-to-zero
options(contrasts = c("contr.sum", "contr.poly"))
# fit model
mod = aov(outcome ~ day + type, data  = df)
# point estimates
dummy.coef(mod)
```

```
## Full coefficients are
##
## (Intercept):       2.868333
## day:                  Day 1       Day 2       Day 3       Day 4
##                 -0.05166667 -0.60166667  0.59833333  0.05500000
## type:                Type A      Type B      Type C
##                  -0.1558333   0.4316667  -0.2758333
```

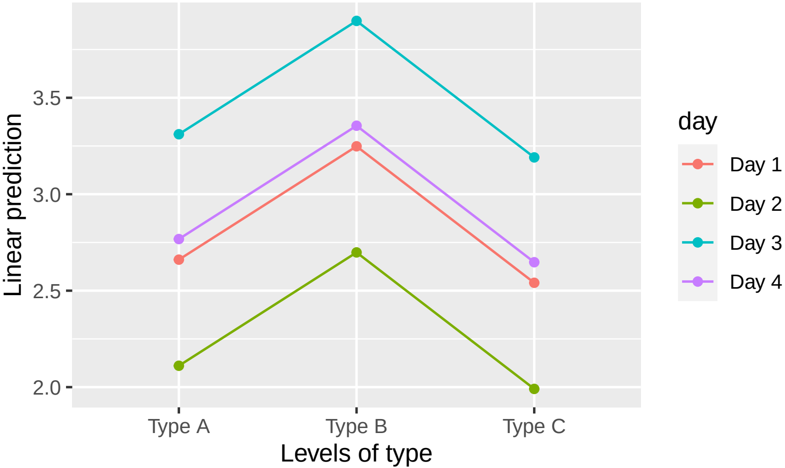
Example: 95% confidence intervals

```
##                   2.5 %      97.5 %
## (Intercept)  2.7760320  2.96063468
## day1        -0.2115373  0.10820396
## day2        -0.7615373 -0.44179604
## day3         0.4384627  0.75820396
## type1       -0.2863672 -0.02529951
## type2        0.3011328  0.56220049
```

No intervals for $\tau_a = -\sum_{i=1}^{a-1} \tau_i$ and $\beta_b = -\sum_{j=1}^{b-1} \beta_j$

Effect plots

```
library(emmeans)
emmip(mod,  day ~ type)
```



Global F tests

Now we have two F tests

- One for τ_i

$$H_{0,\tau} : \tau_i = 0, \text{ for all } i \in \{1, \ldots, a\}$$
$$H_{1,\tau} : \text{ at least one } \tau_i \neq 0$$

- Another one for β_j:

$$H_{0,\beta} : \beta_j = 0, \text{ for all } j \in \{1, \ldots, b\}$$
$$H_{1,\beta} : \text{ at least one } \beta_j \neq 0.$$

Sums of squares

$$\mathrm{SS}_{\mathrm{total}} = \mathrm{SS}_{\mathrm{treat}} + \mathrm{SS}_{\mathrm{block}} + \mathrm{SS}_{\mathrm{error}},$$

where

$$\mathrm{SS}_{\mathrm{total}} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(\overline{Y}_{.j} - \overline{Y})^2$$

$$\mathrm{SS}_{\mathrm{treat}} = br\sum_{i=1}^{a}(\overline{Y}_{i.} - \overline{Y})^2$$

$$\mathrm{SS}_{\mathrm{block}} = ar\sum_{j=1}^{b}(\overline{Y}_{.j} - \overline{Y})^2$$

$$\mathrm{SS}_{\mathrm{error}} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(Y_{ijk} - \widehat{\mu} - \widehat{\tau}_i - \widehat{\beta}_j)^2$$

Under $H_{0,\tau}$, $\overline{Y}_{i.} \approx \overline{Y}$ and $\mathrm{SS}_{\mathrm{treat}}$ will be small; same story with $H_{0,\beta}$ and $\mathrm{SS}_{\mathrm{block}}$

ANOVA table

There are two F statistics: one for the treatment and another one for the block

	df	SS	MS	F	p
Treat	$a-1$	$\mathrm{SS}_{\mathrm{treat}}$	$\mathrm{MS}_{\mathrm{treat}} = \frac{\mathrm{SS}_{\mathrm{treat}}}{a-1}$	$f_{\tau,\mathrm{obs}} = \frac{\mathrm{MS}_{\mathrm{treat}}}{\mathrm{MS}_{\mathrm{error}}}$	p_τ
Block	$b-1$	$\mathrm{SS}_{\mathrm{block}}$	$\mathrm{MS}_{\mathrm{block}} = \frac{\mathrm{SS}_{\mathrm{block}}}{b-1}$	$f_{\beta,\mathrm{obs}} = \frac{\mathrm{MS}_{\mathrm{block}}}{\mathrm{MS}_{\mathrm{error}}}$	p_β
Error	ν	$\mathrm{SS}_{\mathrm{error}}$	$\mathrm{MS}_{\mathrm{error}} = \frac{\mathrm{SS}_{\mathrm{error}}}{\nu}$		

where $\nu = N - a - b + 1$,

$$p_\tau = P(F_{a-1,\nu} > f_{\tau,\mathrm{obs}}), \qquad p_\beta = P(F_{b-1,\nu} > f_{\beta,\mathrm{obs}}),$$

and $F_{\alpha,\nu}$ is notation for the F-distribution with α and ν degrees of freedom.

Example: ANOVA table

```
summary(mod)
```

```
##             Df Sum Sq Mean Sq F value   Pr(>F)    
## day          3 2.1771  0.7257   42.50 0.000195 ***
## type         2 1.1468  0.5734   33.58 0.000552 ***
## Residuals    6 0.1024  0.0171                     
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
```

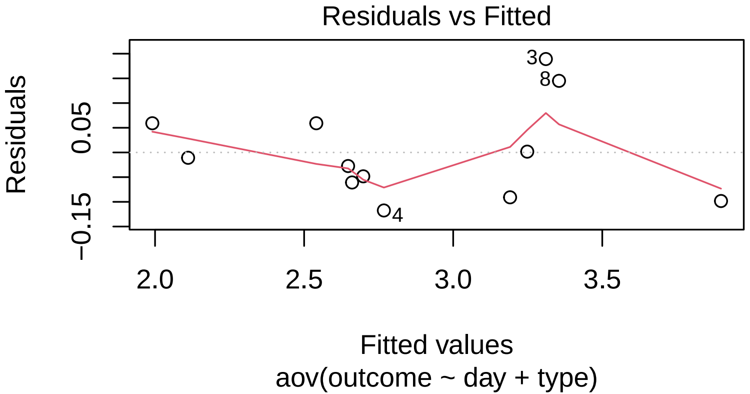
Block and treatment effect are significant at the $\alpha = 0.05$ significance level

Checking model assumptions

- We can check the hypothesis of equality of variances by looking at a plot of fitted values vs residuals: if the assumption is satisfied, the variance on the y-axis shouldn't depend much on where we are on the x-axis
- As before, we can check normality by looking at a qq-plot of the residuals
- Checking independence is hard unless we have a variable that allows us to check for space- or time-dependence, for example
- We assume that the block effect is additive. If $r = 1$, this assumption can't be checked. If $r > 1$, we can check whether an interaction term is needed or not.

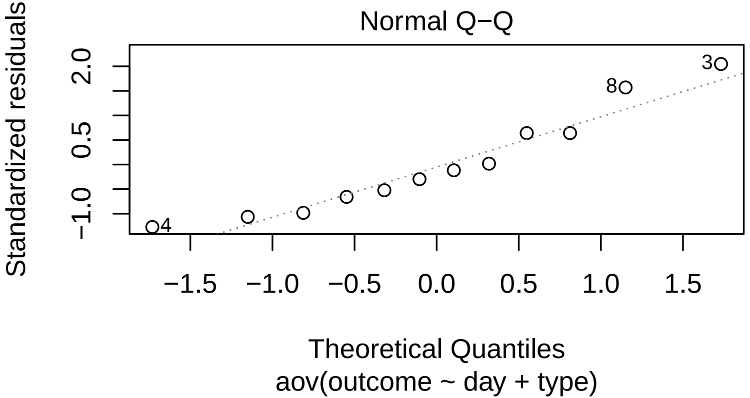
Example: checking equality of variances

```
plot(mod, which = 1)
```



Example: checking normality of residuals

```
plot(mod, which = 2)
```



Pairwise comparisons

- The global F test tells us that there are differences between treatments, but doesn't tell us where the differences are
- We can do pairwise tests to compare treatments; however, we have to be careful and control the type I error rate appropriately
- We can do that with `TukeyHSD`, as we did with completely randomized designs

Example: TukeyHSD

```r
TukeyHSD(mod, which = "type")
```

```
##   Tukey multiple comparisons of means
##     95% family-wise confidence level
##
## Fit: aov(formula = outcome ~ day + type, data = df)
##
## $type
##                    diff        lwr        upr     p adj
## Type B-Type A  0.5875  0.3039958  0.8710042 0.0017250
## Type C-Type A -0.1200 -0.4035042  0.1635042 0.4459693
## Type C-Type B -0.7075 -0.9910042 -0.4239958 0.0006345
```

Significant differences between types A and B and types B and C at the $\alpha = 0.05$ significance level

Two treatments

Two treatments

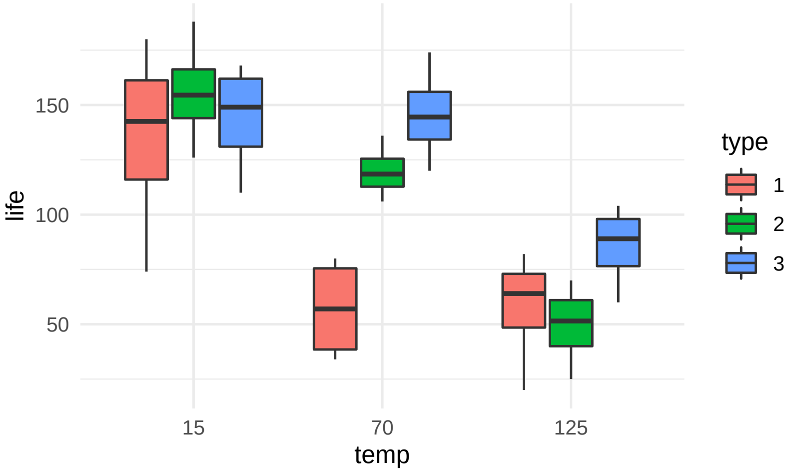
- Now we have two treatments we can control
- We are interested in their effect on the outcome
- The treatments may **interact**: the effect of a treatment may depend on the levels of the other treatment
- To be able to estimate the interaction, we need to have more than one observation for each combination of two treatments

Example: Batteries (Montgomery)

- A company is producing batteries that need to work at different temperatures and for different types of devices
- Battery life is suspected to depend on the temperature and the material that the device is made of (type A, B, or C)
- The company wants to know how temperature and the device affect battery life; they also want to know if there is an interaction between temperature and type of device
- If there is an interaction, it means that the effect of temperature depends on the type of device

Plotting the data

- There are 36 observations: 3 replicates for each combination of type and temperature



Model

$$Y_{ijk} = \mu + \tau_i + \gamma_j + (\tau\gamma)_{ij} + \varepsilon_{ijk}, \qquad \varepsilon_{ijk} \overset{\text{iid}}{\sim} N(0, \sigma^2),$$

with sum-to-zero constraints

$$\sum_{i=1}^{a} \tau_i = \sum_{j=1}^{b} \gamma_j = 0, \qquad \sum_{i=1}^{a} (\tau\gamma)_{ij} = \sum_{j=1}^{b} (\tau\gamma)_{ij} = 0$$

- $i \in \{1, \dots, a\}$ indexes the first treatment, $j \in \{1, \dots, b\}$ indexes the second treatment, and $k \in \{2, \dots, r\}$ indexes replicates
- The errors are independent and normal, the variance σ^2 doesn't depend on the treatment
- $(\tau\gamma)_{ij}$ is the interaction term

Point estimation

Let

$$\overline{Y} = \frac{1}{N}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r} Y_{ijk}, \qquad \overline{Y}_{ij} = \frac{1}{r}\sum_{k=1}^{r} Y_{ijk}$$

$$\overline{Y}_{i.} = \frac{1}{br}\sum_{j=1}^{b}\sum_{k=1}^{r} Y_{ijk}, \qquad \overline{Y}_{.j} = \frac{1}{ar}\sum_{i=1}^{a}\sum_{k=1}^{r} Y_{ijk}$$

Then,

$$\widehat{\mu} = \overline{Y}, \qquad \widehat{(\tau\gamma)}_{ij} = \overline{Y}_{ij} - \widehat{\mu} - \widehat{\tau}_i - \widehat{\gamma}_j$$

$$\widehat{\tau}_i = \overline{Y}_{i.} - \overline{Y}, \qquad \widehat{\gamma}_j = \overline{Y}_{.j} - \overline{Y}$$

and

$$\widehat{\sigma^2} = \frac{1}{N-1}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(Y_{ijk} - \widehat{\mu} - \widehat{\tau}_i - \widehat{\gamma}_j - \widehat{(\tau\gamma)}_{ij})^2$$

Example: point estimation

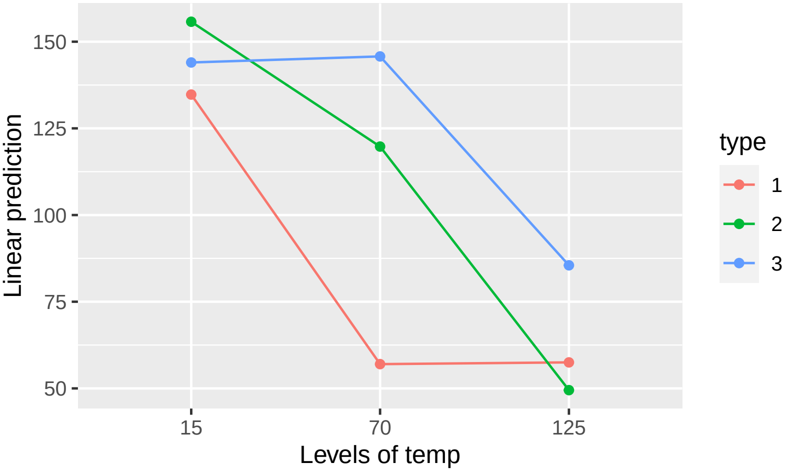
Here's how to find estimates and confidence intervals in R

```
battery = read.csv("https://vicpena.github.io/doe/battery.csv")
battery$type = factor(battery$type)
battery$temp = factor(battery$temp)
options(contrasts = c("contr.sum", "contr.poly"))
mod = aov(life ~ type*temp, data  = battery)
dummy.coef(mod)
confint(mod)
```

Not printing the results here for concreteness

Example: Interaction plot

```
emmip(mod, type ~ temp)
```



Global F tests

We have three F tests

- One for τ_i

$$
\begin{aligned}
H_{0,\tau} &: \tau_i = 0, \text{ for all } i \\
H_{1,\tau} &: \text{ at least one } \tau_i \neq 0
\end{aligned}
$$

- One for γ_j

$$
\begin{aligned}
H_{0,\gamma} &: \gamma_j = 0, \text{ for all } j \\
H_{1,\gamma} &: \text{ at least one } \gamma_j \neq 0
\end{aligned}
$$

- And another one for $(\tau\gamma)_{ij}$

$$
\begin{aligned}
H_{0,\tau\gamma} &: (\tau\gamma)_{ij} = 0, \text{ for all } i, j \\
H_{1,\tau\gamma} &: \text{ at least one } (\tau\gamma)_{ij} \neq 0
\end{aligned}
$$

Sums of squares

$$\mathrm{SS}_{\mathrm{total}} = \mathrm{SS}_\tau + \mathrm{SS}_\gamma + \mathrm{SS}_{\tau\gamma} + \mathrm{SS}_{\mathrm{error}},$$

where

$$\mathrm{SS}_{\mathrm{total}} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(\overline{Y}_{.j} - \overline{Y})^2$$

$$\mathrm{SS}_\tau = br\sum_{i=1}^{a}(\overline{Y}_{i.} - \overline{Y})^2$$

$$\mathrm{SS}_\gamma = ar\sum_{j=1}^{b}(\overline{Y}_{.j} - \overline{Y})^2$$

$$\mathrm{SS}_{\tau\gamma} = r\sum_{i=1}^{a}\sum_{j=1}^{b}(\overline{Y}_{ij} - \overline{Y}_{i.} - \overline{Y}_{.j} + \overline{Y})^2$$

$$\mathrm{SS}_{\mathrm{error}} = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(Y_{ijk} - \overline{Y}_{ij})^2$$

ANOVA table

	df	SS	MS	F	p
τ	$a-1$	SS_τ	$\mathrm{MS}_\tau = \frac{\mathrm{SS}_\tau}{a-1}$	$f_{\tau,\mathrm{obs}} = \frac{\mathrm{MS}_\tau}{\mathrm{MS}_{\mathrm{error}}}$	p_τ
γ	$b-1$	SS_γ	$\mathrm{MS}_\gamma = \frac{\mathrm{SS}_\gamma}{b-1}$	$f_{\gamma,\mathrm{obs}} = \frac{\mathrm{MS}_\gamma}{\mathrm{MS}_{\mathrm{error}}}$	p_γ
$(\tau\gamma)$	$(a-1)(b-1)$	$\mathrm{SS}_{\tau\gamma}$	$\mathrm{MS}_{\tau\gamma} = \frac{\mathrm{SS}_{\tau\gamma}}{(a-1)(b-1)}$	$f_{\tau\gamma,\mathrm{obs}} = \frac{\mathrm{MS}_{\tau\gamma}}{\mathrm{MS}_{\mathrm{error}}}$	$p_{\tau\gamma}$
Error	ν	$\mathrm{SS}_{\mathrm{error}}$	$\mathrm{MS}_{\mathrm{error}} = \frac{\mathrm{SS}_{\mathrm{error}}}{\nu}$		

Example: ANOVA table

```r
summary(mod)
```

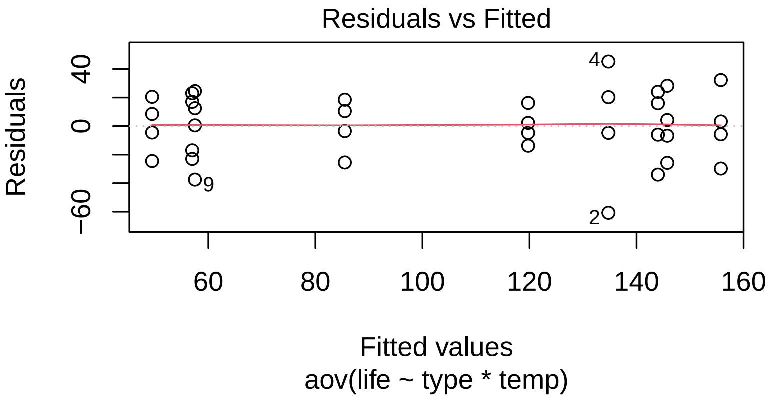
```
##                Df Sum Sq Mean Sq F value   Pr(>F)    
## type            2  10728    5364   7.960  0.00192 ** 
## temp            2  39115   19557  29.020 1.88e-07 ***
## type:temp       4   9670    2417   3.587  0.01803 *  
## Residuals      27  18196     674                     
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1
```

Significant treatment effects and interaction at $\alpha = 0.05$.

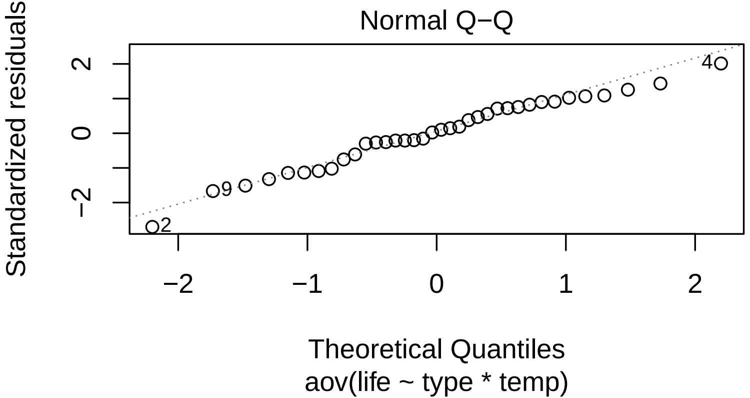
Assumptions

- We still have assumptions of independence, normality, and equality of variances
- We can check them as we did with the blocked design
- Our model has an interaction: if it isn't significant, we can drop it from our model and fit an additive model

Example: checking equality of variances



Example: checking normality



Pairwise comparisons

- As before, global tests don't tell us where the differences are
- For that, we can still use `TukeyHSD`