Tutorial Analysis of Some Agricultural Experiments

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Contents

1 Example 1: Split-plot design with one qualitative and one quantitative level factor

Gomez and Gomez (1984, p. 143) report a rice experiment with three management practices (minimum, optimum, intensive), five different amounts of nitrogen (N) fertilizer (0, 50, 80, 110, 140 kg/ha), and three varieties (V1, V2, V3). The experiment involved variety and management as qualitative treatment factors and nitrogen fertilizer as a quantitative treatment factor. Overall, there were 45 treatments with three replicates in complete replicate blocks. The fertilizer treatments were applied to main plots, the management practices to split-plots and the varieties to split-split-plots.

1.1 Section 1

Section 1 examines treatment effects by fitting qualitative factorial models and the first analysis calculates a full analysis of variance (Table 1) for main plots (nitrogen), split-plots (management) and split-split-plots (variety). Each type of experimental unit (or "stratum") requires a separate error term in the fitted analysis.

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```
library(agriTutorial)
library(magrittr)
library(tidyverse)
library(lmerTest)
library(nlme)
library(emmeans)
library(ggfortify)
library(broom)
library(broom.mixed)
library(kableExtra)
options(contrasts = c('contr.treatment', 'contr.poly'))
```

```
fm1.1 <- aov(yield ~ Replicate + nitrogen * management * variety +
               Error(Replicate/nitrogen/management), rice)

fm1.1.Summary <- broom::tidy(fm1.1)
```

Table 1: *ANOVA Table*

stratum	*term*	*df*	*sumsq*	*meansq*	*statistic*	*p.value*
Replicate	Replicate	2	0.732	0.366		
Replicate:nitrogen	nitrogen	4	61.641	15.410	27.695	0.000
Replicate:nitrogen	Residuals	8	4.451	0.556		
Replicate:nitrogen:management	management	2	42.936	21.468	81.996	0.000
Replicate:nitrogen:management	nitrogen:management	8	1.103	0.138	0.527	0.823
Replicate:nitrogen:management	Residuals	20	5.236	0.262		
Within	variety	2	206.013	103.007	207.867	0.000
Within	nitrogen:variety	8	14.145	1.768	3.568	0.002
Within	management:variety	4	3.852	0.963	1.943	0.115
Within	nitrogen:management:variety	16	3.699	0.231	0.467	0.954
Within	Residuals	60	29.732	0.496		

The second analysis (Table 2 [1]) uses a REML mixed model analysis to find treatment means and SE's for each marginal treatment classification averaged over all the other treatment factors, together with estimates of pairwise contrasts of treatment means and the SE's of the pairwise treatment comparisons. This analysis fits the full set of nitrogen-by-variety interaction effects assuming additive management effects and the fit of the model is tested by a graphical plot of the model residuals. Residual plots provide an important check on model assumptions but many more options for model testing are available and further methods for diagnostic testing are examined in the subsequent examples.

```
fm1.2 <- lmer(yield ~ Replicate + management + nitrogen * variety +
                (1|Replicate:Main) + (1|Replicate:Main:Sub), data = rice)
fm1.2.ANOVA <- anova(fm1.2, ddf = "Kenward-Roger", type = 1)
```

```
fm1.3 <- lmer(yield ~ Replicate + nitrogen + management + variety + nitrogen:variety +
                (1|Replicate:Main) + (1|Replicate:Main:Sub), data = rice)
fm1.3.ANOVA <- anova(fm1.3, ddf = "Kenward-Roger", type = 1)

emmeans::emmeans(fm1.3, ~ nitrogen)
```

[1] Thanks to Mehrshad Barary (mehrshad.barary@dpi.nsw.gov.au) for pointing out some problems in the original vignette.

Table 2: *Mixed Model ANOVA*

	Sum Sq	***Mean Sq***	***NumDF***	***DenDF***	***F value***	***Pr(>F)***
Replicate	0.531	0.266	2	8	0.658	0.544
management	42.936	21.468	2	28	53.150	0.000
nitrogen	44.746	11.186	4	8	27.695	0.000
variety	206.013	103.007	2	80	255.021	0.000
nitrogen:variety	14.145	1.768	8	80	4.377	0.000

```
 nitrogen emmean    SE df lower.CL upper.CL
 0          5.38 0.144  8     5.05     5.72
 50         6.22 0.144  8     5.89     6.55
 80         7.00 0.144  8     6.66     7.33
 110        6.94 0.144  8     6.61     7.27
 140        7.23 0.144  8     6.90     7.56

Results are averaged over the levels of: Replicate, management, variety
Degrees-of-freedom method: kenward-roger
Confidence level used: 0.95

emmeans::emmeans(fm1.3, ~ variety)

 variety emmean    SE   df lower.CL upper.CL
 V1         5.13 0.101 39.7     4.92     5.33
 V2         6.40 0.101 39.7     6.19     6.60
 V3         8.14 0.101 39.7     7.94     8.34

Results are averaged over the levels of: Replicate, nitrogen, management
Degrees-of-freedom method: kenward-roger
Confidence level used: 0.95

emmeans::emmeans(fm1.3, ~ nitrogen * variety)

 nitrogen variety emmean    SE   df lower.CL upper.CL
 0        V1        4.51 0.225 39.7     4.06     4.97
 50       V1        4.76 0.225 39.7     4.31     5.22
 80       V1        5.83 0.225 39.7     5.38     6.29
 110      V1        5.44 0.225 39.7     4.99     5.90
 140      V1        5.08 0.225 39.7     4.62     5.53
 0        V2        5.16 0.225 39.7     4.71     5.62
 50       V2        6.02 0.225 39.7     5.56     6.47
 80       V2        6.59 0.225 39.7     6.13     7.04
 110      V2        6.92 0.225 39.7     6.47     7.38
 140      V2        7.29 0.225 39.7     6.83     7.74
 0        V3        6.48 0.225 39.7     6.02     6.93
 50       V3        7.88 0.225 39.7     7.43     8.34
 80       V3        8.56 0.225 39.7     8.11     9.02
 110      V3        8.44 0.225 39.7     7.99     8.90
 140      V3        9.34 0.225 39.7     8.88     9.79

Results are averaged over the levels of: Replicate, management
Degrees-of-freedom method: kenward-roger
Confidence level used: 0.95
```

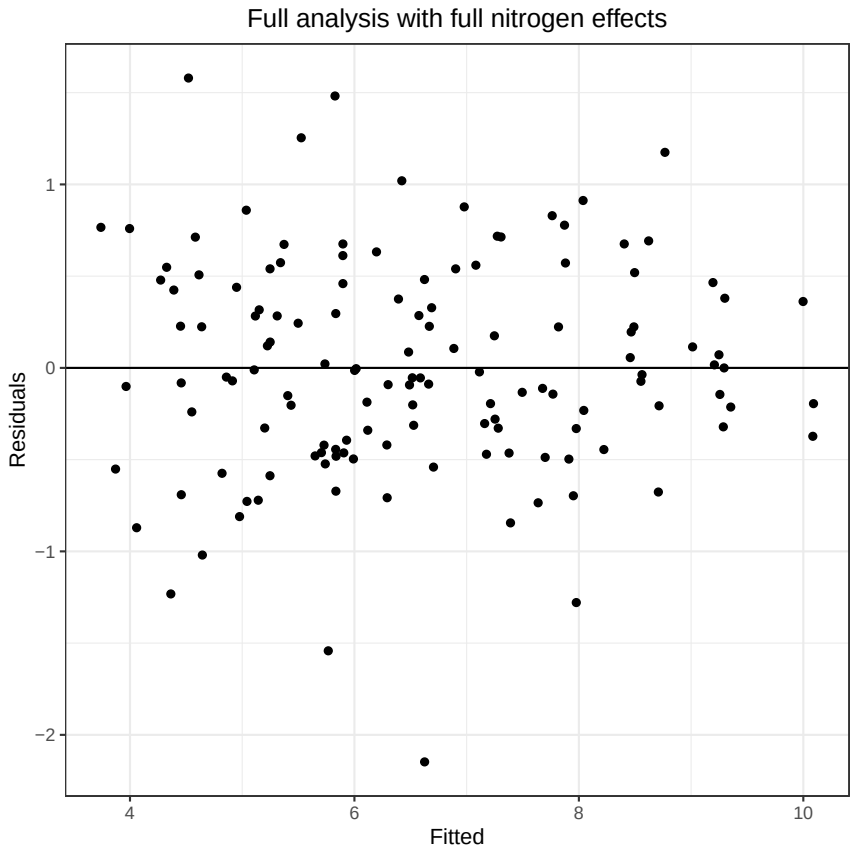
```
emmeans::contrast(
        emmeans::emmeans(fm1.3, ~ nitrogen|variety)
      , alpha = 0.05
      , method = "pairwise"
      )
```

```
variety = V1:
 contrast  estimate    SE   df t.ratio p.value
 0 - 50      -0.251 0.318 39.7 -0.788  0.9326
 0 - 80      -1.322 0.318 39.7 -4.158  0.0015
 0 - 110     -0.932 0.318 39.7 -2.930  0.0420
 0 - 140     -0.565 0.318 39.7 -1.776  0.4012
 50 - 80     -1.071 0.318 39.7 -3.370  0.0138
 50 - 110    -0.681 0.318 39.7 -2.142  0.2230
 50 - 140    -0.314 0.318 39.7 -0.988  0.8591
 80 - 110     0.390 0.318 39.7  1.228  0.7356
 80 - 140     0.757 0.318 39.7  2.382  0.1416
 110 - 140    0.367 0.318 39.7  1.154  0.7768

variety = V2:
 contrast  estimate    SE   df t.ratio p.value
 0 - 50      -0.853 0.318 39.7 -2.684  0.0744
 0 - 80      -1.426 0.318 39.7 -4.485  0.0006
 0 - 110     -1.762 0.318 39.7 -5.542  <.0001
 0 - 140     -2.126 0.318 39.7 -6.686  <.0001
 50 - 80     -0.572 0.318 39.7 -1.800  0.3877
 50 - 110    -0.908 0.318 39.7 -2.857  0.0500
 50 - 140    -1.272 0.318 39.7 -4.002  0.0023
 80 - 110    -0.336 0.318 39.7 -1.057  0.8270
 80 - 140    -0.700 0.318 39.7 -2.202  0.2002
 110 - 140   -0.364 0.318 39.7 -1.145  0.7819

variety = V3:
 contrast  estimate    SE   df t.ratio p.value
 0 - 50      -1.403 0.318 39.7 -4.413  0.0007
 0 - 80      -2.086 0.318 39.7 -6.561  <.0001
 0 - 110     -1.965 0.318 39.7 -6.181  <.0001
 0 - 140     -2.857 0.318 39.7 -8.989  <.0001
 50 - 80     -0.683 0.318 39.7 -2.147  0.2209
 50 - 110    -0.562 0.318 39.7 -1.767  0.4064
 50 - 140    -1.454 0.318 39.7 -4.575  0.0004
 80 - 110     0.121 0.318 39.7  0.380  0.9954
 80 - 140    -0.772 0.318 39.7 -2.428  0.1290
 110 - 140   -0.893 0.318 39.7 -2.808  0.0561

Results are averaged over the levels of: Replicate, management
Degrees-of-freedom method: kenward-roger
P value adjustment: tukey method for comparing a family of 5 estimates
```

```
emmeans::contrast(
    emmeans::emmeans(fm1.3, ~ variety|nitrogen)
  , alpha = 0.05
  , method = "pairwise"
)
```

```
nitrogen = 0:
 contrast estimate  SE df t.ratio p.value
 V1 - V2    -0.650 0.3 80  -2.169 0.0828
 V1 - V3    -1.965 0.3 80  -6.559 <.0001
 V2 - V3    -1.315 0.3 80  -4.390 0.0001

nitrogen = 50:
 contrast estimate  SE df t.ratio p.value
 V1 - V2    -1.253 0.3 80  -4.181 0.0002
 V1 - V3    -3.117 0.3 80 -10.405 <.0001
 V2 - V3    -1.865 0.3 80  -6.225 <.0001

nitrogen = 80:
 contrast estimate  SE df t.ratio p.value
 V1 - V2    -0.754 0.3 80  -2.516 0.0366
 V1 - V3    -2.729 0.3 80  -9.109 <.0001
 V2 - V3    -1.975 0.3 80  -6.593 <.0001

nitrogen = 110:
 contrast estimate  SE df t.ratio p.value
 V1 - V2    -1.480 0.3 80  -4.940 <.0001
 V1 - V3    -2.998 0.3 80 -10.007 <.0001
 V2 - V3    -1.518 0.3 80  -5.068 <.0001

nitrogen = 140:
 contrast estimate  SE df t.ratio p.value
 V1 - V2    -2.211 0.3 80  -7.379 <.0001
 V1 - V3    -4.258 0.3 80 -14.212 <.0001
 V2 - V3    -2.047 0.3 80  -6.833 <.0001

Results are averaged over the levels of: Replicate, management
Degrees-of-freedom method: kenward-roger
P value adjustment: tukey method for comparing a family of 3 estimates
```

```
fm1.3.Augment <- broom.mixed::augment(fm1.3)

ggplot(data = fm1.3.Augment, mapping = aes(x = .fitted, y = .resid)) +
  geom_point() +
  geom_hline(yintercept = 0) +
  labs(
      x = "Fitted"
    , y = "Residuals"
    , title = "Full analysis with full nitrogen effects") +
  theme_bw() +
  theme(plot.title = element_text(hjust = 0.5))
```



The third analysis (Table 3) shows a mixed model analysis of the full factorial model fitted by REML using the lmer function of the lme4 package. Generally with mixed models, determination of the denominator degrees of freedom for Wald-type F- and t-statistics becomes an issue, and here we use the method proposed by Kenward and Roger (1997).

```
fm1.4 <- lmer(yield ~ Replicate + nitrogen * management * variety + (1|Replicate:Main) +
                (1|Replicate:Main:Sub), data = rice)
fm1.4.ANOVA <- anova(fm1.4, ddf = "Kenward-Roger", type = 1)
```

Table 3: *Mixed Model ANOVA*

	Sum Sq	***Mean Sq***	***NumDF***	***DenDF***	***F value***	***Pr(>F)***
Replicate	0.575	0.288	2	8	0.658	0.544
nitrogen	48.424	12.106	4	8	27.695	0.000
management	42.936	21.468	2	20	49.114	0.000
variety	206.013	103.007	2	60	235.653	0.000
nitrogen:management	1.103	0.138	8	20	0.315	0.951
nitrogen:variety	14.145	1.768	8	60	4.045	0.001
management:variety	3.852	0.963	4	60	2.203	0.079
nitrogen:management:variety	3.699	0.231	16	60	0.529	0.921

1.2 Section 2

Section 2 examines treatment effects by fitting polynomial models and the first step calculates a full set of four raw polynomials for the 5-levels of N.

```
fm1.5 <- lmer(yield ~ Replicate + management + variety * (nrate + I(nrate^2) +
           I(nrate^3) + I(nrate^4)) +
          (1|Replicate:Main) + (1|Replicate:Main:Sub), data = rice)
fm1.5.ANOVA <- anova(fm1.5, ddf = "Kenward-Roger", type = 1)
```

Table 4: *Mixed Model ANOVA*

	Sum Sq	***Mean Sq***	***NumDF***	***DenDF***	***F value***	***Pr(>F)***
Replicate	0.531	0.266	2	8	0.658	0.544
management	42.936	21.468	2	28	53.150	0.000
variety	206.013	103.007	2	80	255.021	0.000
nrate	40.624	40.624	1	8	100.575	0.000
I(nrate^2)	2.490	2.490	1	8	6.164	0.038
I(nrate^3)	0.038	0.038	1	8	0.094	0.767
I(nrate^4)	1.594	1.594	1	8	3.947	0.082
variety:nrate	9.861	4.930	2	80	12.206	0.000
variety:I(nrate^2)	0.804	0.402	2	80	0.995	0.374
variety:I(nrate^3)	2.783	1.392	2	80	3.446	0.037
variety:I(nrate^4)	0.696	0.348	2	80	0.862	0.426

The second step fits a mixed model polynomial analysis of nitrogen effects assuming additive management effects (Table 7). In this analysis, most of the nitrogen treatment effect can be explained by linear and quadratic trend effects. but it is important to note that there is a non-negligible Variety x Cubic N interaction effect. This suggests that not all the varieties responded in a similar way to the N treatments and that some further analysis of the data may be required (see also the N plots of individual varieties and replicates in Fig 1).

```
fm1.6 <- lmer(yield ~ Replicate + management + variety * nrate + I(nrate^2) +
                (1|Replicate:Main) + (1|Replicate:Main:Sub), data = rice)

fm1.6.Coef <- summary(fm1.6, ddf = "Kenward-Roger")$coef
```

Table 5: *Model Coefficients*

	Estimate	***Std. Error***	***df***	***t value***	***Pr(>|t|)***
(Intercept)	3.839	0.248	31.463	15.488	0.000
ReplicateR2	0.118	0.173	10.000	0.683	0.510
ReplicateR3	-0.059	0.173	10.000	-0.343	0.739
managementOptimum	0.586	0.137	28.000	4.286	0.000
managementIntensive	1.376	0.137	28.000	10.071	0.000
varietyV2	0.537	0.254	86.000	2.113	0.038
varietyV3	2.009	0.254	86.000	7.897	0.000
nrate	0.016	0.005	12.376	3.157	0.008
I(nrate^2)	0.000	0.000	10.000	-2.263	0.047
varietyV2:nrate	0.010	0.003	86.000	3.412	0.001
varietyV3:nrate	0.013	0.003	86.000	4.684	0.000

The third step fits the required model for the actual fitted model coefficients (Table 8). When estimating model effects, only effects that are significant for the fitted model or that are marginal to those effects

(functional marginality) should be included in the model therefore only linear and quadratic nitrogen effects are included in this model. The fitted model for the nitrogen effects fits the actual nitrogen levels used in the experiment therefore this model provides the required coefficients for the actual applied nitrogen levels.

```
# fm1.6.Coef[ ,1, drop = FALSE]

# Intercepts
fm1.6.Coef[1, 1] + sum(fm1.6.Coef[2:3, 1])/3 + sum(fm1.6.Coef[4:5, 1])/3

[1] 4.512349

fm1.6.Coef[1, 1] + sum(fm1.6.Coef[2:3, 1])/3 + sum(fm1.6.Coef[4:5, 1])/3 +
  fm1.6.Coef[6, 1]

[1] 5.049778

fm1.6.Coef[1, 1] + sum(fm1.6.Coef[2:3, 1])/3 + sum(fm1.6.Coef[4:5, 1])/3 +
  fm1.6.Coef[7, 1]

[1] 6.52096

# Linear Slopes
fm1.6.Coef[8, 1]

[1] 0.01612922

fm1.6.Coef[8, 1] +  fm1.6.Coef[10, 1]

[1] 0.02575925

fm1.6.Coef[8, 1] +  fm1.6.Coef[11, 1]

[1] 0.02935101

# Quadratic Slopes
fm1.6.Coef[9, 1]

[1] -7.528912e-05
```

1.3 Section 3

Section 3 provides checks on some of the assumptions underlying the blocks-by-treatments model.

The first analysis in this section shows a complete partition of the blocks-by-treatments interaction effects into factorial mean square terms where all the terms that contain a replicate:variety interaction effect are estimates of the split-split-plot error variance. If the blocks-by-treatments assumptions are valid, all the estimates of the split-split-plot error variance are expected to have the same error mean square. However, the Replicate:variety effect has a mean square of 1.54 on 4 degrees of freedom whereas the Replicate:management:variety:nitrogen effect has a mean square of 0.26 on 32 degrees of freedom. The ratio of these mean squares is 5.92 with an F-probability of 0.00110 on 4 and 32 degrees of freedom, which means that the Replicate:variety interaction effect is significantly inflated relative to the Replicate:management:variety:nitrogen effect. This shows that the assumptions underlying the blocks-by-treatments analysis of the model are invalid with a high level of probability.

The 4 degrees of freedom in the Replicate:variety interaction effect are the differences between the three varieties differenced between the three replicate blocks. Fig S1 shows graphical plots of variety effects in

each replicate block averaged over management effects, and there is clear evidence that the effects of Variety 1 in blocks 1 and 2 were different from the effects of Variety 1 in block 3.

The second analysis in Section 3 shows a complete partition of the blocks-by-treatments interaction effects into factorial mean square terms ignoring Variety 1. This analysis shows a reasonably good fit to the assumed additive block which supports the hypothesis that the non-additivity of the block-and-treatment effects in the full unrestricted analysis is mainly due to Variety 1.

```
fm1.7 <- aov(yield ~ Replicate*management * variety * nitrogen, rice)
fm1.7.Summary <- broom::tidy(fm1.7)
```

Table 6: *ANOVA*

term	*df*	*sumsq*	*meansq*
Replicate	2	0.732	0.4
management	2	42.936	21.5
variety	2	206.013	103.0
nitrogen	4	61.641	15.4
Replicate:management	4	0.460	0.1
Replicate:variety	4	6.153	1.5
management:variety	4	3.852	1.0
Replicate:nitrogen	8	4.451	0.6
management:nitrogen	8	1.103	0.1
variety:nitrogen	8	14.145	1.8
Replicate:management:variety	8	2.221	0.3
Replicate:management:nitrogen	16	4.777	0.3
Replicate:variety:nitrogen	16	13.125	0.8
management:variety:nitrogen	16	3.699	0.2
Replicate:management:variety:nitrogen	32	8.233	0.3

```
Rice1 <-
  rice %>%
  dplyr::group_by(Replicate, nitrogen, variety) %>%
  dplyr::summarise(Yield = mean(yield, na.rm = TRUE))

WideRice1 <-
  Rice1 %>%
  tidyr::spread(key = nitrogen, value = Yield) %>%
  dplyr::ungroup() %>%
  dplyr::select(-Replicate, -variety)
```

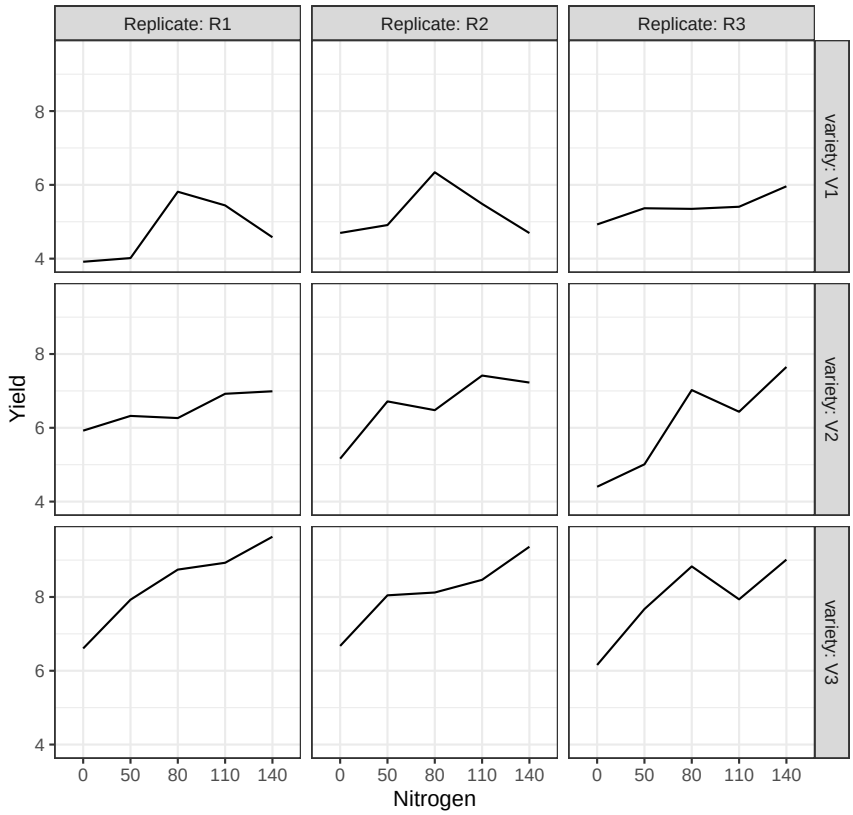
Table 7: *Means Data*

Replicate	*nitrogen*	*variety*	*Yield*
R1	0	V1	3.9
R1	0	V2	5.9
R1	0	V3	6.6
R1	50	V1	4.0
R1	50	V2	6.3
R1	50	V3	7.9

R1	80	V1	5.8
R1	80	V2	6.3
R1	80	V3	8.7
R1	110	V1	5.4
R1	110	V2	6.9
R1	110	V3	8.9
R1	140	V1	4.6
R1	140	V2	7.0
R1	140	V3	9.6
R2	0	V1	4.7
R2	0	V2	5.2
R2	0	V3	6.7
R2	50	V1	4.9
R2	50	V2	6.7
R2	50	V3	8.0
R2	80	V1	6.3
R2	80	V2	6.5
R2	80	V3	8.1
R2	110	V1	5.5
R2	110	V2	7.4
R2	110	V3	8.5
R2	140	V1	4.7
R2	140	V2	7.2
R2	140	V3	9.4
R3	0	V1	4.9
R3	0	V2	4.4
R3	0	V3	6.2
R3	50	V1	5.4
R3	50	V2	5.0
R3	50	V3	7.7
R3	80	V1	5.3
R3	80	V2	7.0
R3	80	V3	8.8
R3	110	V1	5.4
R3	110	V2	6.4
R3	110	V3	7.9
R3	140	V1	6.0
R3	140	V2	7.6
R3	140	V3	9.0

```
ggplot(data = Rice1, mapping = aes(x = nitrogen, y = Yield,  group = Replicate)) +
  geom_line() +
  facet_grid(variety ~ Replicate, labeller = label_both) +
  labs(
        x = "Nitrogen"
      , y = "Yield"
      , title = "Fig S1. Variety response to nitrogen for individual replicate blocks"
      ) +
  theme_bw() +
  theme(plot.title = element_text(hjust = 0.5))
```

Fig S1. Variety response to nitrogen for individual replicate blocks



The final analysis in Section 3 shows an analysis of variance of the treatment effects ignoring Variety 1. In this analysis, the management:variety interaction effect becomes significant at the 0.00992 probability level compared with a non-significant management:variety interaction effect in the analysis of the full data set.

Such anomalies are not uncommon in the analysis of real data sets and it is the task of the statistician to identify anomalies as and when they occur. Factorial designs can be very powerful for practical research but, as demonstrated with this data set, the analysis of such designs is complex and anomalies can be easily missed. Unless an anomaly is due to an easily identified cause such as an incorrectly recorded data point, it is likely that the anomaly will need to be investigated by further discussion with the research workers. It is a mistake to suppose that data from a designed experiment can be analysed statistically in isolation from the research workers who conducted the experiment.

```
riceV2V3 <-
  rice %>%
  dplyr::filter(variety != "V1") %>%
  droplevels()

fm1.8 <- aov(yield ~ Replicate*management * variety * nitrogen, riceV2V3)
fm1.8.ANOVA <- broom::tidy(fm1.8)
```

```
fm1.9 <- aov(yield ~ Replicate + management * variety * nitrogen +
               Error(Replicate/Main/Sub), riceV2V3)
fm1.9.ANOVA <- broom::tidy(fm1.9)
```

Table 8: *ANOVA Table*

term	*df*	*sumsq*	*meansq*
Replicate	2	2.995	1.5
management	2	26.136	13.1
variety	1	68.447	68.4
nitrogen	4	63.989	16.0
Replicate:management	4	0.868	0.2
Replicate:variety	2	0.518	0.3
management:variety	2	3.682	1.8
Replicate:nitrogen	8	6.975	0.9
management:nitrogen	8	0.842	0.1
variety:nitrogen	4	1.776	0.4
Replicate:management:variety	4	1.243	0.3
Replicate:management:nitrogen	16	5.288	0.3
Replicate:variety:nitrogen	8	4.435	0.6
management:variety:nitrogen	8	3.219	0.4
Replicate:management:variety:nitrogen	16	4.030	0.3

Table 9: *ANOVA Table*

stratum	*term*	*df*	*sumsq*	*meansq*	*statistic*	*p.value*
Replicate	Replicate	2	2.995	1.498		
Replicate:Main	nitrogen	4	63.989	15.997	18.348	0.0
Replicate:Main	Residuals	8	6.975	0.872		
Replicate:Main:Sub	management	2	26.136	13.068	42.456	0.0
Replicate:Main:Sub	management:nitrogen	8	0.842	0.105	0.342	0.9
Replicate:Main:Sub	Residuals	20	6.156	0.308		
Within	variety	1	68.447	68.447	200.819	0.0
Within	management:variety	2	3.682	1.841	5.401	0.0
Within	variety:nitrogen	4	1.776	0.444	1.303	0.3
Within	management:variety:nitrogen	8	3.219	0.402	1.181	0.3
Within	Residuals	30	10.225	0.341		

2 Example 2: Lack-of-fit and marginality for a single quantitative treatment factor

Petersen (1994, p. 125) describes an experiment conducted to assess the effects of five different quantities of N-fertiliser (0, 35, 70, 105 and 140 kg N/ha) on root dry matter yield of sugar beet (t/ha) with three complete replications laid out in three randomized complete blocks. One objective of this experiment was to determine the amount of fertilizer for maximizing yield.

The first stage fits a full polynomial analysis of variance based on polynomial contrasts which are fitted in sequence from the lowest to the highest. This is equivalent to the analysis shown in Tables 4 and 5 of Piepho and Edmondson (2018) except that a complete partition into single degree of freedom polynomial contrasts is shown here compared with the pooled 'lack of fit' term shown in Tables 4 and 5.

```
fm2.1 <- lm(yield ~ Replicate + nrate + I(nrate^2) + I(nrate^3) + I(nrate^4), data = beet)
fm2.1.ANOVA <- anova(fm2.1)
```

Table 10: *ANOVA Table*

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(>F)*
Replicate	2	26.321	13.161	3.712	0.072
nrate	1	651.468	651.468	183.736	0.000
I(nrate^2)	1	260.504	260.504	73.471	0.000
I(nrate^3)	1	1.587	1.587	0.448	0.522
I(nrate^4)	1	0.004	0.004	0.001	0.974
Residuals	8	28.365	3.546		

The second stage fits a quadratic regression model with linear and quadratic terms only. This model provides the model coefficients, standard errors and the confidence intervals shown in Table 6 of Piepho and Edmondson (2018). A set of diagnostic plots are fitted for the fitted quadratic regression model to check the validity of the model assumptions.

```
fm2.2 <- lm(yield ~ Replicate + nrate + I(nrate^2), data = beet)
fm2.2.Coef <- summary(fm2.2)$coef
```

Table 11: *Model Coefficients*

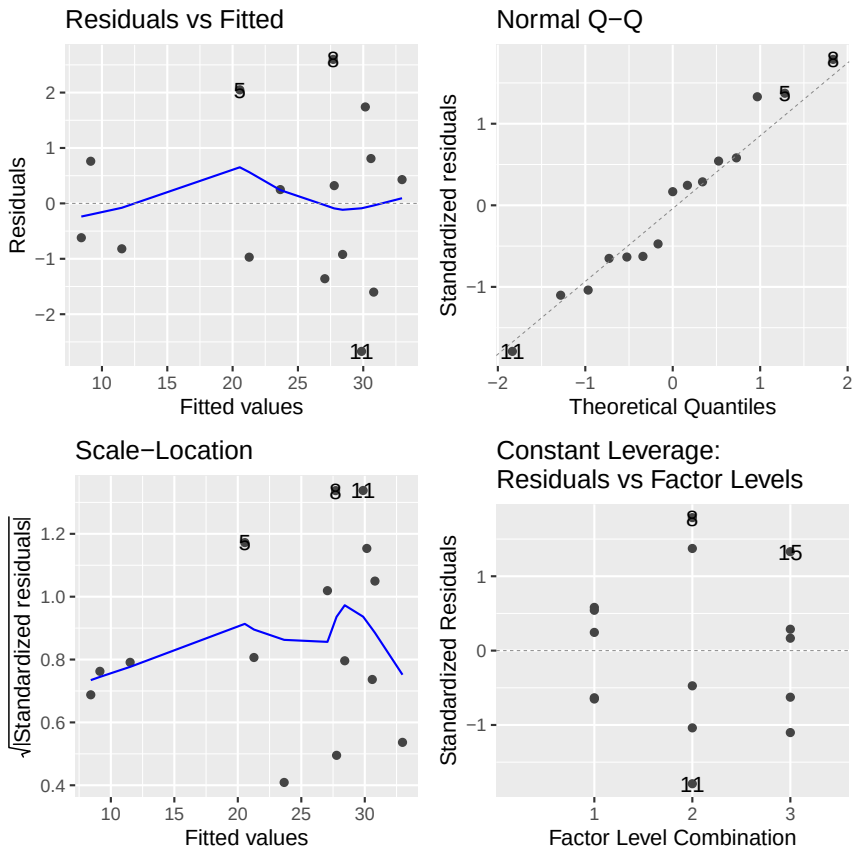
	Estimate	*Std. Error*	*t value*	*Pr(>|t|)*
(Intercept)	9.1	1.133	8.066	0.000
Replicate2	-0.7	1.095	-0.658	0.526
Replicate3	2.4	1.095	2.174	0.055
nrate	0.4	0.032	13.125	0.000
I(nrate^2)	0.0	0.000	-9.325	0.000

```
fm2.2.Coef[1, 1] + sum(fm2.2.Coef[2:3, 1])/3

[1] 9.692381

fm2.2.Coef[4, 1]

[1] 0.4177687
```

```
fm2.2.Coef[5, 1]

[1] -0.002033042

confint(fm2.2, level = 0.95)

                   2.5 %       97.5 %
(Intercept)  6.614421038 11.663674200
Replicate2  -3.159020996  1.719020996
Replicate3  -0.059020996  4.819020996
nrate        0.346848911  0.488688503
I(nrate^2)  -0.002518805 -0.001547278
```

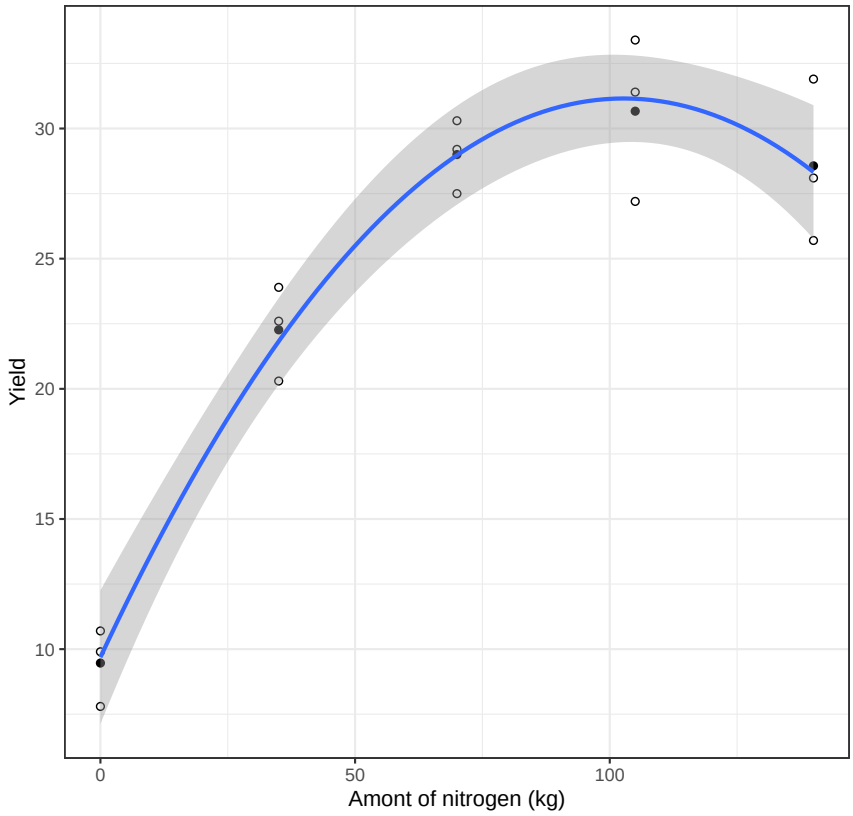
Finally, a smoothed quadratic graph of the yield versus the N rate is plotted to show the goodness of fit of the quadratic regression model. This plot corresponds to plot Fig 3 in Piepho and Edmondson (2018).

```
ggplot2::autoplot(fm2.2)
```




```
ggplot(data = beet, mapping = aes(x = nrate, y = yield)) +
  geom_point(shape = 1) +
  stat_summary(fun.y = mean, geom = "point") +
  geom_smooth(method = lm, formula = y ~ poly(x, 2)) +
  labs(
        x = "Amont of nitrogen (kg)"
      ,  y = "Yield"
      , title = "Fig 3 Yield versus N for sugar beet with 95 percent confidence band"
      ) +
  theme_bw() +
  theme(plot.title = element_text(hjust = 0.5))
```

Fig 3 Yield versus N for sugar beet with 95 percent confidence band



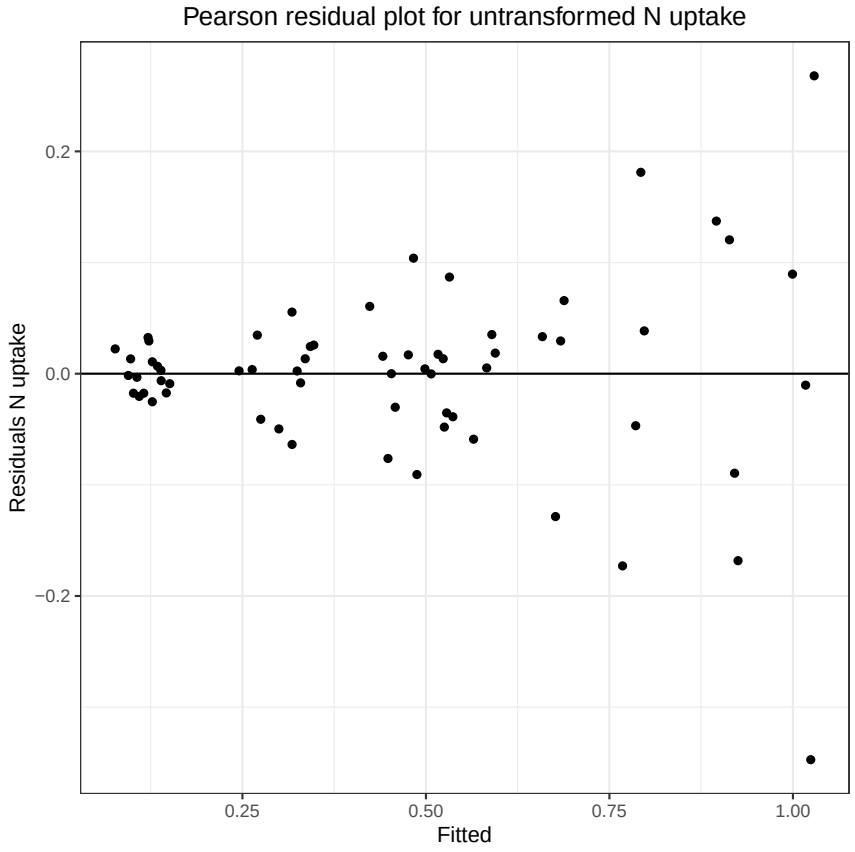
3 *Example 3: Polynomial regression model with two quantitative level treatment factors*

Gomez and Gomez (1984, p. 401) report a two-factor nitrogen uptake greenhouse experiment on rice involving duration of water stress (W) and level of nitrogen application (N) with four complete replicates of each treatment. The experiment had four water-stress levels (0, 10, 20 and 40 days) applied as main-plot treatments and four nitrogen rates (0, 90, 180 and 270 kg/ha) applied as sub-plot treatments. The four sub-plot treatments were randomized within main plots and the four main plot treatments were randomized within complete replicate blocks.

The first stage shows a Pearson residual plot of the untransformed N uptake data versus a Pearson residual plot of the log transformed N uptake data. Comparison of the two plots shows that the untransformed residuals increase as the fitted values increase whereas the log transformed N uptake residuals are approximately constant over the full range of the fitted values. This shows that a log transformation of the N uptake data gives a dependent variate with constant variance over the full range of fitted values which shows that a simple unweighted analysis of variance is valid for the effects of the treatment factors.

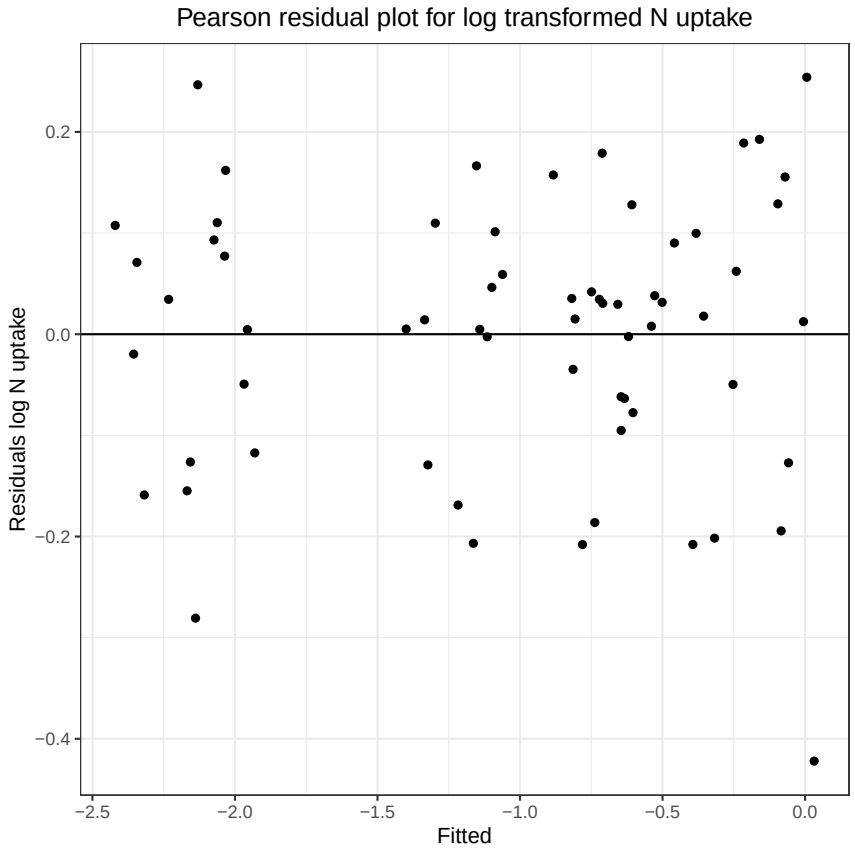
```
fm3.1 <- lmer(uptake ~ Replicate + Nitrogen * Water +
                (1|Replicate:Main), data = greenrice)
```

```
fm3.1.Augment <- broom.mixed::augment(fm3.1)

ggplot(data = fm3.1.Augment, mapping = aes(x = .fitted, y = .resid)) +
  geom_point() +
  geom_hline(yintercept = 0) +
  labs(
      x = "Fitted"
    , y = "Residuals N uptake"
    , title = "Pearson residual plot for untransformed N uptake") +
  theme_bw() +
  theme(plot.title = element_text(hjust = 0.5))
```



```
fm3.2 <- lmer(loguptake ~ Replicate + Nitrogen * Water +
                (1|Replicate:Main), data = greenrice)
```

```
fm3.2.Augment <- broom.mixed::augment(fm3.2)

ggplot(data = fm3.2.Augment, mapping = aes(x = .fitted, y = .resid)) +
  geom_point() +
  geom_hline(yintercept = 0) +
  labs(
    x = "Fitted"
    , y = "Residuals log N uptake"
    , title = "Pearson residual plot for log transformed N uptake") +
  theme_bw() +
  theme(plot.title = element_text(hjust = 0.5))
```




```
fm3.3 <- lmer(loguptake ~ N + W + Nitrogen * Water +
                (1|Replicate) + (1|Replicate:Main), data = greenrice)
fm3.3.ANOVA <- anova(fm3.3, ddf = "Kenward-Roger", type = 1)
fm3.3.Summary <- summary(fm3.3, ddf = "Kenward-Roger", type = 1)$coef
```

```
fm3.4 <- lmer(loguptake ~ N * W + I(N^2) + I(W^2) +
                Nitrogen * Water + (1|Replicate) + (1|Replicate:Main), data = greenrice)
fm3.4.Coef <-summary(fm3.4, ddf = "Kenward-Roger", type = 1)$coef
greenrice2 <- broom.mixed::augment(fm3.4)
```

Table 12: *ANOVA Table*

	Sum Sq	***Mean Sq***	***NumDF***	***DenDF***	***F value***	***Pr(>F)***
N	4.653	4.653	1	36	183.807	0
W	25.524	25.524	1	9	1008.297	0
Nitrogen	0.630	0.315	2	36	12.437	0
Water	2.739	1.370	2	9	54.105	0
Nitrogen:Water	1.318	0.146	9	36	5.786	0

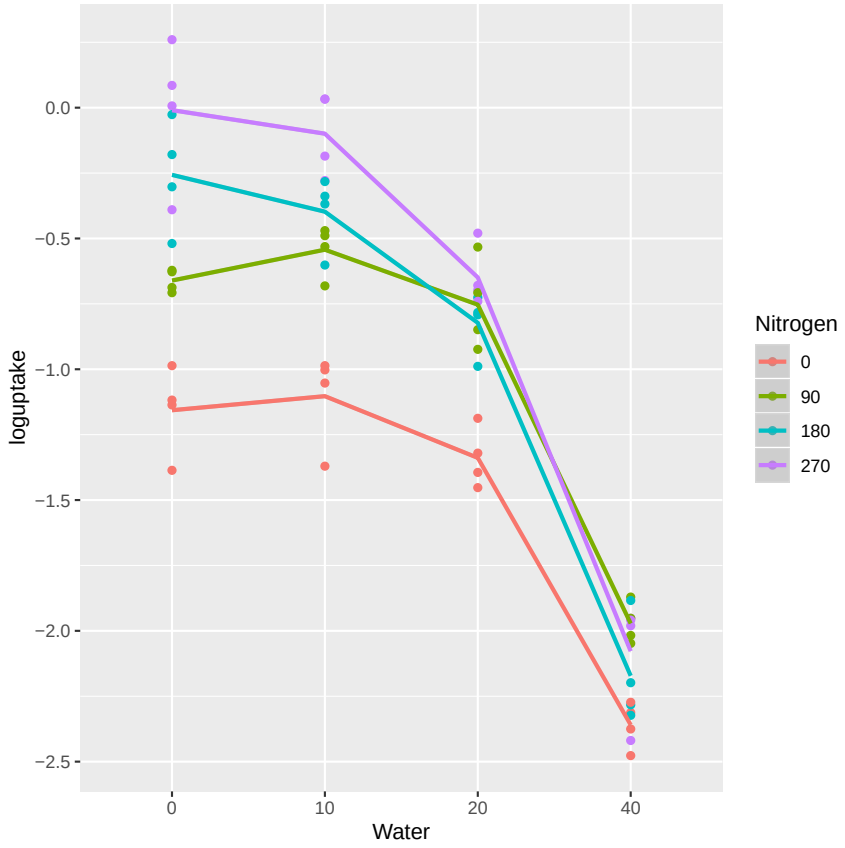
Table 13: *Model Coefficients*

	Estimate	***Std. Error***	***df***	***t value***	***Pr(>|t|)***
(Intercept)	-1.157	0.080	47.898	-14.452	0.000
N	0.004	0.000	36.000	10.197	0.000
W	-0.030	0.003	44.308	-10.691	0.000
Nitrogen90	0.113	0.099	36.000	1.143	0.261
Nitrogen180	0.135	0.099	36.000	1.361	0.182
Water10	0.354	0.101	44.308	3.495	0.001
Water20	0.419	0.097	44.308	4.304	0.000
Nitrogen90:Water10	0.064	0.159	36.000	0.404	0.689
Nitrogen180:Water10	-0.195	0.159	36.000	-1.223	0.229
Nitrogen270:Water10	-0.144	0.159	36.000	-0.903	0.372
Nitrogen90:Water20	0.090	0.159	36.000	0.564	0.576
Nitrogen180:Water20	-0.384	0.159	36.000	-2.411	0.021
Nitrogen270:Water20	-0.458	0.159	36.000	-2.876	0.007
Nitrogen90:Water40	-0.108	0.159	36.000	-0.681	0.500
Nitrogen180:Water40	-0.712	0.159	36.000	-4.477	0.000
Nitrogen270:Water40	-0.865	0.159	36.000	-5.439	0.000

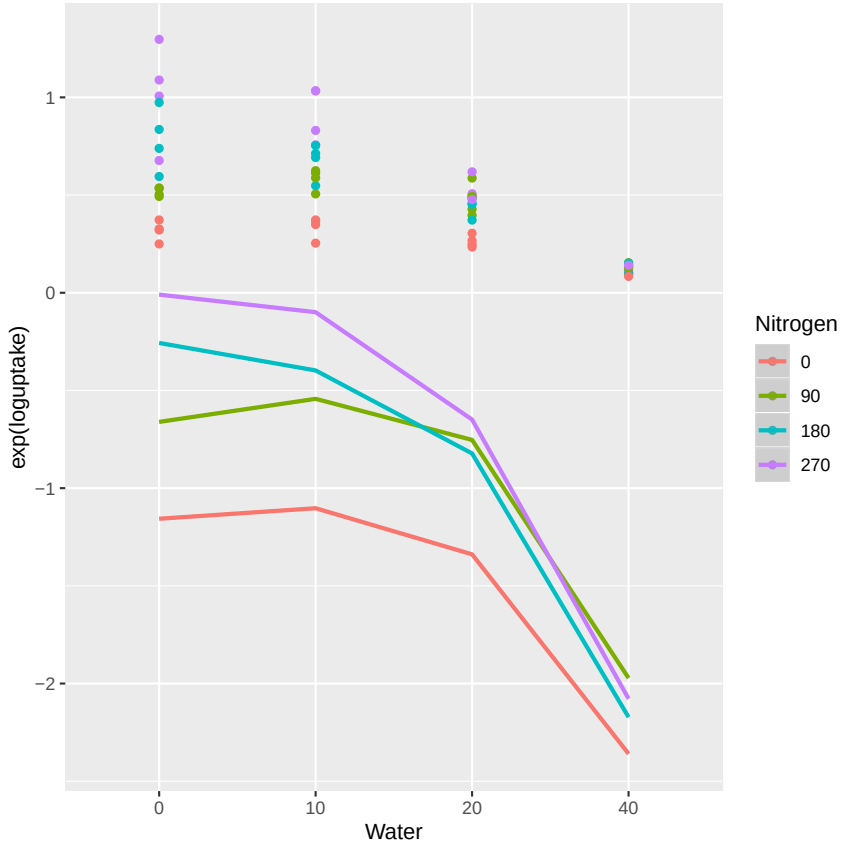
Table 14: *Model Coefficients*

	Estimate	***Std. Error***	***df***	***t value***	***Pr(>|t|)***
(Intercept)	-1.157	0.080	47.898	-14.452	0.000
N	0.006	0.002	36.000	3.995	0.000
W	0.012	0.010	44.308	1.170	0.248
I(N^2)	0.000	0.000	36.000	-1.361	0.182
I(W^2)	-0.001	0.000	44.308	-4.304	0.000
Nitrogen90	-0.022	0.119	36.000	-0.183	0.856
Water10	0.040	0.104	44.308	0.383	0.704
N:W	0.000	0.000	36.000	-5.439	0.000
Nitrogen90:Water10	0.136	0.156	36.000	0.872	0.389
Nitrogen180:Water10	-0.050	0.155	36.000	-0.325	0.747
Nitrogen270:Water10	0.073	0.143	36.000	0.507	0.615
Nitrogen90:Water20	0.234	0.155	36.000	1.514	0.139
Nitrogen180:Water20	-0.095	0.155	36.000	-0.615	0.542
Nitrogen270:Water20	-0.025	0.138	36.000	-0.181	0.858
Nitrogen90:Water40	0.180	0.140	36.000	1.284	0.207
Nitrogen180:Water40	-0.135	0.140	36.000	-0.965	0.341

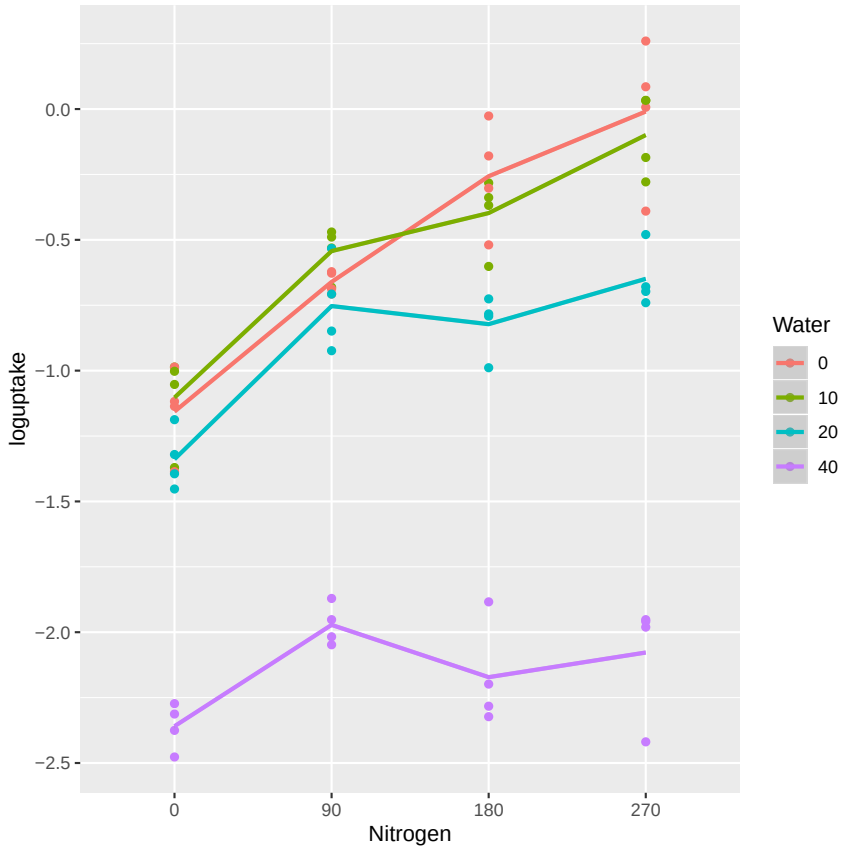
```
ggplot(
    data = greenrice2
  , mapping = aes(x = Water, y = loguptake, color = Nitrogen, group = Nitrogen)) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```



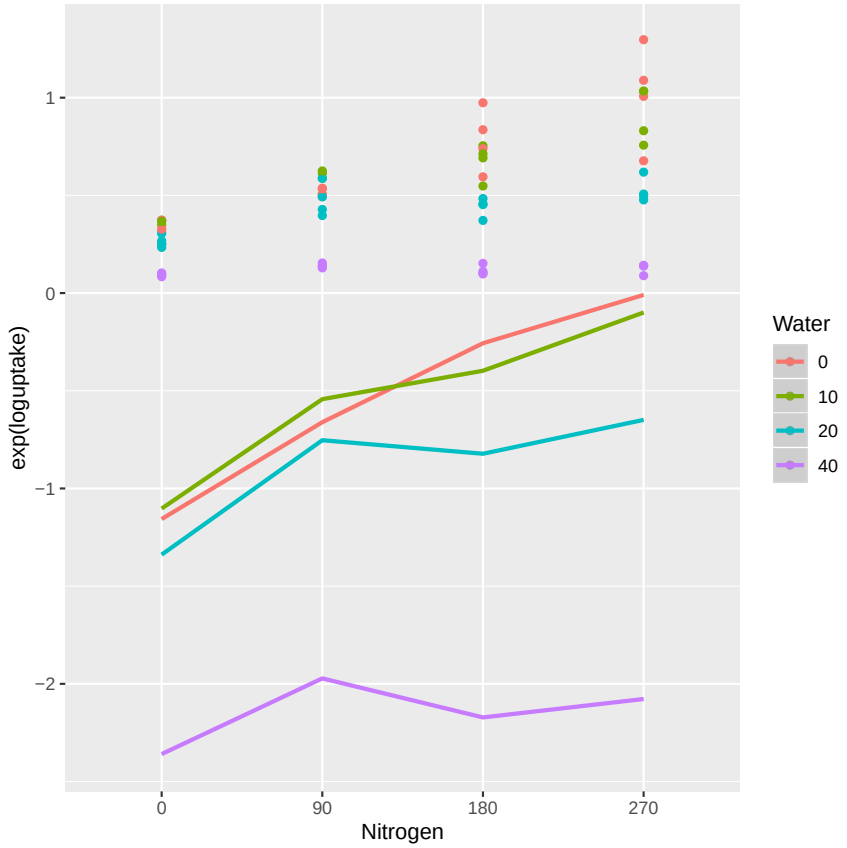

```
ggplot(
        data = greenrice2
      , mapping = aes(x = Water, y = exp(loguptake), color = Nitrogen, group = Nitrogen)) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```




```
ggplot(
        data = greenrice2
      , mapping = aes(x = Nitrogen, y = loguptake, color = Water, group = Water)) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```



```
ggplot(
       data = greenrice2
    , mapping = aes(x = Nitrogen, y = exp(loguptake), color = Water, group = Water)) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```




```
fm3.5 <- lmer(loguptake ~ N * W + I(N^2) + I(W^2) +
                (1|Replicate) + (1|Replicate:Main), data = greenrice)
fm3.5.Coef <- summary(fm3.5, ddf = "Kenward-Roger", type = 1)$coef
```

Table 15: *Model Coefficients*

	Estimate	***Std. Error***	***df***	***t value***	***Pr(>|t|)***
(Intercept)	-1.160	0.064	47.806	-18.187	0.000
N	0.007	0.001	45.000	8.731	0.000
W	0.018	0.006	12.919	3.196	0.007
I(N^2)	0.000	0.000	45.000	-3.582	0.001
I(W^2)	-0.001	0.000	10.000	-9.694	0.000
N:W	0.000	0.000	45.000	-6.365	0.000

4 Example 4: One qualitative treatment factor with repeated measurements over time

Milliken and Johnson (1992, p. 429) discuss data which they describe as repeated leaf index measurements on sorghum. Their data comprises five replicate blocks of four sorghum varieties and they assume equally spaced repeated measurements on each plot in each block on five consecutive occasions starting two weeks after emergence. No further information is given but it appears that the data is artificial rather than real. Although real data is more authentic, it can sometimes be useful to discuss the analysis of an example data set from the literature, even when the data is artificial. Milliken & Johnson discuss a multivariate analysis of variance (MANOVA) for this data but MANOVA take no account of the ordered relationship between repeated observations or the likely correlation structure of the data and here we discuss a generalized least squares (GLS) method that is specifically intended to account for the underlying structure of repeated measures data. The interested reader can, if desired, compare the GLS method of analysis with the MANOVA analysis dicussed by Milliken and Johnson (1992) in Chapter 13 of their book.

4.1 Section 1

Section 1 calculates polynomials for weeks and blocks using the poly() function. Two sets of polynomials for weeks, raw and orthogonal, are calculated and saved as sorghum$rawWeeks and sorghum$polWeeks respectively. Orthogonal polynomials for blocks are calculated and saved as sorghum$polBlocks. It is important to note that the poly() function calculates all polynomial contrasts up to the required degree but does NOT include the zero-degree polynomial. Additionally, the block variable varblock is saved as a factor factblock.

```
## independent uncorrelated random plots
fm4.1 <- nlme::gls(y ~ factweek * (Replicate + variety), sorghum)
fm4.1.ANOVA <- anova(fm4.1)
fm4.1.glance <- broom::glance(fm4.1)
fm4.1.Variogram <- nlme::Variogram(fm4.1)
```

Table 16: *ANOVA Table*

	numDF	*F-value*	*p-value*
(Intercept)	1	80947.1	0.000
factweek	4	220.9	0.000
Replicate	4	358.9	0.000
variety	3	334.9	0.000
factweek:Replicate	16	1.8	0.049
factweek:variety	12	4.5	0.000

Table 17: *Model Summary*

sigma	*df*	*logLik*	*AIC*	*BIC*	*df.residual*
0.152	40	1.869	78.261	164.129	60

4.2 Section 2

Section 2 compares five different correlation structures for the repeated measures analysis using the gls() function of the nlme package. Each analysis fits a full factorial model for the variety-by-weeks and blocks-by-weeks effects assuming block and treatment additivity. The goodness of fit of the five models is compared

by AIC statistics where the smaller the AIC the better the fit. Here, the AR(1)+nugget model fitted by the corExp() function gave the best fitting model. See help(corExp)for further information about the corExp() function. Note that corSymm represents a general correlation structure and will, presumably, give an analysis similar to a multivariate analysis of variance. Although this structure appears to give the best fit according to the negative log likelihood statistic, this criterion takes no account of the number of estimated variance parameters p in the variance model which, in the case of the corSymm model, is p = 15, compared to only p = 2 for the AR(1) model. When assessed by the AIC statistic, the corSymm model gave the least good fit of any of the non-null correlation structures which is strong evidence that the multivariate analysis of variance method discussed by Milliken and Johnson (1992) will lack power.

```
## corCompSymm compound symmetry
fm4.2 <- nlme::gls(y ~ factweek * (Replicate + variety),
                   corr = corCompSymm(form = ~ varweek|factplot), sorghum)
fm4.2.ANOVA <- anova(fm4.2)
fm4.2.glance <- broom::glance(fm4.2)
fm4.2.Variogram <- nlme::Variogram(fm4.2)
```

Table 18: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	21284.9	0
factweek	4	738.2	0
Replicate	4	94.4	0
variety	3	88.1	0
factweek:Replicate	16	6.1	0
factweek:variety	12	15.0	0

Table 19: *Model Summary*

sigma	***df***	***logLik***	***AIC***	***BIC***	***df.residual***
0.152	40	22.81	38.379	126.342	60

Table 20: *Variogram*

variog	***dist***	***n.pairs***
0.146	1	80
0.181	2	60
0.214	3	40
0.243	4	20

4.3 Section 3

Section 3 fits a full regression model over the five weeks of repeated measures and tests for possible variety and variety-by-weeks interactions effects. The weeks factor is decomposed into individual polynomial contrasts (see Table A2 and Table 14) to test the significance of each individual variety-by-weeks polynomial effect. The analysis of polynomial contrasts shows that the variety-by-weeks interaction is due mainly to the degree-1 = variety:rawWeeks[,1] and the degree-2 = variety:rawWeeks[,2] effects, although there is also some evidence of higher-degree variety-by-weeks interaction effects. The analysis also shows the corExp()

range and nugget statistics for the full fitted model and these are used to calculate the correlation coefficient usingthe formula rho=(1-nugget)*exp(-1/range). Note that this formula is different from the the formula used in Tables A1 and A2 and will give a different value of rho: see help(corExp).

```
## corExp without nugget
fm4.3 <- nlme::gls(y ~ factweek * (Replicate + variety),
                   corr = corExp(form = ~ varweek|factplot), sorghum)
fm4.3.ANOVA <- anova(fm4.3)
fm4.3.glance <- broom::glance(fm4.3)
fm4.3.Variogram <- nlme::Variogram(fm4.3)
```

Table 21: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	26108.4	0.000
factweek	4	272.5	0.000
Replicate	4	112.8	0.000
variety	3	102.2	0.000
factweek:Replicate	16	3.2	0.001
factweek:variety	12	10.3	0.000

Table 22: *Model Summary*

sigma	***df***	***logLik***	***AIC***	***BIC***	***df.residual***
0.149	40	22.978	38.045	126.007	60

Table 23: *Variogram*

variog	***dist***	***n.pairs***
0.153	1	80
0.189	2	60
0.223	3	40
0.255	4	20

4.4 Section 4

Section 4 fits a quadratic regression model for weeks assuming the degree-3 and degree-4 polynomial week effects are zero. The average effects of blocks are fitted by polBlocks and the interactions between the blocks and the weeks are fitted by polBlocks:(rawWeeks[,1] + rawWeeks[,2] + polWeeks[,3]+ polWeeks[,4]). The gls() algorithm requires the same polynomial weeks contrasts in both the blocks and the varieties models which is why raw degree-1 and degree-2 weeks contrasts have been used for the blocks-by-weeks interaction model. However, orthogonal polynomials have better numerical stability than raw polynomials so orthogonal polynomial contrasts have been used for the degree-3 and degree-4 weeks contrasts. The summary analysis shows all variety effects as differences from the intercept which, in this analysis, is variety 1 therefore all model effects in Table 15 can be derived by adding appropriate effects to the intercept. If SED's are required, these must be calculated from the variance/covariance matrix which can be extracted by the code vcov(). Using this matrix, the SED for variety differences was calculated to be 0.172, the SED

for the variety-by-linear weeks slope parameters was calculated to be 0.117 and the SED for the variety-by-quadratic weeks slope parameters was calculated to be 0.0192. These estimates are approximately 2-3 percent larger than those shown in Table 15 but it is not clear if the discrepancies are due to the model specification or to a difference between the R and the SAS software. Possibly the implementation of the Kenward-Roger method of adjusting the denominator d.f. and the estimated variance-covariance matrix of the estimated fixed effects might be different for the two algorithms. The range, nugget and correlation coefficient are extracted and displayed and a graphical plot of the studentized residuals from the quadratic regression model is also shown.

```
##  corExp with nugget
fm4.4 <- nlme::gls(y ~ factweek * (Replicate + variety),
                   corr = corExp(form = ~ varweek|factplot, nugget = TRUE), sorghum)
fm4.4.ANOVA <- anova(fm4.4)
fm4.4.glance <- broom::glance(fm4.4)
fm4.4.Variogram <- nlme::Variogram(fm4.4)
```

Table 24: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	22278.1	0
factweek	4	447.1	0
Replicate	4	97.7	0
variety	3	88.7	0
factweek:Replicate	16	4.2	0
factweek:variety	12	12.6	0

Table 25: *Model Summary*

sigma	***df***	***logLik***	***AIC***	***BIC***	***df.residual***
0.15	40	24.26	37.479	127.536	60

Table 26: *Variogram*

variog	***dist***	***n.pairs***
0.150	1	80
0.186	2	60
0.220	3	40
0.251	4	20

4.5 Section 5

Section 5 fits a quadratic regression model for the variety-by-week interaction effects assuming a full degree-4 model for both the weeks regression model and for the blocks-by-weeks interaction model. The quadratic regression model in Section 4 corresponds to the regression model used for Tables 14 and 15 of Piepho and Edmondson (2018) but the range = 3397131013 and nugget = 0.4605535 of this model are very different from the range = 10.35774 and nugget = 0.1720444 of the full factorial model. For robust smoothed prediction, the treatments model must be as parsimonious as possible and a degree-2 regression model for the variety-by-weeks effects seems reasonable, even though there is some evidence (Table 14

and Table A2) of significant higher-degree variety-by-weeks interaction effects. However, as shown in the analysis in Section 4, there is quite strong evidence of degree-3 and degree-4 polynomial weeks effects therefore the assumption of a degree-2 regression model for weeks is problematic. In this section, we fit a more general model that assumes a quadratic regression model for weeks-by-varieties effects and a full degree-4 regression model for weeks and weeks-by-blocks effects. With this model, the values of the auto-correlation parameters are: range = 42.75763, nugget = 0.3586337 and correlation = 0.6265403 which are much closer to the autocorrelation parameters from the full factorial model than are those from Section 4. As this model fits a full degree-4 polynomial model both for weeks and for block-by-weeks effects, it is not necessary to use polynomial blocks contrasts and instead we fit the replcate block effects by using the Replicate blocks factor.

```
##  corSymm unstructured
fm4.5 <- nlme::gls(y ~ factweek * (Replicate + variety),
                   corr = corSymm(form = ~ 1|factplot),
                   weights = varIdent(form = ~ 1|varweek), sorghum)
fm4.5.ANOVA <- anova(fm4.5)
fm4.5.glance <- broom::glance(fm4.5)
fm4.5.Variogram <- nlme::Variogram(fm4.5)
```

Table 27: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	57534.1	0
factweek	4	594.2	0
Replicate	4	217.6	0
variety	3	144.7	0
factweek:Replicate	16	4.0	0
factweek:variety	12	12.2	0

Table 28: *Model Summary*

sigma	***df***	***logLik***	***AIC***	***BIC***	***df.residual***
0.141	40	31.45142	47.097	162.286	60

Table 29: *Variogram*

variog	***dist***	***n.pairs***
0.142	1	80
0.179	2	60
0.211	3	40
0.280	4	20

Comment The model fitted in Section 5 appears to be the best model available based on the generalized least squares method but it is clear from the graphical plots of studentized residuals that the fitted data contains outliers that are not well accommodated by the fitted model. If the data was from a real experiment, further information about the data might be available but as the data seems to be artificial this option is not available. In this situation, various robust methods of model fitting or regression analysis that can accommodate non-standard distributions or model outliers are available. However, these methods are beyond the scope of this tutorial and will not be discussed further here.

Table 30: Models Summary

Model	*sigma*	*df*	*logLik*	*AIC*	*BIC*	*df.residual*
ID	0.152	40	1.869	78.261	164.129	60
CS	0.152	40	22.810	38.379	126.342	60
AR(1)	0.149	40	22.978	38.045	126.007	60
AR(1) + nugget	0.149	40	22.978	38.045	126.007	60
UN	0.141	40	31.451	47.097	162.286	60

```
fm4.6 <- nlme::gls(
  y ~ (factblock+variety) * (varweek + I(varweek^2) + I(varweek^3) + I(varweek^4))
, corr = corExp(form = ~ varweek | factplot, nugget = TRUE)
, sorghum)

fm4.6.ANOVA <- anova(fm4.6)
fm4.6.Coef <- broom::tidy(fm4.6)
fm4.6.vcov <- vcov(fm4.6)


fm4.6.Par <-
  tibble::tibble(
    "Parameter" = c("Range", "Nugget", "rho")
    , "Value"     = c(
      coef(fm4.6$modelStruct$corStruct, unconstrained = FALSE)[1]
      , coef(fm4.6$modelStruct$corStruct, unconstrained = FALSE)[2]
      , (1-coef(fm4.6$modelStruct$corStruct, unconstrained = FALSE)[2])*
        exp(-1/coef(fm4.6$modelStruct$corStruct, unconstrained = FALSE)[1])
    )
  )

fm4.6.ACF <- nlme::ACF(fm4.6)
```

Table 31: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	22278.1	0.000
factblock	4	97.7	0.000
variety	3	88.7	0.000
varweek	1	1687.5	0.000
I(varweek^2)	1	62.7	0.000
I(varweek^3)	1	18.1	0.000
I(varweek^4)	1	20.0	0.000
factblock:varweek	4	12.4	0.000
factblock:I(varweek^2)	4	1.7	0.163
factblock:I(varweek^3)	4	0.1	0.988
factblock:I(varweek^4)	4	2.7	0.042
variety:varweek	3	21.2	0.000
variety:I(varweek^2)	3	16.6	0.000
variety:I(varweek^3)	3	7.7	0.000
variety:I(varweek^4)	3	4.8	0.005

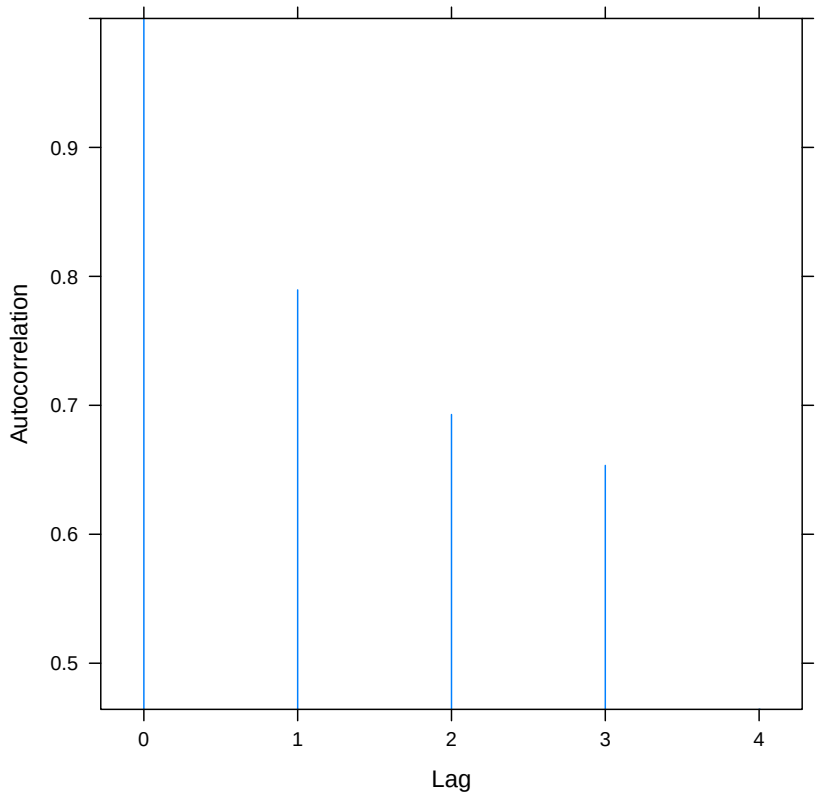
Table 32: *Model Coefficients*

	term	*estimate*	*std.error*	*statistic*	*p.value*
1	(Intercept)	1.530	0.705	2.171	0.034
2	factblock2	0.652	0.788	0.828	0.411
3	factblock3	0.950	0.788	1.206	0.233
4	factblock4	0.725	0.788	0.920	0.361
5	factblock5	0.423	0.788	0.536	0.594
6	variety2	2.708	0.705	3.843	0.000
7	variety3	0.398	0.705	0.565	0.574
8	variety4	3.204	0.705	4.547	0.000
9	varweek	6.701	1.287	5.205	0.000
10	I(varweek^2)	-4.147	0.772	-5.371	0.000
11	I(varweek^3)	0.959	0.186	5.171	0.000
12	I(varweek^4)	-0.077	0.015	-4.987	0.000
13	factblock2:varweek	-1.690	1.439	-1.174	0.245
14	factblock3:varweek	-2.835	1.439	-1.969	0.054
15	factblock4:varweek	-3.392	1.439	-2.356	0.022
16	factblock5:varweek	-4.256	1.439	-2.957	0.004
17	factblock2:I(varweek^2)	1.014	0.863	1.175	0.245
18	factblock3:I(varweek^2)	1.710	0.863	1.981	0.052
19	factblock4:I(varweek^2)	2.127	0.863	2.464	0.017
20	factblock5:I(varweek^2)	2.567	0.863	2.974	0.004
21	factblock2:I(varweek^3)	-0.239	0.207	-1.150	0.255
22	factblock3:I(varweek^3)	-0.407	0.207	-1.961	0.055
23	factblock4:I(varweek^3)	-0.509	0.207	-2.456	0.017
24	factblock5:I(varweek^3)	-0.609	0.207	-2.936	0.005
25	factblock2:I(varweek^4)	0.019	0.017	1.117	0.268
26	factblock3:I(varweek^4)	0.034	0.017	1.945	0.056
27	factblock4:I(varweek^4)	0.042	0.017	2.434	0.018
28	factblock5:I(varweek^4)	0.050	0.017	2.917	0.005
29	variety2:varweek	-3.519	1.287	-2.733	0.008
30	variety3:varweek	0.067	1.287	0.052	0.958
31	variety4:varweek	-4.313	1.287	-3.350	0.001
32	variety2:I(varweek^2)	2.207	0.772	2.859	0.006
33	variety3:I(varweek^2)	0.249	0.772	0.323	0.748
34	variety4:I(varweek^2)	2.549	0.772	3.302	0.002
35	variety2:I(varweek^3)	-0.535	0.186	-2.883	0.005
36	variety3:I(varweek^3)	-0.074	0.186	-0.401	0.690
37	variety4:I(varweek^3)	-0.572	0.186	-3.082	0.003
38	variety2:I(varweek^4)	0.045	0.015	2.890	0.005
39	variety3:I(varweek^4)	0.006	0.015	0.378	0.707
40	variety4:I(varweek^4)	0.044	0.015	2.825	0.006

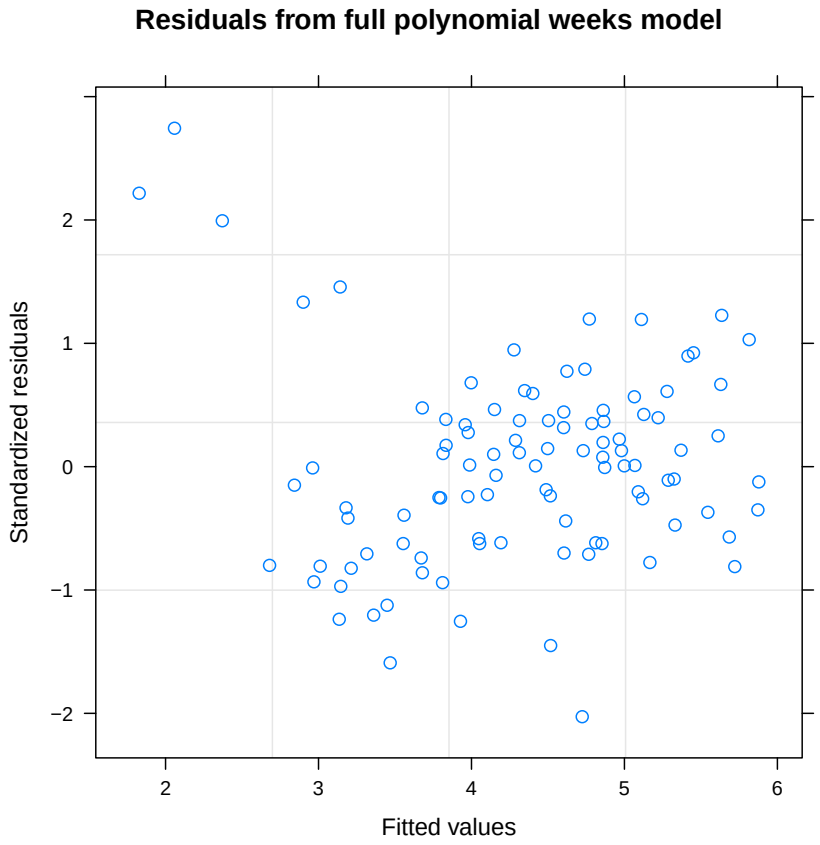
Table 33: *Structured Parameters*

Parameter	***Value***
Range	10.358
Nugget	0.172
rho	0.752

```
plot(fm4.6.ACF)
```




```
plot(fm4.6, sub.caption = NA, main = "Residuals from full polynomial weeks model")
```



```r
fm4.7 <- nlme::gls(
  y ~  polBlocks + variety + rawWeeks[,1] + rawWeeks[,2] +
      polBlocks:(rawWeeks[,1] + rawWeeks[,2]+ polWeeks[,3] + polWeeks[,4]) +
      variety:(rawWeeks[,1] + rawWeeks[,2])
 , corr = corExp(form = ~ varweek | factplot, nugget=TRUE), sorghum)
fm4.7.ANOVA <- anova(fm4.7)
fm4.7.Coef <- broom::tidy(fm4.7)
fm4.7.vcov <- vcov(fm4.7)

fm4.7.Par <-
  tibble::tibble(
    "Parameter" = c("Range", "Nugget", "rho")
    , "Value"     = c(
      coef(fm4.7$modelStruct$corStruct, unconstrained = FALSE)[1]
      , coef(fm4.7$modelStruct$corStruct, unconstrained = FALSE)[2]
      , (1-coef(fm4.7$modelStruct$corStruct, unconstrained = FALSE)[2])*
        exp(-1/coef(fm4.7$modelStruct$corStruct, unconstrained = FALSE)[1])
    )
  )

fm4.7.ACF <- nlme::ACF(fm4.7)
```

Table 34: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	21284.9	0.000
polBlocks	4	94.4	0.000
variety	3	88.1	0.000
rawWeeks[, 1]	1	1548.2	0.000
rawWeeks[, 2]	1	29.8	0.000
polBlocks:rawWeeks[, 1]	4	11.3	0.000
polBlocks:rawWeeks[, 2]	4	0.8	0.533
polBlocks:polWeeks[, 3]	4	0.0	0.998
polBlocks:polWeeks[, 4]	4	1.0	0.408
variety:rawWeeks[, 1]	3	19.1	0.000
variety:rawWeeks[, 2]	3	8.2	0.000

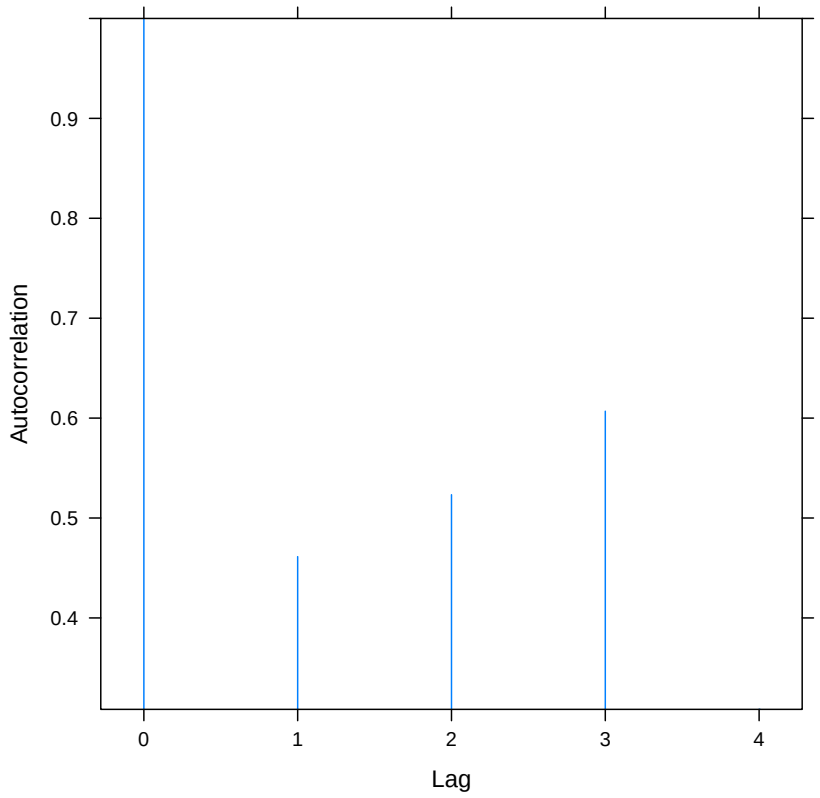
Table 35: *Model Coefficients*

	term	*estimate*	*std.error*	*statistic*	*p.value*
1	(Intercept)	4.679	0.122	38.414	0.000
2	polBlocks1	-6.445	0.609	-10.583	0.000
3	polBlocks2	-1.259	0.609	-2.067	0.043
4	polBlocks3	-0.110	0.609	-0.180	0.858
5	polBlocks4	0.369	0.609	0.605	0.547
6	variety2	0.785	0.172	4.556	0.000
7	variety3	0.073	0.172	0.425	0.672
8	variety4	0.501	0.172	2.907	0.005
9	rawWeeks[, 1]	-0.379	0.083	-4.569	0.000
10	rawWeeks[, 2]	-0.004	0.014	-0.316	0.753
11	polBlocks1:rawWeeks[, 1]	0.050	0.414	0.122	0.904
12	polBlocks2:rawWeeks[, 1]	-0.326	0.414	-0.787	0.434
13	polBlocks3:rawWeeks[, 1]	-0.357	0.414	-0.862	0.392
14	polBlocks4:rawWeeks[, 1]	-0.485	0.414	-1.170	0.246
15	polBlocks1:rawWeeks[, 2]	0.077	0.068	1.129	0.263
16	polBlocks2:rawWeeks[, 2]	0.052	0.068	0.772	0.443
17	polBlocks3:rawWeeks[, 2]	0.033	0.068	0.481	0.632
18	polBlocks4:rawWeeks[, 2]	0.070	0.068	1.035	0.304
19	polBlocks1:polWeeks[, 3]	-0.210	1.134	-0.185	0.854
20	polBlocks2:polWeeks[, 3]	0.220	1.134	0.194	0.847
21	polBlocks3:polWeeks[, 3]	-0.205	1.134	-0.181	0.857
22	polBlocks4:polWeeks[, 3]	0.195	1.134	0.172	0.864
23	polBlocks1:polWeeks[, 4]	2.238	1.134	1.974	0.053
24	polBlocks2:polWeeks[, 4]	-0.425	1.134	-0.375	0.709
25	polBlocks3:polWeeks[, 4]	0.089	1.134	0.078	0.938
26	polBlocks4:polWeeks[, 4]	0.045	1.134	0.040	0.968
27	variety2:rawWeeks[, 1]	0.107	0.117	0.915	0.363
28	variety3:rawWeeks[, 1]	0.645	0.117	5.500	0.000
29	variety4:rawWeeks[, 1]	0.388	0.117	3.312	0.001
30	variety2:rawWeeks[, 2]	-0.001	0.019	-0.060	0.953
31	variety3:rawWeeks[, 2]	-0.079	0.019	-4.122	0.000
32	variety4:rawWeeks[, 2]	-0.051	0.019	-2.639	0.010

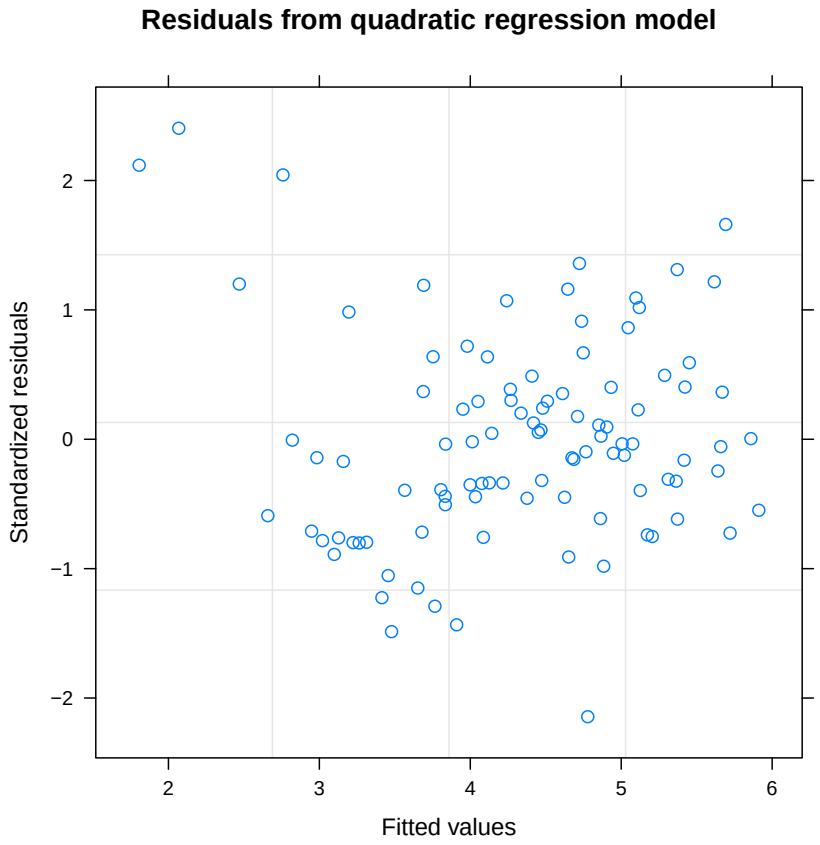
Table 36: *Structured Parameters*

Parameter	*Value*
Range	2.83988e+09
Nugget	4.61000e-01
rho	5.39000e-01

```
plot(fm4.7.ACF)
```




```
plot(fm4.7, sub.caption = NA, main = "Residuals from quadratic regression model")
```



```r
fm4.8 <-  nlme::gls(
  y ~ Replicate * (rawWeeks[,1] + rawWeeks[,2] + polWeeks[,3] + polWeeks[,4]) +
      variety * (rawWeeks[,1] + rawWeeks[,2])
 ,  corr = corExp(form = ~ varweek | factplot, nugget = TRUE), sorghum)
fm4.8.ANOVA <- anova(fm4.8)
fm4.8.Coef <- broom::tidy(fm4.8)
fm4.8.vcov <- vcov(fm4.8)

fm4.8.Par <-
  tibble::tibble(
    "Parameter" = c("Range", "Nugget", "rho")
    , "Value"     = c(
      coef(fm4.8$modelStruct$corStruct, unconstrained = FALSE)[1]
      , coef(fm4.8$modelStruct$corStruct, unconstrained = FALSE)[2]
      , (1-coef(fm4.8$modelStruct$corStruct, unconstrained = FALSE)[2])*
        exp(-1/coef(fm4.8$modelStruct$corStruct, unconstrained = FALSE)[1])
    )
  )

fm4.8.ACF <- nlme::ACF(fm4.8)
```

Table 37: *ANOVA Table*

	numDF	***F-value***	***p-value***
(Intercept)	1	21467.3	0.000
Replicate	4	95.0	0.000
rawWeeks[, 1]	1	1811.8	0.000
rawWeeks[, 2]	1	40.0	0.000
polWeeks[, 3]	1	10.2	0.002
polWeeks[, 4]	1	10.6	0.002
variety	3	88.2	0.000
Replicate:rawWeeks[, 1]	4	13.2	0.000
Replicate:rawWeeks[, 2]	4	1.1	0.380
Replicate:polWeeks[, 3]	4	0.0	0.996
Replicate:polWeeks[, 4]	4	1.4	0.244
rawWeeks[, 1]:variety	3	22.4	0.000
rawWeeks[, 2]:variety	3	11.0	0.000

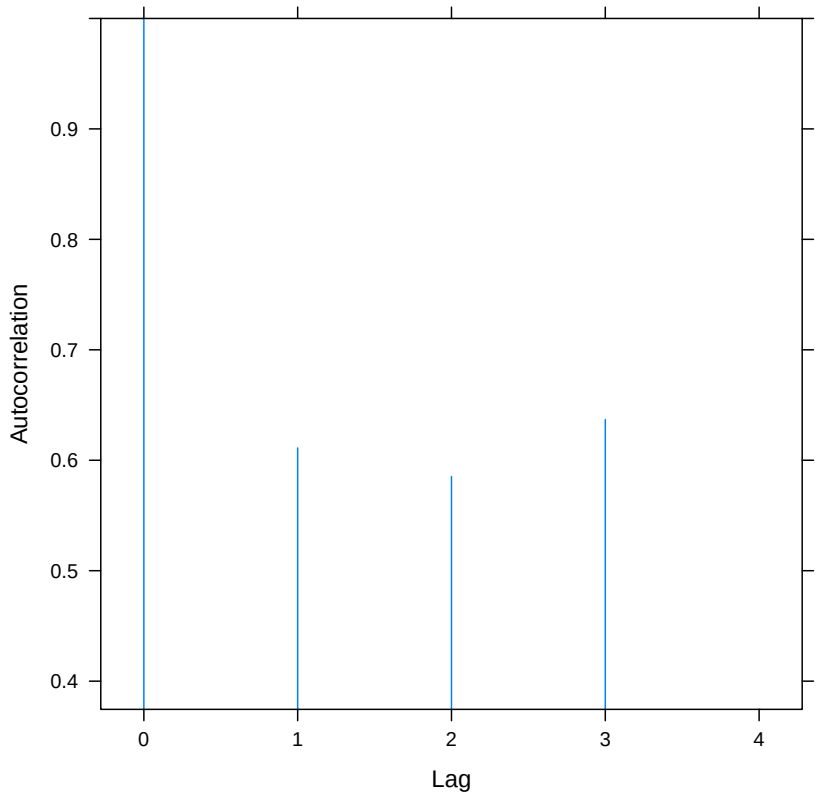
Table 38: *Model Coefficients*

	term	*estimate*	*std.error*	*statistic*	*p.value*
1	(Intercept)	5.456	0.155	35.228	0.000
2	Replicate2	-0.302	0.173	-1.747	0.085
3	Replicate3	-0.569	0.173	-3.286	0.002
4	Replicate4	-1.183	0.173	-6.831	0.000
5	Replicate5	-1.838	0.173	-10.617	0.000
6	rawWeeks[, 1]	-0.412	0.102	-4.050	0.000
7	rawWeeks[, 2]	-0.009	0.017	-0.566	0.573
8	polWeeks[, 3]	0.385	0.217	1.780	0.080
9	polWeeks[, 4]	-0.686	0.216	-3.180	0.002
10	variety2	0.786	0.155	5.075	0.000
11	variety3	0.074	0.155	0.475	0.636
12	variety4	0.505	0.155	3.260	0.002
13	Replicate2:rawWeeks[, 1]	0.051	0.114	0.449	0.655
14	Replicate3:rawWeeks[, 1]	-0.005	0.114	-0.044	0.965
15	Replicate4:rawWeeks[, 1]	0.159	0.114	1.401	0.166
16	Replicate5:rawWeeks[, 1]	-0.036	0.114	-0.319	0.751
17	Replicate2:rawWeeks[, 2]	-0.006	0.019	-0.347	0.730
18	Replicate3:rawWeeks[, 2]	0.010	0.019	0.540	0.591
19	Replicate4:rawWeeks[, 2]	-0.005	0.019	-0.260	0.796
20	Replicate5:rawWeeks[, 2]	0.026	0.019	1.416	0.161
21	Replicate2:polWeeks[, 3]	-0.124	0.306	-0.404	0.687
22	Replicate3:polWeeks[, 3]	-0.071	0.306	-0.231	0.818
23	Replicate4:polWeeks[, 3]	-0.095	0.306	-0.312	0.756
24	Replicate5:polWeeks[, 3]	-0.088	0.306	-0.289	0.774
25	Replicate2:polWeeks[, 4]	0.247	0.305	0.811	0.420
26	Replicate3:polWeeks[, 4]	0.430	0.305	1.412	0.163
27	Replicate4:polWeeks[, 4]	0.539	0.305	1.767	0.082
28	Replicate5:polWeeks[, 4]	0.645	0.305	2.117	0.038
29	rawWeeks[, 1]:variety2	0.106	0.102	1.045	0.300
30	rawWeeks[, 1]:variety3	0.644	0.102	6.340	0.000
31	rawWeeks[, 1]:variety4	0.386	0.102	3.800	0.000
32	rawWeeks[, 2]:variety2	-0.001	0.017	-0.058	0.954
33	rawWeeks[, 2]:variety3	-0.079	0.017	-4.765	0.000
34	rawWeeks[, 2]:variety4	-0.050	0.017	-3.040	0.003

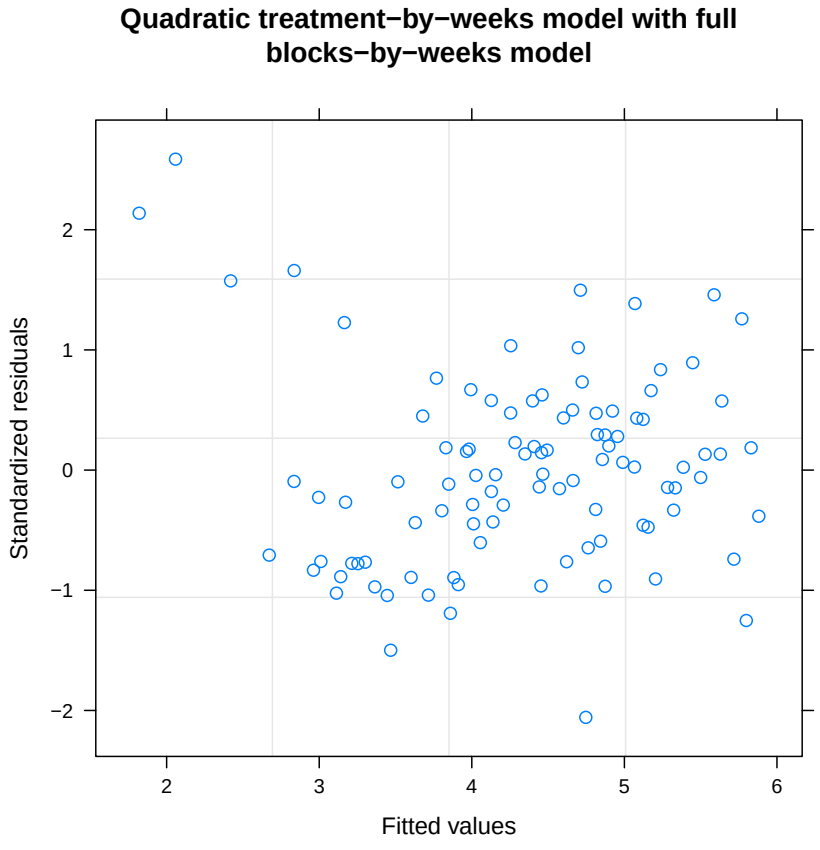
Table 39: *Structured Parameters*

Parameter	*Value*
Range	42.758
Nugget	0.359
rho	0.627

```
plot(fm4.8.ACF)
```




```
plot(fm4.8,sub.caption = NA, main = "Quadratic treatment-by-weeks model with full
blocks-by-weeks model")
```



5 Example 5: Transformation of treatment levels to improve model fit

Mead (1990, p. 323) describes an experiment on spacing effects with turnips, which was laid out in three complete blocks. Five different seed rates (0.5, 2, 8, 20, 32 lb/acre) were tested in combination with four different row widths (4, 8, 16, 32 inches), giving rise to a total of 20 treatments.

Transformation of the dependent variable will often stabilize the variance of the observations whereas transformation of the regressor variables will often simplify the fitted model. In this example, the fit of a regression model based on the original seed rate and row width variables is compared with the fit of a regression model based on the log transformed seed rates and log transformed row widths. In each case, the model lack-of-fit is examined by assessing the extra variability explained when the Density and Spacing treatment factors and their interactions are added to the quadratic regression models. All yields are logarithmically transformed to stabilize the variance.

The first analysis fits a quadratic regression model of log yields on the untransformed seed rates and row widths (Table 16) while the second analysis fits a quadratic regression model of log yields on the log transformed seed rates and log transformed row widths (Table 17). The analysis of variance of the first model shows that significant extra variability is explained by the Density and Spacing factors and this shows that a quadratic regression model is inadequate for the untransformed regressor variables. The analysis of variance of the second model, however, shows no significant extra variability explained by the Density and Spacing factors and this shows that the quadratic regression model with the log transformed regressor variables gives a good fit to the data and therefore is the preferred model for the observed data.

```
fm5.1 <- lm(log_yield ~ Replicate + density * rowspacing +
              I(density^2) + I(rowspacing^2) + Density * Spacing
            , turnip)
fm5.1.ANOVA <- anova(fm5.1)
```

Table 40: *ANOVA Table*

	Df	*Sum Sq*	*Mean Sq*	*F value*	*Pr(>F)*
Replicate	2	3.417	1.708	43.617	0.000
density	1	14.120	14.120	360.486	0.000
rowspacing	1	0.518	0.518	13.219	0.001
I(density^2)	1	6.178	6.178	157.737	0.000
I(rowspacing^2)	1	0.224	0.224	5.712	0.022
Density	2	5.350	2.675	68.293	0.000
Spacing	1	0.175	0.175	4.472	0.041
density:rowspacing	1	0.447	0.447	11.414	0.002
Density:Spacing	11	0.551	0.050	1.278	0.274
Residuals	38	1.488	0.039		

```
fm5.2 <- lm(log_yield ~ Replicate + log(density) * log(rowspacing) +
              I(log(density)^2) + I(log(rowspacing)^2) +
              Density * Spacing, turnip)
fm5.2.ANOVA <- anova(fm5.2)
```

The superiority of the model with the log transformed regressor variables is confirmed by comparing the fit of the quadratic regression model for the untransformed regressor variables (Figs 8 and 9) versus the fit of the quadratic regression model for the log transformed regressor variables (Figs 10 and 11).

Table 41: *ANOVA Table*

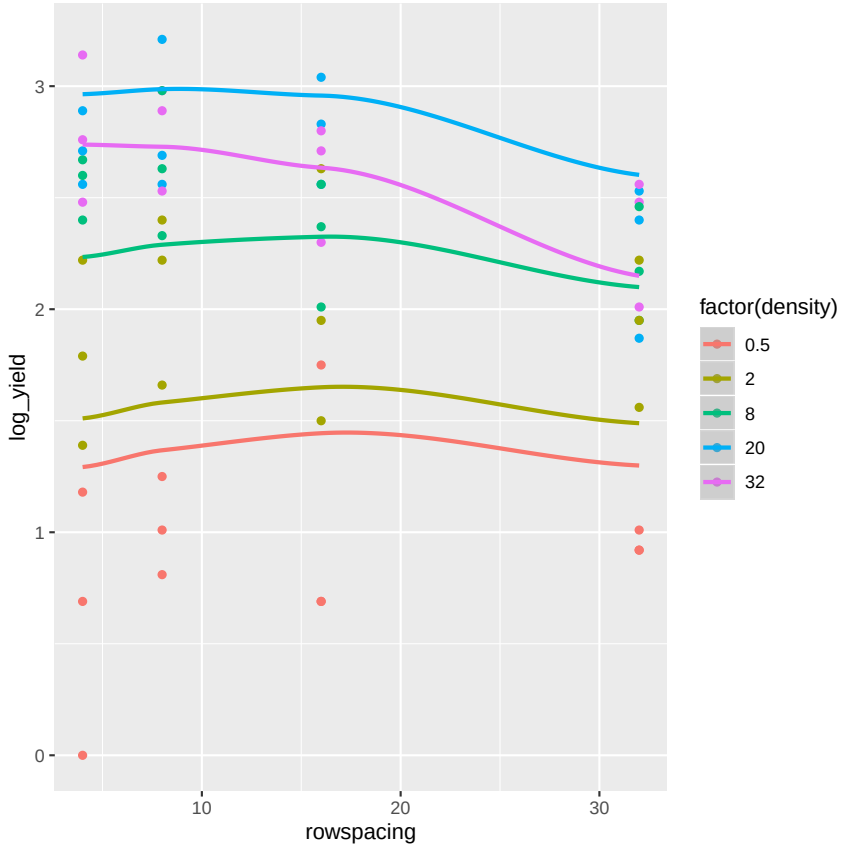
	Df	Sum Sq	Mean Sq	F value	Pr(>F)
Replicate	2	3.417	1.708	43.617	0.000
log(density)	1	23.477	23.477	599.396	0.000
log(rowspacing)	1	0.280	0.280	7.156	0.011
I(log(density)^2)	1	2.100	2.100	53.619	0.000
I(log(rowspacing)^2)	1	0.610	0.610	15.575	0.000
Density	2	0.070	0.035	0.897	0.416
Spacing	1	0.026	0.026	0.672	0.417
log(density):log(rowspacing)	1	0.750	0.750	19.157	0.000
Density:Spacing	11	0.247	0.022	0.574	0.838
Residuals	38	1.488	0.039		

```
fm5.3 <- lm(log_yield ~ density * rowspacing + I(density^2) +
              I(rowspacing^2) , turnip)
fm5.3.Coef <- broom::tidy(fm5.3)
turnip1 <- broom::augment(fm5.3, turnip)
```

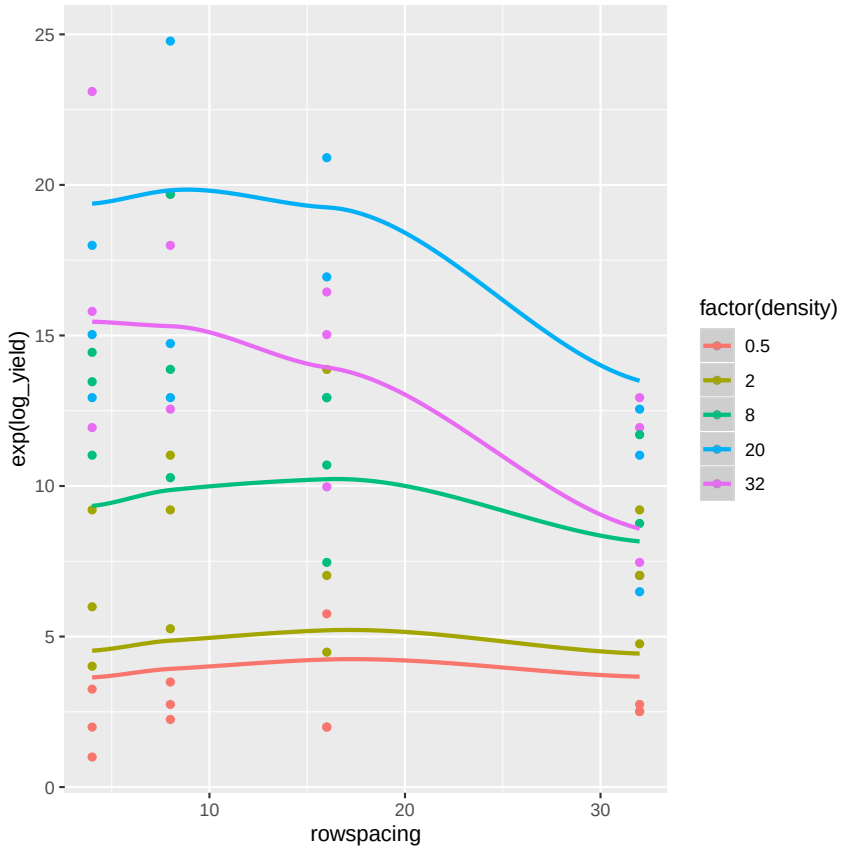
Table 42: *Model Coefficients*

	term	estimate	std.error	statistic	p.value
1	(Intercept)	1.115	0.224	4.985	0.000
2	density	0.156	0.021	7.477	0.000
3	rowspacing	0.028	0.028	1.000	0.322
4	I(density^2)	-0.003	0.001	-5.512	0.000
5	I(rowspacing^2)	-0.001	0.001	-1.049	0.299
6	density:rowspacing	-0.001	0.000	-1.483	0.144

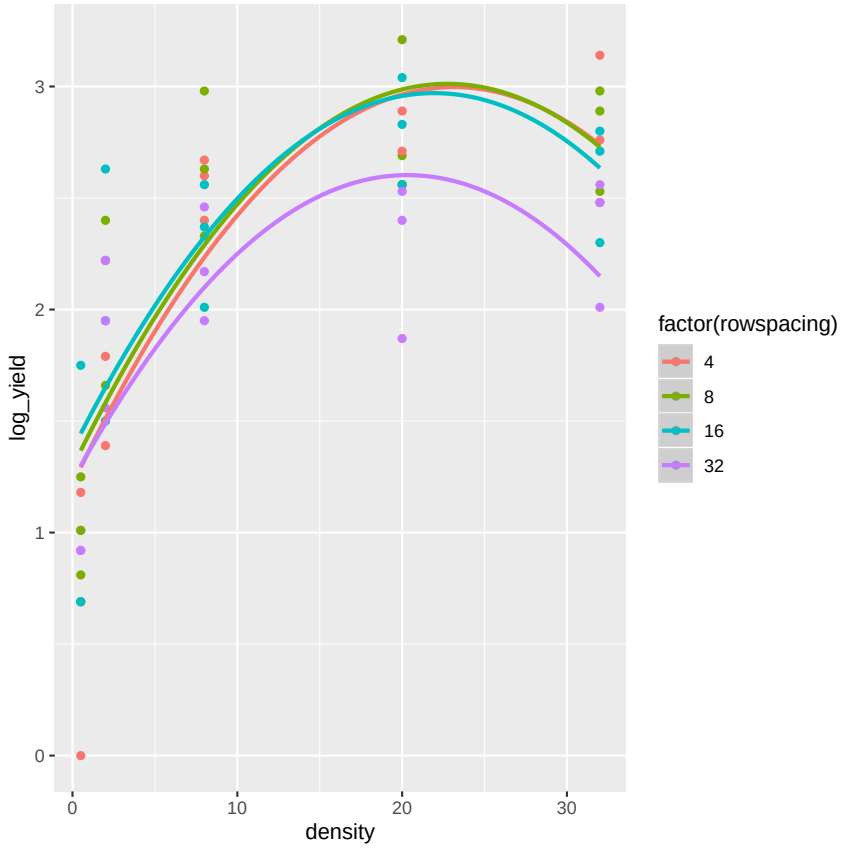
```
ggplot(data = turnip1,
     mapping = aes(x = rowspacing, y = log_yield,
                   color = factor(density), group = factor(density))) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```




```
ggplot(data = turnip1,
       mapping = aes(x = rowspacing, y = exp(log_yield),
                     color = factor(density), group = factor(density))) +
  geom_point() +
  geom_smooth(mapping = aes(y =exp(.fitted)), method = "loess")
```



```
ggplot(data = turnip1,
       mapping = aes(x = density, y = log_yield,
                     color = factor(rowspacing), group = factor(rowspacing))) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```




```
ggplot(data = turnip1,
       mapping = aes(x = density, y = exp(log_yield),
                     color = factor(rowspacing), group = factor(rowspacing))) +
  geom_point() +
  geom_smooth(mapping = aes(y =exp(.fitted)), method = "loess")
```

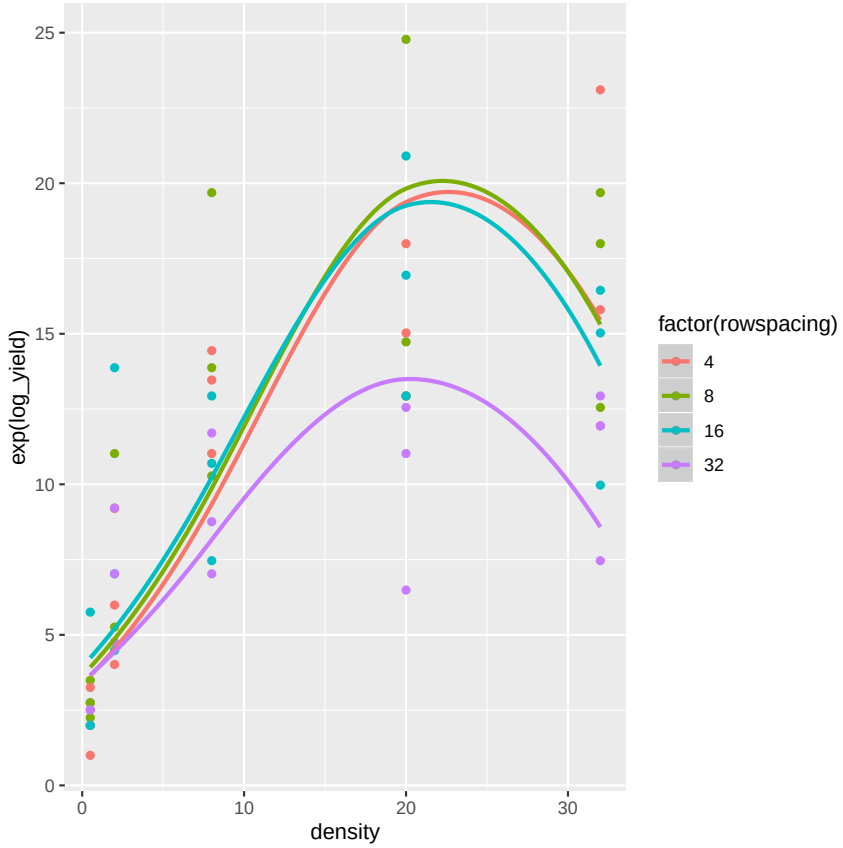
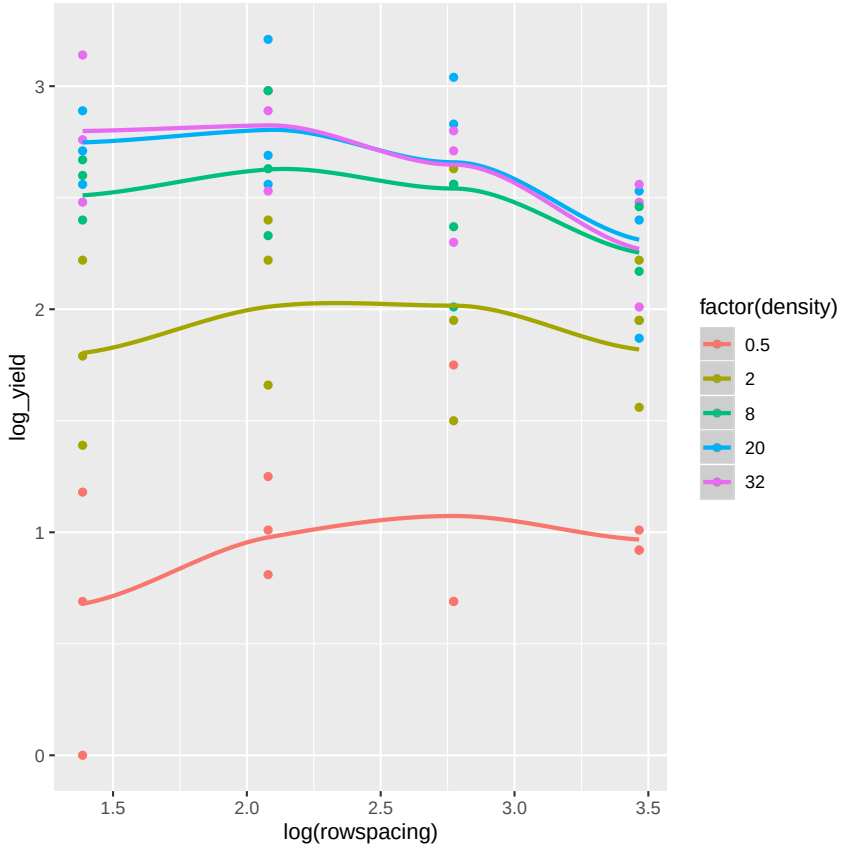


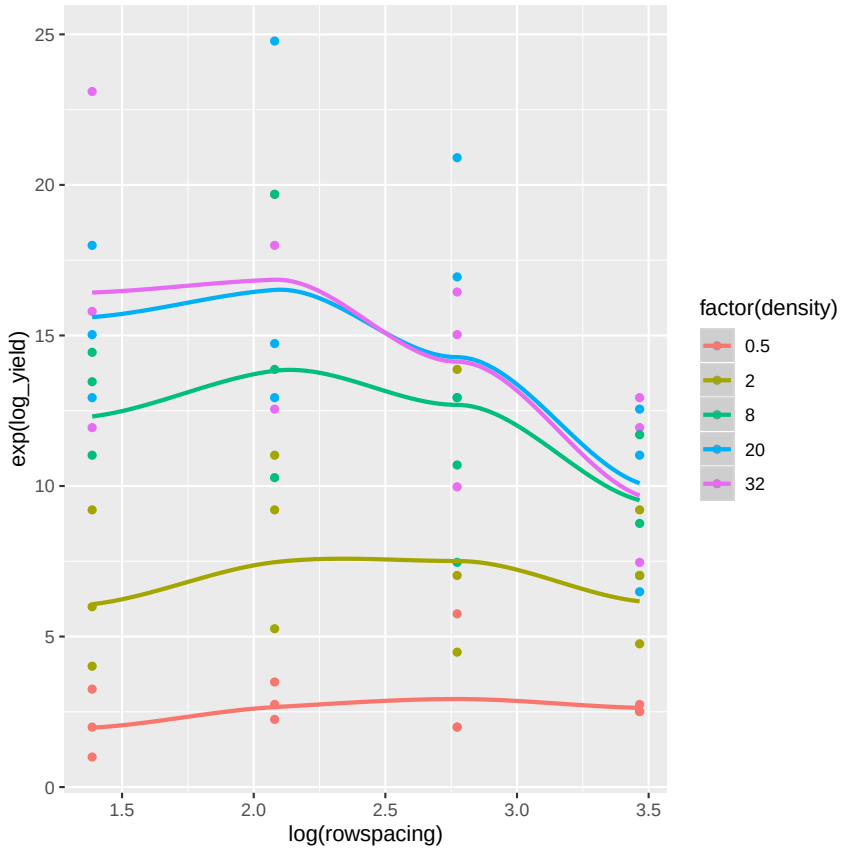
Fig 12a shows diagnostic plots for the fit of a quadratic model with untransformed regressor variables while Fig 12b shows corresponding diagnostic plots for the fit of a quadratic model with loge transformed regressor variables. Each of the four types of diagnostic plots in the two figures shows an improvement in fit for the transformed versus the untransformed regressor variables.

```
fm5.4 <- lm(log_yield ~ log(density) * log(rowspacing) +
              I(log(density)^2) + I(log(rowspacing)^2),
            turnip)
fm5.4.Coef <- broom::tidy(fm5.4)
turnip2 <- broom::augment(fm5.4, turnip)
```

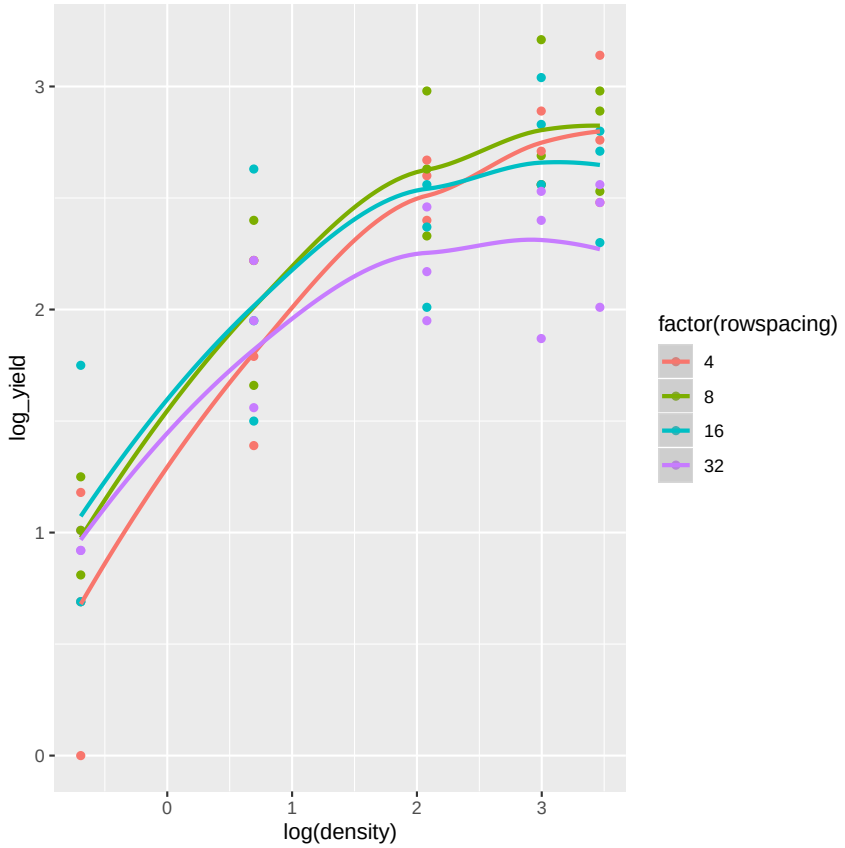
```
ggplot(data = turnip2,
       mapping = aes(x = log(rowspacing), y = log_yield,
                     color = factor(density), group = factor(density))) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```



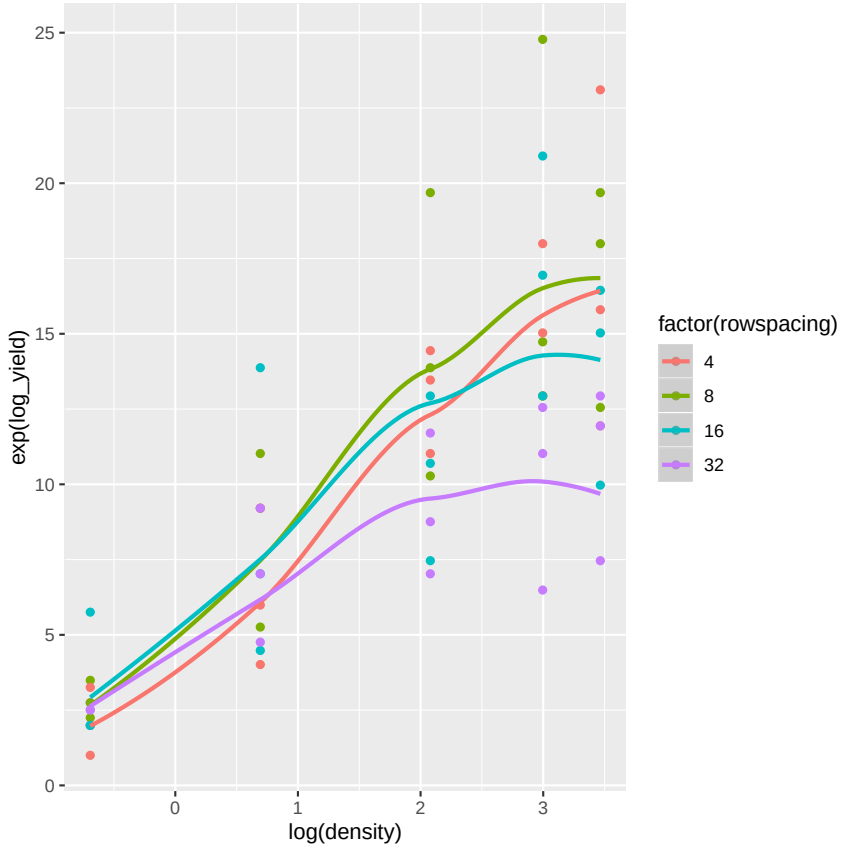

```
ggplot(data = turnip2,
       mapping = aes(x = log(rowspacing), y = exp(log_yield),
                     color = factor(density), group = factor(density))) +
  geom_point() +
  geom_smooth(mapping = aes(y =exp(.fitted)), method = "loess")
```



```
ggplot(data = turnip2,
       mapping = aes(x = log(density), y = log_yield,
                     color = factor(rowspacing), group = factor(rowspacing))) +
  geom_point() +
  geom_smooth(mapping = aes(y =.fitted), method = "loess")
```

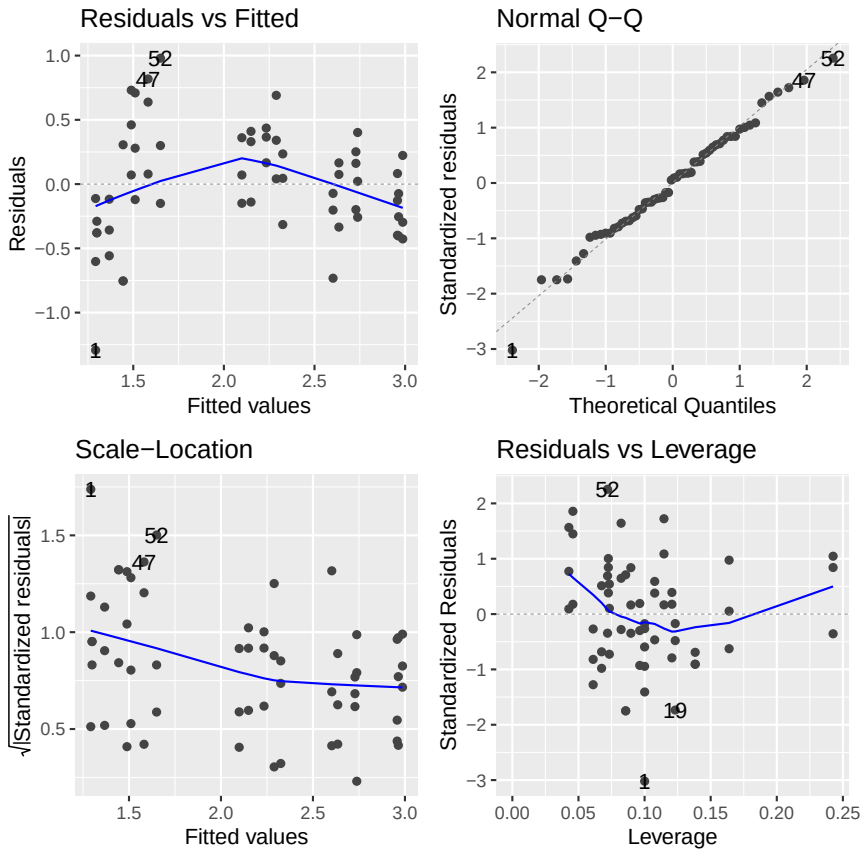



```
ggplot(data = turnip2,
       mapping = aes(x = log(density), y = exp(log_yield),
                     color = factor(rowspacing), group = factor(rowspacing))) +
  geom_point() +
  geom_smooth(mapping = aes(y = exp(.fitted)), method = "loess")
```



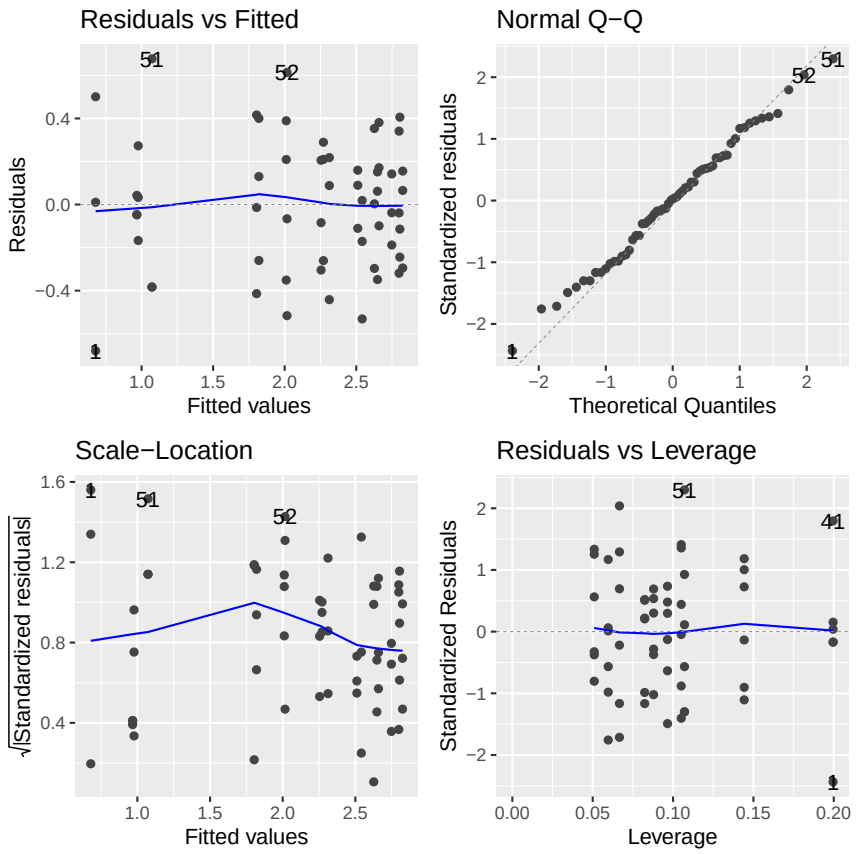

```
fm5.5 <- lm(log_yield ~ density * rowspacing +
              I(density^2) + I(rowspacing^2),
            turnip)
```

```
ggplot2::autoplot(fm5.5)
```



```
fm5.6 <- lm(log_yield ~ log(density) * log(rowspacing) +
              I(log(density)^2) + I(log(rowspacing)^2),
            turnip)
```

```
ggplot2::autoplot(fm5.6)
```



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