Regression Models for Quantitative and Qualitative Predictors

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Linear Regression Models - Lecture 10

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General Linear Regression Model

• Independent responses of the form $Y_i \sim N(\mu_i, \sigma^2)$, where

$$\mu_i = \mathbf{X}_i^{\top} \boldsymbol{\beta}$$

for some known vector of explanatory variables $\mathbf{X}_i^{ op} = (X_{i1}, \dots, X_{ip})$.

- Unknown parameter vector $\boldsymbol{\beta} = (\beta_0, \dots, \beta_{P-1})^{\top}$, where P < N.
- This is the linear model and is usually written as

$$Y = X\beta + \varepsilon$$

(in vector notation) where

$$\mathbf{Y} = \left(\begin{array}{c} Y_1 \\ \vdots \\ Y_N \end{array} \right), \quad \mathbf{X} = \left(\begin{array}{c} x_1^\top \\ \vdots \\ x_N^\top \end{array} \right), \quad \boldsymbol{\beta} = \left(\begin{array}{c} \beta_0 \\ \vdots \\ \beta_{P-1} \end{array} \right), \quad \boldsymbol{\varepsilon} = \left(\begin{array}{c} \varepsilon_1 \\ \vdots \\ \varepsilon_N \end{array} \right),$$

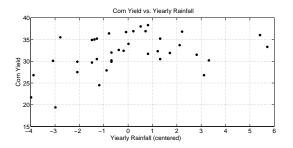
where $\varepsilon_i \stackrel{i.i.d.}{\sim} N(0, \sigma^2)$, for i = 1, 2, ..., N.

Building Regression Models

- One of the first steps in the construction of a regression model is to *hypothesize* the form of the regression function.
- We can dramatically expand the scope of our regression models by including specially constructed explanatory variables.
- These include indicator variables, interaction terms, transformed variables, and higher order terms.

Yield and Rainfall

 Data was collected on the yearly rainfall and corn yield at a farm during a 38 year period.



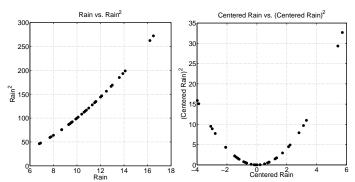
- There exits a curvilinear relationship between the variables.
- The relationship appears to be quadratic.

Polynomial Regression Models

- Polynomial regression models are useful when there is reason to believe the relationship between two variables is curvilinear.
- The general form for the polynomial regression model with one explanatory variable is:

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \ldots + \beta_P X_i^P + \varepsilon_i$$

- The order of the model, P, is the highest power used for the explanatory variable.
- Prior to performing polynomial regression it is recommended to *center* the observations by removing their mean, i.e., exchange X_i with $X_i \bar{X}$ to minimize problems with multicollinearity.



Alternative format

- Regression coefficients in polynomial regression are often written in an alternative format.
- We write

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \varepsilon_i$$

as

$$Y_i = \beta_0 + \beta_1 X_i + \beta_{11} X_i^2 + \varepsilon_i$$

Yield and Rainfall

- Let Y be the yield and X the yearly rainfall.
- Since the relationship is *quadratic*, we use poly. regression of order 2.
- Predicted response:

$$\hat{Y}_{i} = \beta_{0} + \beta_{1}X_{i} + \beta_{11}X_{i}^{2} + \varepsilon_{i}
\hat{Y} = 33.06 + 1.06X - 0.23X^{2}$$

Re-expression

- After fitting a polynomial regression model, we often re-express it using the original variables.
- The fitted model:

$$\hat{Y}_i = b_0 + b_1 X_i + b_{11} X_i^2$$

becomes

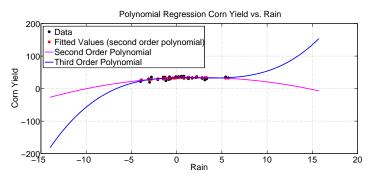
$$\hat{Y}_i = b_0' + b_1' X_i + b_{11}' X_i^2$$

where

$$b_0' = b_0 - b_1 \bar{X} + b_{11} \bar{X}^2, \quad , b_1' = b_1 - 2b_{11} \bar{X}, \quad b_{11}' = b_{11}$$

Comments

- Be careful when choosing the order of the polynomial regression model, as it is easy to over-fit the model.
- For a problem with N data points, a polynomial of order N 1 will pass through all N points.
- However, such a model will not be useful for predicting future values.
- Extrapolation is particularly hazardous when using polynomial regression.
- Polynomial regression may provide good fits for the data at hand but may turn in unexpected directions when extrapolated beyond the range of the data.



Interaction Regression Models

• A regression model with P-1 explanatory variables contains additive effects if the regression function can be written in the form:

$$\mathbb{E}(Y) = f(X_1) + f(X_2) + \ldots + f(X_{P-1}).$$

Example:

$$\mathbb{E}(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2.$$

- Two explanatory variables are said to interact if the effect that one of them has on the mean response depends on the value of the other.
- A simple way of modelling interaction is by including a bilinear interaction term (e.g., X_1X_2).

Interaction Regression Models

For example:

$$\mathbb{E}(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2.$$

- The interpretation of the coefficients β_1 and β_2 differ due to the inclusion of the interaction term.
- The change in mean response with a unit increase in X_1 , when X_2 is fixed, is $\beta_1 + \beta_3 X_2$.
- Hence, the effect of X_1 , for a given level of X_2 , will depend on the value of X_2 .
- The same relationship holds for X_1 .

Polynomial Regression Models

The regression model:

$$Y_{i} = \beta_{0} + \beta_{1}X_{1i} + \beta_{11}X_{1i}^{2} + \beta_{2}X_{2i} + \beta_{22}X_{2i}^{2} + \beta_{22}X_{1i}X_{2i} + \varepsilon_{i}$$

where

$$X_{1i}
ightarrow X_{1i} - \bar{X}_1, \qquad X_{2i}
ightarrow X_{2i} - \bar{X}_2$$

is a second order model with two explanatory variables.

Categorical Explanatory Variables

- So far we have only used quantitative explanatory variables in our regression models.
- However, often the explanatory variables we are interested in are categorical (e.g., gender, weekday, hair color).
- We can use indicator variables, or dummy variables to denote the values of the categorical variable.
- There are a number of ways of quantitatively identifying the classes of a categorical variable.
- Often the most appropriate is to use indicator variables that take on the values 0 and 1, i.e., $X_i = 1$ if the observation belongs to group A, and 0 otherwise.

Illustration

- Suppose we have data on two variables X_1 and Y collected for two separate groups (A and B).
- Define X_2 to be an *indicator* variable that is equal to 1 if the observation belongs to group A and 0 if it belongs to group B.
- Consider the regression model:

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \varepsilon_i.$$

• The mean response for

Group
$$A: \mathbb{E}(Y) = (\beta_0 + \beta_2) + \beta_1 X_1$$

Group
$$B: \mathbb{E}(Y) = \beta_0 + \beta_1 X_1$$

 The groups are allowed to have different intercepts, but must have the same slope.

Inference

 To determine whether the mean of Y differs between the two groups, after controlling for the other explanatory variable, test:

$$H_0: \beta_2 = 0$$
 versus $H_a: \beta_2 \neq 0$

• If we reject H_0 , there is evidence of a significant difference in means between the groups.

Insulating foam

- Data was collected to see whether a certain type of insulating foam had an effect on the ambient formaldehyde (CH₂O) concentration inside a house.
- As the amount of CH₂O was also influenced by the amount of air that can move through the house via windows and cracks, an air tightness rating (between 0-10) was determined for each house.
- Let Y be the CH_2O concentration, X_1 the air tightness of the house and X_2 equal to 1 if foam is present in the house and 0 otherwise.
- Model: $Y = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \varepsilon_i$.
- Is there a *difference* in the average concentration of CH_2O between homes of equal air tightness but different insulation?

- Predicted Response: $\hat{Y} = 31.37 + 2.85X_1 + 9.31X_2$.
- Test: $H_0: \beta_2 = 0$ versus $H_1: \beta_2 \neq 0$
- From the output: t = 4.37, p-value = 0.0003
- There is *strong* evidence that homes with foam insulation have *higher CH*₂O concentration.

Varying Slopes and Intercepts

- In the previous example we used an indicator variable to model differences in the *intercept* between groups.
- Sometimes we also want the *slopes* of the regression model to differ between groups.
- This can be done by including an *interaction* term together with an indicator variable in the model.

Illustration

- Suppose we have data on two variables X_1 and Y collected for two groups (A and B).
- Let X_2 be equal to 1 if the observation belongs to group A and 0 if it belongs to group B.
- Consider a regression model with *interactions*:

$$Y = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \beta_3 X_{1i} X_{2i} + \varepsilon_i.$$

The response surface:

Group *A*:
$$\mathbb{E}(Y) = (\beta_0 + \beta_2) + (\beta_1 + \beta_3)X_1$$

Group *B*: $\mathbb{E}(Y) = \beta_0 + \beta_1 X_1$

• Picture! Both the intercept and slope are allowed to vary.

Inference

• Testing whether the two regression equations are *identical* involves the following hypothesis:

$$H_0: \beta_2 = \beta_3 = 0$$
 versus $H_1:$ Both not equal to 0.

- Perform this test using a t-test.
- Perform this test using a general linear *F*-test.

Varying slopes

- We have looked at regression models where:
 - the *intercept* is allowed to *vary* between groups.
 - the intercept and slope are allowed to vary across groups.
- How about the case where the slope varies but not the intercept?

Illustration

- Suppose we have data on two variables X_1 and Y collected for two groups (A and B).
- Let X_2 be equal to 1 if the observation belongs to group A and 0 if it belongs to group B.
- Consider a regression model with interactions:

$$Y = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{1i} X_{2i} + \varepsilon_i.$$

• The response surface:

Group
$$A$$
: $\mathbb{E}(Y) = \beta_0 + (\beta_1 + \beta_2)X_1$
Group B : $\mathbb{E}(Y) = \beta_0 + \beta_1X_1$

• Picture! The slopes are allowed to vary, but not the intercepts.

Inference

 Testing whether the two regression equations are identical involves the following hypothesis:

$$H_0: \beta_2 = 0$$
 versus $H_1: \beta_2 \neq 0$.

- Perform this test using a t-test.
- To determine whether the effect of the foam depends on air tightness include an interaction term.
- Predicted Response: $\hat{Y} = 30.00 + 3.12X_1 + 12.48X_2 0.62X_1X_2$

Results

- Test: $H_0: \beta_2 = \beta_3 = 0$ versus $H_1:$ Both not equal to 0.
- Reject H₀.
- There is strong evidence that the foam insulation has an effect on the CH₂O concentration.
- Test individual regression coefficients:

$$H_0: \beta_2 = 0$$
 $H_0: \beta_3 = 0$ $H_1: \beta_2 \neq 0$ $H_1: \beta_3 \neq 0$. From the output: From the output: $t = 2.79$ $t = -0.81$ $p - value = 0.0113$ $p - value = 0.4292$

• The intercept appears to differ, but not slope.

Multiple classes

- Sometimes a categorical variable can take more than 2 possible values.
- A categorical variable with c classes is best represented using c-1 separate indicator variables.
- This provides a more flexible model than coding the different classes using a single variable.
- Illustration: Create a model relating profit, Y, to bank size, X_1 , and bank type (Commercial, Mutual savings or Savings and loans).

Model I

• If bank type is coded as a variable X_2 with values

Comercial:

Mutual Savings:

Savings & Ioan:

3

• The regression model: $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \varepsilon_i$.

The mean response for

Comercial:
$$\mathbb{E}(Y) = (\beta_0 + \beta_2) + \beta_1 X_1$$

Mutual Savings:
$$\mathbb{E}(Y) = (\beta_0 + 2\beta_2) + \beta_1 X_1$$

Savings & loan:
$$\mathbb{E}(Y) = (\beta_0 + 3\beta_2) + \beta_1 X_1$$

- This approach is not very effective and/or very realistic.
- The difference in profit between Commercial and Mutual savings banks is β_2 . Similarly, the difference between Savings & loan and Mutual saving banks must also be equal to β_2 .

Model II

• If bank type is coded as *two* variables X_2 and X_3 with values

$$X_2$$
 X_3

Comercial: 1

Mutual Savings: 0 1

Savings & loan: 0 0

- The regression model: $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \beta_3 X_{3i} + \varepsilon_i$.
- The mean response for

Comercial: $\mathbb{E}(Y) = (\beta_0 + \beta_2) + \beta_1 X_1$

Mutual Savings: $\mathbb{E}(Y) = (\beta_0 + \beta_3) + \beta_1 X_1$

Savings & loan: $\mathbb{E}(Y) = \beta_0 + \beta_1 X_1$

This approach is more flexible.

ANOVA and ANCOVA

- In analysis of variance (ANOVA) models all explanatory variables are categorical.
- In analysis of covariance (ANCOVA) models there are both quantitative and categorical variables. The explanatory variable of interest is categorical and the quantitative variables are included primarily to reduce variation.

Analysis of Variance

• The one-way analysis of variance (ANOVA) model is given by

$$Y_{jk} = \mu_j + \varepsilon_{jk},$$

for $j=1,\ldots,J$ and $k=1,\ldots,N_j$, where the ε_{jk} 's are i.i.d. and follow a $N(0,\sigma^2)$ distribution.

• It can be used to test:

$$H_0: \mu_1 = \mu_2 = \ldots = \mu_J$$
 versus $H_a:$ Not all means equal.

- Example: Consider measuring yields of plants under a *control* condition and J-1 different *treatment* conditions.
- The explanatory variable (factor) has J levels, and the response variables at level j are Y_{j1}, \ldots, Y_{jn_i} .

One-way analysis of variance (ANOVA)

The model that the responses are independent with

$$Y_{jk} \sim N(\mu_j, \sigma^2), \quad j = 1, \dots, J; \quad k = 1, \dots, N_j$$

is of linear model form, with

Cereal grain example

• Six samples of each of *four* types of cereal grain were analyzed to determine the *thiamin* content, resulting in the following data:

• Is there evidence of a *difference* in mean thiamin content between the grain types?

ANOVA and Regression

- ANOVA can be formulated and performed within the multiple regression framework.
- The variable 'grain type' can be included in the regression model using a series of indicator variables.
- If a variable has K levels, we need K-1 indicator variables in order to represent it properly.

Cereal grain

• Since there are 4 levels we need to define 3 indicator variables:

Groups	X_1	X_2	X_3
Wheat:	1	0	0
Barley	0	1	0
Maize	0	0	1
Oats	0	0	0

- The regression model: $Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \beta_3 X_{3i} + \varepsilon_i$.
- The mean response for

Wheat
$$\mathbb{E}(Y) = \beta_0 + \beta_1$$

Barley $\mathbb{E}(Y) = \beta_0 + \beta_2$
Maize $\mathbb{E}(Y) = \beta_0 + \beta_3$
Oats $\mathbb{E}(Y) = \beta_0$

- Each group has its own mean response.
- The standard ANOVA null hypothesis $H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4$ is equivalent to testing the hypothesis

$$H_0: \beta_1 = \beta_2 = \beta_3 = 0$$

in the regression model.

- For the above test, F = 3.957, p-value = 0.02293.
- Moderately strong evidence of a difference in mean thiamin content between the four grain types.

 An alternative parameterization, emphasizing the differences between treatments, is

$$Y_{jk} = \mu + \alpha_j + \varepsilon_{jk}, \quad j = 1, \dots, J; \quad k = 1, \dots, N_j$$

where

- \bullet μ is the baseline or mean effect
- α_i is the effect of the j^{th} treatment (or the control j=1).
- Notice that the parameter vector $(\mu, \alpha_1, \alpha_2, \dots, \alpha_J)^{\top}$ is not identifiable, since replacing μ with $\mu + 10$ and α_j by $\alpha_j 10$ gives the same model. Either a
 - corner point constraint $\alpha_1 = 0$ is used to emphasise the differences from the control, or the
 - sum-to-zero constraint $\sum_{j=1}^{J} N_j \alpha_j = 0$ can be used to make the model identifiable.
- R uses corner point constraints.

- If $N_i = K$, say, for all j, the data are said to be balanced.
- We are usually interested in comparing the null model

$$H_0: Y_{jk} = \mu + \varepsilon_{jk}$$

with that given above, which we call H_1 ; i.e., we wish to test whether the treatment conditions have an effect on the plant yield:

$$H_0: \boldsymbol{\alpha} = 0$$
, where $\alpha = (\alpha_1, \dots, \alpha_J)$, against $H_1: \boldsymbol{\alpha} \neq 0$.

• Check that the MLE fitted values, under H_1 , are

$$\hat{Y}_{jk} = \bar{Y}_j \equiv \frac{1}{N_j} \sum_{k=1}^{N_j} Y_{jk},$$

whatever parameterization is chosen, and, under H_0 , are

$$\hat{\hat{Y}}_{jk} = \bar{Y} \equiv \frac{1}{N} \sum_{j=1}^J N_j \bar{Y}_j, \quad \text{ where } N = \sum_{j=1}^J N_j.$$

ullet Our linear model theory says that we should test H_0 by referring

$$F = \frac{\frac{1}{J-1} \sum_{j=1}^{J} N_j (\bar{Y}_j - \bar{Y})^2}{\frac{1}{N-J} \sum_{j=1}^{J} \sum_{k=1}^{N_j} (Y_{jk} - \bar{Y}_j)^2} \equiv \frac{\frac{1}{J-1} S_2}{\frac{1}{N-J} S_1}$$

to $F_{J-1,N-J}$, where S_1 is the "within groups" sum of squares and S_2 is the "between groups" sum of squares.

• In (familiar) tabular form

Source of variation	Degrees of freedom	Sum of squares	$\emph{F}-$ statistic
Between groups	J-1	S_2	$F = \frac{\frac{1}{J-1}S_2}{\frac{1}{N-J}S_1}$
Within groups	N-J	S_1	N-J
Total	N-1	$\sum_{j=1}^{J} \sum_{k=1}^{N_j} (y_{jk} - \bar{y})^2$	

Two-way ANOVA

• Suppose now that we have two factors having I, J levels respectively, and that our model for independent responses $\{Y_{ijk}\}$ is

$$Y_{ijk}=\mu+lpha_i+eta_j+arepsilon_{ijk},$$
 for $i=1,\ldots,I;\;\;j=1,\ldots,J;\;\;k=1,\ldots,N_{ij},$ where $arepsilon_{iik}\sim N(0,\sigma^2).$

- For example, Y_{ijk} might represent the exam score of the k^{th} individual of sex $i \in \{M,F\}$ taking course j.
- This model is called an additive two-way ANOVA model because it is assumed that the effects of the different factors are additive.
- Possible identifiability constraints are

$$\sum_{i=1}^{J} \alpha_i = \sum_{i=1}^{J} \beta_j = 0 \qquad \text{or} \qquad \alpha_1 = \beta_1 = 0.$$

Again, R uses the latter corner point constraint.

 Let this model correspond to the hypothesis H₃. We might be interested in testing

$$H_0: \alpha_i = \beta_j = 0$$
 for all $i = 1, \dots, I; j = 1, \dots, J$
 $H_1: \alpha_i = 0$ for all $i = 1, \dots, I$
 $H_2: \beta_i = 0$ for all $j = 1, \dots, J$.

For simplicity, assume that $N_{ii} = K$, say.

 The expressions for the MLE under each model depends on the identifiability constraint imposed, but the fitted values are the same and the residual sum of squares in each case is:

$$\begin{split} &SSE(H_0) = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} (Y_{ijk} - \bar{Y})^2 & \text{where} & \bar{Y} \equiv \bar{Y}_{+++} = \frac{1}{IJK} \sum_{i=1}^{J} \sum_{j=1}^{K} \sum_{k=1}^{K} Y_{ijk} \\ &SSE(H_1) = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} (Y_{ijk} - \bar{Y}_{+j+})^2 & \text{where} & \bar{Y}_{+j+} = \frac{1}{IK} \sum_{i=1}^{I} \sum_{k=1}^{K} Y_{ijk} \\ &SSE(H_2) = \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} (Y_{ijk} - \bar{Y}_{i++})^2 & \text{where} & \bar{Y}_{i++} = \frac{1}{JK} \sum_{i=1}^{I} \sum_{k=1}^{K} Y_{ijk} \\ &SSE(H_3) = \sum_{i=1}^{I} \sum_{i=1}^{J} \sum_{k=1}^{K} (Y_{ijk} - \bar{Y}_{ijk})^2 & \text{where} & \bar{Y}_{ijk} = \bar{Y}_{i++} + \bar{Y}_{+j+} - \bar{Y}. \end{split}$$

These can be used to calculate F-statistics in a way similar to two-way ANOVA.

Interactions

- In the two-way ANOVA model we assumed that the effects of the factors were additive.
- We may also want to check for the presence of interaction between the two effects, using the model

$$Y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk}.$$

Sometimes γ_{ij} is notated as $(\alpha\beta)_{ij}$ to more explicitly denote the interaction of α and β .

- Possible identifiability constraints include
 - \bullet $\alpha_1 = \beta_1 = 0$, $\gamma_{1j} = 0$ for all j, and $\gamma_{i1} = 0$ for all i, or alternatively
 - ② $\sum_{i=1}^{I} \alpha_i = \sum_{j=1}^{J} \beta_j = 0$, $\sum_{i=1}^{I} \gamma_{ij} = 0$ for each j, and $\sum_{j=1}^{J} \gamma_{ij} = 0$ for each j.

One can show that

$$\begin{split} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} \left(Y_{ijk} - \bar{Y}_{+++} \right)^2 &= JK \sum_{i=1}^{I} \left(\bar{Y}_{i++} - \bar{Y}_{+++} \right)^2 + JK \sum_{j=1}^{J} \left(\bar{Y}_{+j+} - \bar{Y}_{+++} \right)^2 \\ &+ K \sum_{i=1}^{I} \sum_{j=1}^{J} \left(\bar{Y}_{ij+} - \bar{Y}_{i++} - \bar{Y}_{+j+} + \bar{Y}_{+++} \right)^2 \\ &+ \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} \left(Y_{ijk} - \bar{Y}_{ij+} \right)^2 \end{split}$$

That is the total sum squares is decomposed into that due to row differences, that due to column differences, that due to interaction, and that within cells. The test

$$H_0: \gamma_{ii} = 0$$
 for all i, j vs. $H_1: \gamma_{ii} \neq 0$ for some i, j

is based upon an $F_{(l-1)(J-1),IJ(K-1)}$ distributed test statistic given by

$$F = \frac{\left[K \sum_{i=1}^{J} \sum_{j=1}^{J} (\bar{Y}_{ij+} - (\bar{Y}_{i++} + \bar{Y}_{+j+} - \bar{Y}_{+++}))^{2}\right] / [(I-1)(J-1)]}{\left[\sum_{i=1}^{J} \sum_{j=1}^{J} \sum_{k=1}^{K} (Y_{ijk} - \bar{Y}_{ij+})^{2}\right] / [J(K-1)]}$$

- If an interaction is present, the interpretation is that the effect of the first factor on the response depends on the level of the second factor.
- For example, the response might be a "tastiness score" for a cake which depends on the factors of (1) baking time and (2) baking temperature.
- Interaction effects are most easily seen via plots, e.g., plot the responses Y_{ijk} against j, for each level of i. The statistical way is via an F-test (see anova2_int.R).