Statistical Design and Analysis of Experiments

Part Three

Lecture notes

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List of contents, cont.

Supplements

General ANOVA models

An example with a random factor

A factorial experiment carried out and placed randomly on 3 batches of material selected randomly among many possible batches (complete randomization assumed):

Batch	pH = 6			pH = 7		
	1%	2%	3%	1%	2%	3%
I	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$
II	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$
III	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$	$y_1\ y_2$

$$Y_{ijkl} = \mu + p_i + c_j + pc_{ij} + B_k + PB_{ik} + CB_{jk} + PCB_{ijk} + E_{ijkl}$$

etc. Random terms are written with capital letters.

p_i is a parameter (a number). A deterministic (fixed) factor

B_k is a random factor fx: $B_k \in N(0, \sigma_B^2)$

PB_{ik} is a random interaction term fx: $PB_{ik} \in N(0, \sigma_{BP}^2)$

A more reasonable (useful) model:

$$\boxed{Y_{ijkl} = \mu + p_i + c_j + pc_{ij} + B_k + E_{ijkl}}$$

In ANOVA test PCB, CB and PB terms first in order to reduce model to a more interpretable or reasonable model (without interaction between the deterministic factor(s) and the random factor(s)).

If the batches in the example essentially are blocks (restricted randomization) care should be exercised in interpreting the F-tests (see Montgomery p. 123).

For such blocks both physical placement and time sequence, for example, can be randomized.

The ANOVA table and the EMS column

The analysis of variance table for the above complete model has the following appearance.

Source of variation	Name of term	SSQ	d.f.	S^2	Expected mean square $= \text{EMS} = E\{S^2\}$
pH	p_i		1	S_p^2	$18\phi_p + 6\sigma^2_{PB} + 2\sigma^2_{PCB} + \sigma^2_E$
concentr.	c_j		2	S_c^2	$12\phi_c + 4\sigma^2_{CB} + 2\sigma^2_{PCB} + \sigma^2_E$
pc-interaction	pc_{ij}		2	S_{pc}^2	$6\phi_{pc} + 2\sigma^2_{PCB} + \sigma^2_E$
Batch	B_k		2	S_B^2	$12\sigma^2_B + 6\sigma^2_{PB} + 4\sigma^2_{CB} + 2\sigma^2_{PCB} + \sigma^2_E$
PB-interaction	PB_{ik}		2	S_{PB}^2	$6\sigma^2_{PB} + 2\sigma^2_{PCB} + \sigma^2_E$
CB-interaction	CB_{jk}		4	S_{CB}^2	$4\sigma^2_{CB} + 2\sigma^2_{PCB} + \sigma^2_E$
PCB-interaction	PCB_{ijk}		4	S_{PCB}^2	$2\sigma^2_{PCB} + \sigma^2_E$
Error	E_{ijkl}		18	S_E^2	σ^2_E
Total			35		

The EMS values determine how tests and component of variance estimates are constructed. What happens if the reduced model (PB=CB=PCB=0) is used?

The EMS-column, balanced design, 'unrestricted model' method

$$Y_{ijkl} = \mu + p_i + c_j + pc_{ij} + B_k + PB_{ik} + CB_{jk} + PCB_{ijk} + E_{ijkl}$$

Where do the various components appear								
EMS:	ϕ_p	ϕ_c	ϕ_{pc}	σ^2_B	σ^2_{PB}	σ^2_{CB}	σ^2_{PCB}	σ^2_E
p_i	$+$				$+$		$+$	$+$
c_j		$+$				$\boxed{+}$	$+$	$+$
pc_{ij}			$+$				$+$	$+$
B_k				$+$	$+$	$\boxed{+}$	$+$	$+$
PB_{ik}					$+$		$+$	$+$
CB_{jk}						$\boxed{+}$	$+$	$+$
PCB_{ijk}							$+$	$+$
$Error$								$+$

Rule: <u>*Random*</u> *terms of higher order which include the term itself* contribute to the EMS for a term (σ^2_{CB} contribute to the EMS for c and B and itself, see the $\boxed{+}$'s in the table).

The coefficient for a variance component is the number of observations per 'level' of the corresponding model term, for example:

p_i : 18 observations per level ($i \sim$ one pH level in the data table)

PB_{ik} : 6 observations per level (one ik-combination $=$ one pH$\times$Batch combination)

What are the coefficients								
EMS:	ϕ_p	ϕ_c	ϕ_{pc}	σ^2_B	σ^2_{PB}	σ^2_{CB}	σ^2_{PCB}	σ^2_E
p_i	18				6		2	1
c_j		12				4	2	1
pc_{ij}			6				2	1
B_k				12	6	4	2	1
PB_{ik}					6		2	1
CB_{jk}						4	2	1
PCB_{ijk}							2	1
$Error$								1

Good small examples: see slides 14.1-14.5 .

Example like 13-2 in Montgomery

Test item	Operator 1=Hansen	2=Jensen	3=Ulrich
1	y_1 y_2	y_1 y_2	y_1 y_2
:	:	:	:
:	:	:	:
20	y_1 y_2	y_1 y_2	y_1 y_2

$$Y_{ijk} = \mu + T_i + O_j + TO_{ij} + E_{ijk}$$

The model has 4 components of variance

$T_i \in N(0, \sigma^2_T)$, $O_j \in N(0, \sigma^2_O)$, $TO_{ij} \in N(0, \sigma^2_{TO})$, $E_{ijk} \in N(0, \sigma^2_E)$

$$\boxed{\text{Var}\{Y\} = \sigma^2_T + \sigma^2_O + \sigma^2_{TO} + \sigma^2_E}$$

The idea of the experiment is to assess these variances.

The ANOVA strategy: The EMS column

ANOVA table for example 13-2

Source		SSQ	d.f.	s²	E$\{s^2\}$
Test items	T_i	1185.43	19	63.39	$\sigma^2_E + 2\sigma^2_{TO} + 6\sigma^2_T$
Operators	O_j	2.62	2	1.31	$\sigma^2_E + 2\sigma^2_{TO} + 40\sigma^2_O$
TO-interaction	TO_{ij}	27.05	38	0.71	$\sigma^2_E + 2\sigma^2_{TO}$
Residual	E_{ijk}	59.50	60	0.992	σ^2_E
Total		1274.59	119		

How should we test the model. What does the E$\{s^2\}$ column tell us? Which terms first? How is the TO_{ij}-term tested?

How are the main effects T_i and O_j tested dependent on whether the TO_{ij}-term is significant or not?

Can we estimate σ^2_E (how?) and σ^2_{TO} (how?).

How are σ^2_T and σ^2_O estimated dependent on whether the TO_{ij}-term is significant or not?

The ANOVA

1: Test TO_{ij} : $F(38,60) = 0.71/0.992 = 0.71$ is not significant (< 1)

2: If σ^2_{OT} clearly insignificant, then reduce the model and pool variances (look at EMS column to see how)

ANOVA table for example 13-2, reduced model

Source	SSQ	d.f.	s²	E$\{s^2\}$	F-value
Test items	1185.43	19	63.39	$\sigma^2_E + 6\sigma^2_T$	72.0
Operators	2.62	2	1.31	$\sigma^2_E + 40\sigma^2_O$	1.49
Residual	86.55	98	0.88	σ^2_E	
Total	1274.59	119			

3: The O_j term is not significant. However, it could still be interesting to estimate all variance components, at this point:

$$\widehat{\sigma}^2_E = s^2_E = 0.88 = 0.94^2$$

$$\widehat{\sigma}^2_T = (s^2_T - s^2_E)/6 = (63.39 - 0.88)/6 = 10.42 = 3.23^2$$

$$\widehat{\sigma}^2_O = (s^2_O - s^2_E)/40 = (1.31 - 0.88)/40 = 0.011 = 0.10^2$$

Conclusion

$$\sigma^2_O \simeq 0 \Longrightarrow Y_{ijk} \longrightarrow Y_{ik} = \mu + T_i + E_{ik}$$

Revised estimates:

$$\widehat{\sigma}^2_E = \frac{SSQ_O + SSQ_E}{2+98} = \frac{2.62 + 86.55}{2+98} = 0.89 = 0.94^2$$

$$\widehat{\sigma}^2_T = (s^2_T - \widehat{\sigma}^2_E)/6 = (63.39 - 0.89)/6 = 10.42 = 3.23^2$$

Mixed effect ANOVA

ANOVA table for mixed model

Source	SSQ	d.f.	s²	E$\{s^2\}$
Test items (T_i)				$\sigma^2_E + 2\sigma^2_{TC} + 6\sigma^2_T$
Coatings (c_j)				$\sigma^2_E + 2\sigma^2_{TC} + 40\phi_c$
TC-interaction (TC_{ij})				$\sigma^2_E + 2\sigma^2_{TC}$
Residual (E_{ijk})				σ^2_E
Total				

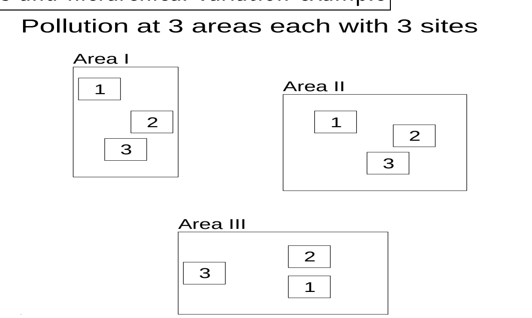
$$Y_{ijk} = \mu + T_i + c_j + TC_{ij} + E_{ijk}$$

c_j : unknown constants: $\{c_1, \ldots, c_a\}$ (with a levels). Define $\phi_c = \Sigma_{j=1}^{a} c_j^2/(a-1)$.

TC_{ij}, are unrestricted random variables as in the 'Unrestricted Mixed Model' described in Montgomery at page 498 and 504 (as used in SAS fx).

Notation : capital letters $\sim$ random terms, small letters $\sim$ deterministic terms.

Random factors and hierarchical variation example



Variation between areas and between sites within areas.

Y = Constant + Area + Site(Area) + Uncertainty(Area,Site)

The variation between 'Areas' is a random variation (there can be many 'Areas').

The effect of Area is called A_i written in capital letters indicating a random variable.

The variation between 'Sites' is a random variation within 'Areas' (indicated by parentheses as Sites(Areas))

The total variation of Y is composed of the variation from 'Area', 'Site(Area)' and the measurement 'Uncertainty' within (Area,Site)

The design is a hierarcial components of variance design :

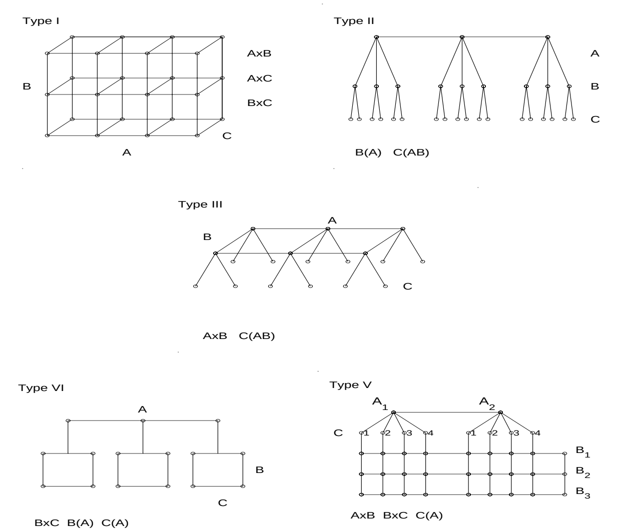
$$Y_{ijk} = \mu + A_i + S(A)_{j(i)} + U(AS)_{k(ij)}$$

sometimes only, when it is obvious that $U(AS)_{k(ij)}$ is the <u>error</u> term

$$Y_{ijk} = \mu + A_i + S(A)_{j(i)} + E_{k(ij)}$$

Assumptions: $A_i \in N(0, \sigma_A^2)$, $S(A)_{j(i)} \in N(0, \sigma_{S(A)}^2)$, $E_{k(ij)} \in N(0, \sigma_E^2)$.

All possible structures for three factors



General notation for models with many factors

Factors are a/A, b/B and c/C etc. If the factor is fixed use a_i, b_j or c_k etc. If it is random use A_i, B_j or C_k etc.

An interaction between a fixed and a random factor, fx between a_i and B_j is random and is called AB_{ij}.

A factor C_k nested within a fixed factor b_j is called $C(b)_{k(j)}$.

A factor C_k nested within a random factor B_j is called $C(B)_{k(j)}$.

A nested factor is practically always random.

The interaction between a_i and $C(b)_{k(j)}$ is called $AC(b)_{ik(j)}$ and is random.

The interaction between a_i and $C(B)_{k(j)}$ is called $AC(B)_{ik(j)}$ and is random

Indices are i, j and k while ℓ denotes repetition no. They can take the values $i = \{1...a\}$, $j = \{1...b\}$, $k = \{1...c\}$ and $\ell = \{1...r\}$.

The residual is denoted $E_{\ell(ijk)}$ and the index ℓ runs within the (ijk) combinations.

EMS tables for all (relevant) three factor models are given from slide Supplement V.1. The various models are organized as types I, II, III, IV and V corresponding to the structures shown on slide 12.1.

All EMS values correspond the 'Alternate Mixed Model', see page 526, where interactions are modeled as unrestricted random variables.

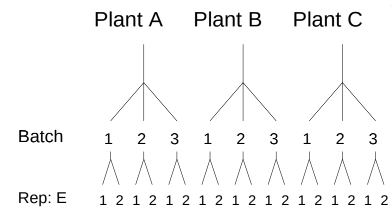
Note: In some cases there are no direct tests for all terms in the model. For example in the model $V.4$ (slide 19.12) there is no direct test for A_i. If, in this model, both AB_{ij} and $C(A)_{k(i)}$ are clearly significant, the approximate F-test (p 505) could be considered.

If, for example, AB_{ij} is not significant, reduce the model and pool the AB_{ij} SSQ with the $BC(A)_{jk(i)}$ SSQ and test the A_i term against the $C(A)_{k(i)}$ term.

In general, do the testing 'bottom up', and in many cases the EMS structure can be simplified and good tests can be constructed.

The approximate F-test is not generally recommendable, since it often has poor power.

A nested (hierarchical) design



Nested design with three batches per plant and two repetitions per batch

$$Y_{ijk} = \mu + P_i + B(P)_{j(i)} + E(PB)_{k(ij)}$$

We often write the error term shorter:

$$Y_{ijk} = \mu + P_i + B(P)_{j(i)} + E_{k(ij)}$$

Both plants and batches are random variables in this model

Another possibility is:

$$Y_{ijk} = \mu + p_i + B(p)_{j(i)} + E_{k(ij)}$$

where the plants are deterministic (fixed). Depends on how plants are selected (explain)

From crossed to nested ANOVA computations

Model: $Y = \mu + A + B(A) + C(AB) + E(ABC)$

$$\begin{array}{ll}
\text{A} \longrightarrow & \text{A} = \text{A} \\ \hline
\text{B} & \\
\text{AB} \longrightarrow & \text{B(A)} = \text{B} + \text{AB} \\ \hline
\text{C} & \\
\text{AC} & \\
\text{BC} & \\
\text{ABC} \longrightarrow & \text{C(AB)} = \text{C} + \text{AC} + \text{BC} + \text{ABC} \\ \hline
\text{E} & \\
\text{AE} & \\
\text{BE} & \\
\text{ABE} & \\
\text{CE} & \\
\text{ACE} & \\
\text{BCE} & \\
\text{ABCE} \longrightarrow & \text{E} = \text{E(ABC)} = \text{E} + \text{AE} + \ldots + \text{ABCE} \\ \hline
\end{array}$$

Applies to SSQ's and d.f.'s

From crossed to nested ANOVA computations

Model: $Y = \mu + A + B + AB + C(A) + BC(A) + E(ABC)$

$$\begin{array}{lll}
\text{A} & \longrightarrow & \text{A} = \text{A} \\
\text{B} & \longrightarrow & \text{B} = \text{B} \\
\text{AB} & \longrightarrow & \text{AB} = \text{AB} \\
\text{C} & & \\
\text{AC} & \longrightarrow & \text{C(A)} = \text{C} + \text{AC} \\
\text{BC} & & \\
\text{ABC} & \longrightarrow & \text{BC(A)} = \text{BC} + \text{BCA} \\
\text{E} & & \\
\text{AE} & & \\
\text{BE} & & \\
\text{ABE} & & \\
\text{CE} & & \\
\text{ACE} & & \\
\text{BCE} & & \\
\text{ABCE} & \longrightarrow & \text{E} = \text{E(ABC)} = \text{E} + \text{AE} + \ldots + \text{ABCE}
\end{array}$$

Example 14-1

Plant A $\sim a_1$				Plant B $\sim a_2$				Plant C $\sim a_3$			
batches				batches				batches			
1	2	3	4	1	2	3	4	1	2	3	4
94	91	91	94	94	93	92	93	95	91	94	96
92	90	93	97	91	97	93	96	97	93	92	95
93	89	94	93	90	95	91	95	93	95	95	94
279	270	278	284	275	285	276	284	285	279	281	285
1111				1120				1130			

$$SSQ_a = \frac{1111^2 + 1120^2 + 1130^2}{12} - \frac{3361^2}{36} = 15.06$$

$$SSQ_{B(a)} = \frac{279^2 + 270^2 + \ldots + 285^2}{3} - \frac{1111^2 + 1120^2 + 1130^2}{12} = 69.92$$

$$f_a = 3 - 1 = 2, \text{ and } f_{B(a)} = 3(4-1) = 9$$

Computational relation : B(a) = B + BA (or B(a) = B + AB)

Crossed computation:

Term	SSQ	d.f.
a	15.06	3-1
B	25.64	4-1
AB	44.28	(3-1)(4-1)
Residual	63.33	12(3-1)
Total	148.31	35

Nested computation:

Term	SSQ	d.f
a	15.06	3-1
B(a)	69.92	3(4-1)
Residual	63.33	12(3-1)
Total	148.31	35

Two more examples: (factors organized A, B, C, D)

1) : CD(aB) = CD + ACD + BCD + ABCD

2) : B(aCD) = B + AB + BC + ABC + BD + ABD + BCD + ABCD

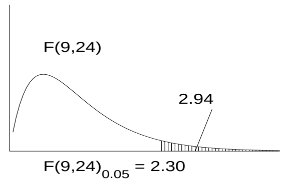
Analysis of variance - detailed

$$Y_{ijk} = \mu + a_i + B(a)_{j(i)} + E_{k(ij)}$$

Source	SSQ	d.f.	s^2	EMS
Plants	15.06	2	7.53	$\sigma_E^2 + 3\sigma_{B(a)}^2 + 12\phi_a$
Batches(plants)	69.92	9	7.77	$\sigma_E^2 + 3\sigma_{B(a)}^2$
Residual	63.33	24	2.64	σ_E^2
Total	148.31	35		

Test batches : $F_{batches} = 7.77/2.64 = 2.94 \sim F(9, 24)$

Variation between batches significant using $\alpha = 0.05$.



Test plants : $F_{plants} = 7.53/7.77 = 0.97 \sim F(2,9)$

Since $F(2,9)_{0.05} = 4.26 > 0.97$ plants are not significantly different

Reduced model, write fx:

$$Y_{ijk} = \mu + B_{ij} + E_{k(ij)}$$

Conclusion for example 14-1

Source	SSQ	d.f.	s^2	EMS
	15.06	2		
	69.92	9		
Batches	84.98	11	7.73	$\sigma_E^2 + 3\sigma_B^2$
Residual	63.33	24	2.64	σ_E^2
Total	148.31	35		

Estimation:

Level: $\widehat{\mu} = 3361/36 = 93.4$

$\widehat{\sigma}_E^2 = 2.64 = 1.63^2$

$\widehat{\sigma}_B^2 = (7.73 - 2.64)/3 = 1.70 = 1.30^2$

Model again : $Y = \mu + B + E$

Var$\{Y\} = \sigma_B^2 + \sigma_E^2 \simeq 2.64 + 1.70 = 2.08^2$

More nested (hierarchical) models

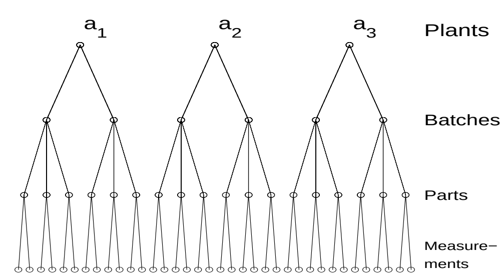
	Plant A (a_1)						Plant B (a_2)						Plant C (a_3)					
Batches	I			II			I			II			I			II		
Parts	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
Data	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y
	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y	y

For each plant two batches are selected. From each batch three parts are formed (selected), and on each part two measurements are performed.

Mathematical model (for fixed plants $\sim a_i$) :

$$Y_{ijk\ell} = \mu + a_i + B(a)_{j(i)} + P(aB)_{k(ij)} + E_{\ell(ijk)}$$

In the design, essentially, 3×2 = 6 different batches are used and 3×2×3 = 18 different parts.

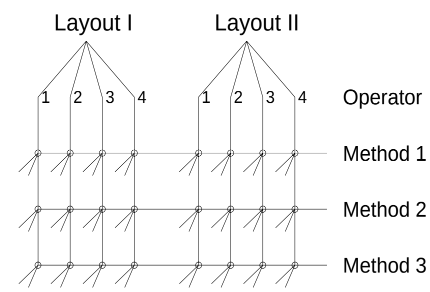


Mixed model, example 14-2 p. 536

Layout	I				II			
Operator	1	2	3	4	1	2	3	4
	KKA	EMB	AHJ	HS	MK	PBB	HM	HR
Method 1	y	y	y	y	y	y	y	y
	y	y	y	y	y	y	y	y
Method 2	y	y	y	y	y	y	y	y
	y	y	y	y	y	y	y	y
Method 3	y	y	y	y	y	y	y	y
	y	y	y	y	y	y	y	y

Eight different operators (indicated by their initials) participated.
The factor 'Operator' is random and nested within 'Layout'.

Design in principle



$$Y_{ijk\nu} = \mu + m_i + l_j + ml_{ij} + O(l)_{k(j)} + MO(l)_{ik(j)} + E_{\nu(ijk)}$$

Note: Totally 8 different operators participated, 4 for each layout.

ANOVA table and expected mean squares computation

Source		SSQ	d.f	s^2	E$\{s^2\}$
Methods	(m)	82.80	3−1	41.4	see
Layouts	(l)	4.08	2−1	4.08	below
Interaction	(m×l)	19.04	2	9.52	
Operators	(O(l))	71.91	6	11.99	
Interaction	(m×O(l))	65.84	12	5.49	
Residual	E	56.00	24	2.33	
Total		299.67	48−1		

Model	3	2	4	2	Expected mean squares					
term	i	j	k	ν	ϕ_m	ϕ_l	ϕ_{ml}	$\sigma^2_{O(l)}$	$\sigma^2_{MO(l)}$	σ^2_E
m_i	0	2	4	2	16				2	1
l_j	3	0	4	2		24		6	2	1
ml_{ij}	0	0	4	2			8		2	1
$O(l)_{k(j)}$	3	1	1	2				6	2	1
$MO(l)_{ik(j)}$	1	1	1	2					2	1
$E_{\nu(ijk)}$	1	1	1	1						1

The first test is:

$F_{MO(l)} = 5.49/2.33 = 2.36 \sim F(12, 24)$

$F(12, 24)_{0.05} = 2.18 < 2.36 \Longrightarrow MO(l)$ term significant (in principle)

Remaining tests can then be based on $s^2_{MO(l)}$ with 12 degrees of freedom

The remaining tests

$F_{O(l)} = 11.99/5.49 = 2.18 \;<\; F(6, 12)_{0.05} = 3.00$

It can be discussed whether the $O(l)$-term should be removed from model.

In principle

$F_{ml} = 9.52/5.49 = 1.73 < \; F(2, 12)_{0.05} = 3.89$

The ml-term is not significant

Test of layouts : $F_l = s^2_l/s^2_{O(l)} = 4.08/11.99 = 0.34 << \; F(1, 6)_{0.05} = 5.99$

$\boxed{\text{Alternatively:}}$

Remove $O(l)$ from model and compute

$s^2_{MO(l)-new} = (65.84 + 71.91)/(12 + 6) = 7.65$, with d.f.$= 12 + 6 = 18$ and then

$F_{ml} = 9.52/7.65 = 1.24 < F(2, 18)_{0.05} = 3.55$

$F_l = 4.08/7.65 = 0.53 << \ F(1, 18)_{0.05} = 8.29$

Same conclusion : ml-interaction and l-effect not significant

The layouts are probably not different !

$\boxed{\text{Test of methods}}$

Directly : $F_m = s^2_m/s^2_{MO(l)} = 7.54 \sim F(2, 12)$

Alternatively : $F_m = s^2_m/s^2_{MO(l)-new} = 5.41 \sim F(2, 18)$

Both cases result in significance

$\boxed{\text{Conclusion:}}$ Layouts are not of importance, but methods and operators are:

$$Y_{ijk\nu} = \mu + m_i + O_k + MO_{ik} + E_{\nu(ik)}$$

$\widehat{\sigma}^2_E = s^2_E = 2.33 = 1.53^2$

$\widehat{\sigma}^2_{MO} = (s^2_{MO} - s^2_E)/2 = \frac{5.49-2.33}{2} = 1.58 = 1.26^2$

$\widehat{\sigma}^2_O = (s^2_O - s^2_{MO})/6 = \frac{11.99-5.49}{6} = 1.08 = 1.04^2$

$\widehat{\mu} = \overline{Y}_{....} = 1252/48 = 26.08$

$\widehat{m}_1 = \overline{Y}_{1...} - \overline{Y}_{....} = 404/16 - 26.08 = -0.83$

$\widehat{m}_2 = \overline{Y}_{2...} - \overline{Y}_{....} = 447/16 - 26.08 = +1.86$

$\widehat{m}_3 = \overline{Y}_{3...} - \overline{Y}_{....} = 401/16 - 26.08 = -1.02$

Significant differences between methods found. The best (fastest assembly time) is no. 3, with estimated mean $26.08 - 1.02 = 25.06$. Three (or two) components of variance identified.

$\boxed{\text{Model with two crossed factors, both fixed}}$

	Temperature		
Concentr.	15^{o}C	25^{o}C	35^{o}C
1%	y y	y y	y y
2%	y y	y y	y y

Two crossed factors both fixed

$$Y_{ijk} = \mu + c_i + t_j + ct_{ij} + E_{k(ij)}$$

Model	a	b	r	EMS			
term	i	j	k	ϕ_c	ϕ_t	ϕ_{ct}	σ^2_E
c_i	0	b	r	br=6			1
t_j	a	0	r		ar=4		1
ct_{ij}	0	0	r			r=2	1
$E_{k(ij)}$	1	1	1				1

In the example
a=2
b=3
r=2

The table also correspond to the EMS-method described slide 19.1.

$\boxed{\text{Two random factors crossed}}$

	Operator		
Batch	Hans	John	Curt
Batch I	y y	y y	y y
Batch II	y y	y y	y y

Two crossed factors both random

$$Y_{ijk} = \mu + B_i + O_j + BO_{ij} + E_{k(ij)}$$

Model	a	b	r	EMS			
term	i	j	k	σ^2_B	σ^2_O	σ^2_{BO}	σ^2_E
B_i	1	b	r	br=6		r=2	1
O_j	a	1	r		ar=4	r=2	1
BO_{ij}	1	1	r			r=2	1
$E_{k(ij)}$	1	1	1				1

In the example
a=2
b=3
r=2

Two factors, one fixed and one random

	Operator		
Method	Joan	Anna	Miriam
m_1	y y	y y	y y
m_2	y y	y y	y y
m_3	y y	y y	y y

Two crossed factors
one fixed
one random

$$Y_{ijk} = \mu + m_i + O_j + MO_{ij} + E_{k(ij)}$$

Model term	a i	b j	r k	EMS ϕ_m	σ_O^2	σ_{MO}^2	σ_E^2
m_i	0	b	r	br=6		r=2	1
O_j	a	1	r		ar=6	r=2	1
MO_{ij}	1	1	r			r=2	1
$E_{k(ij)}$	1	1	1				1

In the example
a=3
b=3
r=2

Two factors, one fixed and one nested and random

Rule: A nested factor will in practice always be random

	Animals		
Gender	1	2	3
Males	y y	y y	y y
Females	y y	y y	y y

Two factors,
one fixed,
one random and
nested

$$Y_{ijk} = \mu + g_i + A(g)_{j(i)} + E_{k(ij)}$$

Model term	a i	b j	r k	EMS ϕ_g	$\sigma_{A(g)}^2$	σ_E^2
g_i	0	b	r	br=6	r=2	1
$A(g)_{j(i)}$	1	1	r		r=2	1
$E_{k(ij)}$	1	1	1			1

In the example
a=2
b=3
r=2

Two random factors, one nested

	Animals		
Litter	1	2	3
L_1	y y y	y y y	y y y
L_2	y y y	y y y	y y y
L_3	y y y	y y y	y y y
L_4	y y y	y y y	y y y

Two factors,
one nested,
both random

$$Y_{ijk} = \mu + L_i + A(L)_{j(i)} + E_{k(ij)}$$

Model term	a i	b j	r k	EMS σ_L^2	$\sigma_{A(L)}^2$	σ_E^2
L_i	0	b	r	br=9	r=3	1
$A(L)_{j(i)}$	1	1	r		r=3	1
$E_{k(ij)}$	1	1	1			1

In the example
a=4
b=3
r=3

For each litter three animals are considered and three measurements are made on each animal. Thus totally 12 animals participated.

Split plot designs

Example: Treatments at different temperatures and using different lengths of times of treatment.

Factorial design

	Temperature			
	20^oC	25^oC	30^oC	35^oC
5 min	217	158	229	223
	188	126	160	201
	162	122	167	182
10 min	233	138	186	227
	201	130	170	181
	170	185	181	201
15 min	175	152	155	156
	195	147	161	172
	213	180	182	199

Naive model : $Y_{ijk} = \mu + t_i + m_j + tm_{ij} + E_{k(ij)}$

Source	SSQ	d.f.	s^2	EMS
Temperatures	12494	3	4165	$\sigma_E^2 + 9\phi_t$
Minutes	566	2	283	$\sigma_E^2 + 12\phi_m$
Interaction	2601	6	434	$\sigma_E^2 + 3\phi_{tm}$
Residual	13670	24	570	σ_E^2
Total	29331	35		

A question of randomization

How should the experiment be carried out ideally. The following shows a randomization scheme:

Complete randomization

	20^{o}C	25^{o}C	30^{o}C	35^{o}C
5 min	25	3	24	26
	7	30	2	10
	12	4	34	11
10 min	13	14	15	8
	6	1	20	32
	22	21	36	23
15 min	17	16	27	35
	5	31	29	9
	18	28	33	19

The table shows the order in which the measurements are performed using complete randomization

Is it thinkable that this is how it was carried out? - No, because it would take a very long time to do so.

How would it often be carried out in practice instead?

A wrong randomization scheme

Carry out one temperature at a time. Only randomization within temperatures:

No randomization
between temperatures

	20^{o}C	25^{o}C	30^{o}C	35^{o}C
5 min	18	1	22	31
	14	9	27	33
	13	2	23	32
10 min	10	4	19	34
	16	8	24	30
	17	5	26	29
15 min	11	3	20	36
	12	7	21	35
	15	6	25	28

The 9 measurements at 25^{o}C are carried out first, then the 9 measurements at 20^{o}C, then 30^{o}C and finally 35^{o}C.

Since all measurements at one temperature level are carried out together one temperature level is also a block!

$$Y_{ijk} = \mu + t_i + B_i(\text{block } i) + m_j + tm_{ij} + E_{k(ij)}$$

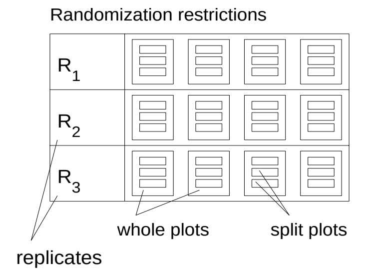
t_i and B_i are confounded. The temperature effect cannot be estimated free from the blocking or tested.

The split plot design

Use three rounds and carry out each temperature at a time. Randomize minutes within temperatures:

Round	Minutes	20^{o}C	25^{o}C	30^{o}C	35 ^{o}C
I	5 min	6	1	7	10
	10 min	4	2	9	11
	15 min	5	3	8	12
II	5 min	14	22	21	17
	10 min	13	23	19	18
	15 min	15	24	20	16
III	5 min	30	25	33	34
	10 min	29	27	32	36
	15 min	28	26	31	35

The three measurements no. $\boxed{\begin{array}{c}\boxed{25}\\ \boxed{27}\\ \boxed{26}\end{array}}$, for example, now form a block: A whole plot with 3 split plots.



The split plot model

Data example for a split plot experiment					
Round	Minutes	20^{o}C	25^{o}C	30^{o}C	35 ^{o}C
I	5 min	217	158	217	217
	10 min	233	138	233	233
	15 min	175	152	175	175
II	5 min	188	126	160	201
	10 min	201	130	170	181
	15 min	195	147	161	172
III	5 min	162	122	167	182
	10 min	170	185	181	201
	15 min	213	180	182	199

$$Y_{ijk\ell} = \mu + R_i + t_j + RT_{ij} + m_k + RM_{ik} + tm_{jk} + RTM_{ijk} + E_{\ell(ijk)}$$

RT_{ij} is called the whole plot error

RTM_{ijk} is called the split plot error

$RT_{ij} = R \times t$-interaction + block-effect(i,j) is a random variable

$RTM_{ijk} = R \times t \times m$-interaction + split-plot-effect(i,j,k)

is also a random variable

ANOVA of split plot experiment

Model term	σ_R^2	ϕ_t	σ_{RT}^2	ϕ_m	σ_{RM}^2	ϕ_{tm}	σ_{RTM}^2	σ_E^2
R_i	12		3		4		1	1
t_j		9	3				1	1
RT_{ij}			3				1	1
m_k				12	4		1	1
RM_{ik}					4		1	1
tm_{jk}						3	1	1
RTM_{ijk}							1	1
$E_{\ell(ijk)}$								1

Source	SSQ	d.f.	s^2	F-test
R_i	1963	2	982	
t_j	12494	3	4165	$F_t = 4165/296 \sim F(3,6)$
RT_{ij}	1774	6	296	
m_k	566	2	283	$F_m = 283/1755 \sim F(2,4)$
RM_{ik}	7021	4	1755	
tm_{jk}	2601	6	434	$F_{tm} = 434/243 \sim F(6,12)$
RTM_{ijk}	2912	12	243	
$E_{\ell(ijk)}$	0	0	–	
Total	29331	35		

It is problematic, that the RM_{ik} term is so large. It would be reasonable if it was small to test the m_k term against the split plot error term RTM_{ijk}.

Under all circumstances, the temperature (t_j) is significant, but the time (m_k) is not.

Repeated measures design

Characteristics: Several treatments applied to the same “individual”:

Treat-ment	Individual number 1	2	...	...	n
1	y_{11}	y_{12}			y_{1n}
2	y_{21}	y_{22}			y_{2n}
...	...	...	...	...	...
...	...	...	...	...	...
a	y_{a1}	y_{a2}			y_{an}

The design is not completely randomized. Randomization can sometimes be made within individuals (persons), sometimes not (time). Measurements on the same individual are correlated - the time sequence may be important.

Partition of sums of squares in the simplest case

$$Y_{ijk} = \mu + a_i + P_j + AP_{ij} + E_{k(ij)}$$

$\Sigma_{j=1}^{n} a(\overline{Y}_{.j} - \overline{Y}_{..})^2 =$ Variation between individuals

$\Sigma_{i=1}^{a} \Sigma_{j=1}^{n} (Y_{ij} - \overline{Y}_{.j})^2 =$ variation within individuals

$= \Sigma_{i=1}^{a} n(\overline{Y}_{i.} - \overline{Y}_{..})^2 + \Sigma_{i=1}^{a} \Sigma_{j=1}^{n} (Y_{ij} - \overline{Y}_{i.} - \overline{Y}_{.j} + \overline{Y}_{..})^2$

$SSQ_{Treatments} + SSQ_{Uncertainty}$

ANOVA technique if correlation within individuals is neglected

Model term	EMS ϕ_a	σ_P^2	σ_{AP}^2	σ_E^2
a_i	n		1	1
P_j		a	1	1
AP_{ij}			1	1
$E_{k(ij)}$				1

For k $=1$ there is no estimate for σ_E^2 (no degrees of freedom).

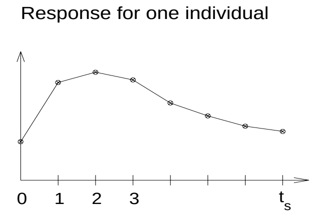
E$\{s_{AP}^2\} = \sigma_{AP}^2 + \sigma_E^2$ (confounding of AP_{ij} and $E_{k(ij)}$)

The design can analyzed as a two-way ANOVA with one fixed and one random factor if the correlation within individuals is small (not too many treatments per individual).

A more realistic repeated measures design

Often used in the development of drugs

Treatment group	Individual	Time 1	2	3	...	...	t_s
No dose (vehicle)	1	y	y	y	...	...	y
	2	y	y	y	...	...	y
	3	y	y	y	...	...	y
Low dose	4	y	y	y	...	...	y
	5	y	y	y	...	...	y
	6	y	y	y	...	...	y
Medium dose	7	y	y	y	...	...	y
	8	y	y	y	...	...	y
	9	y	y	y	...	...	y
High dose	10	y	y	y	...	...	y
	11	y	y	y	...	...	y
	12	y	y	y	...	...	y



Repeated measures model with time effect

$$Y_{ijk\ell} = \mu + a_i + P(a)_{j(i)} + t_k + at_{ik} + PT(a)_{jk(i)} + E_{\ell(ijk)}$$

Model term		EMS ϕ_a	$\sigma_{P(a)}^2$	ϕ_t	ϕ_{at}	$\sigma_{PT(a)}^2$	σ_E^2
a_i	= treatments	pt	t			1	1
$P(a)_{j(i)}$	= individuals		t			1	1
t_k	= time			ap		1	1
at_{ik}					p	1	1
$PT(a)_{jk(i)}$						1	1
$E_{\ell(ijk)}$							1

No estimate for σ_E^2 (no degrees of freedom)

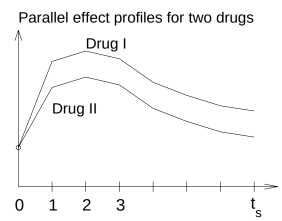
The model structure corresponds to a type $V.1$ model.

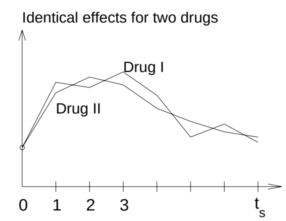
The time point '0' is special (no effect start value)

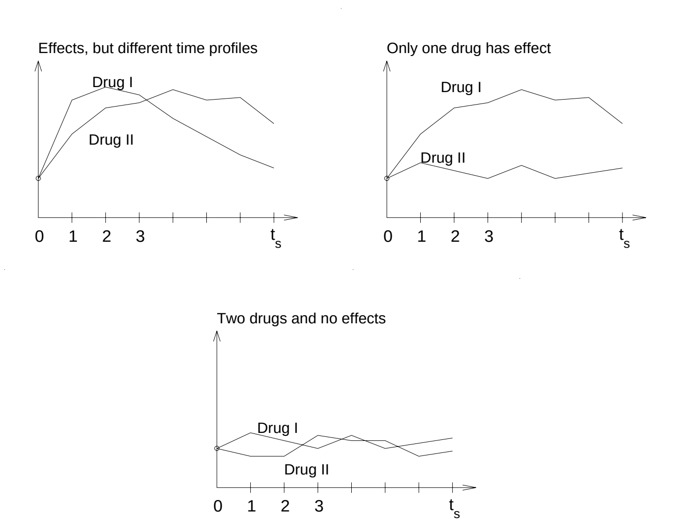
A special problem is time$\times$treatment interaction as illustrated below

A model for the (auto-) correlation within individuals is generally needed

Time Effect profiles







A repeated measures example - two measurements per individual

Group	Individuals	Pretest: t_1	Post-test: t_2
Training program I a_1	1	26.25	29.50
	2	24.33	27.62
	3	22.52	25.71
	4	29.33	31.55
	5	28.90	31.35
	6	25.13	29.07
	7	29.33	31.15
Training program II a_2	8	27.47	28.74
	9	25.19	26.11
	10	23.53	25.45
	11	24.57	25.58
	12	26.88	27.70
	13	27.86	28.82
	14	28.09	28.99
Training program III a_3	15	22.27	22.52
	16	21.55	21.79
	17	23.31	23.53
	18	30.03	30.21
	19	28.17	28.65
	20	28.09	28.33
	21	27.55	27.86

Description and model

3 groups of 7 persons are presented to 3 training programs and their throwing velocities are measured before and after the training

The 21 individuals are randomly allocated to the groups

$$Y_{ijk\ell} = \mu + a_i + P(a)_{j(i)} + t_k + at_{ik} + PT(a)_{jk(i)} + E_{\ell(ijk)}$$

a_i = treatments, $P(a)_{j(i)}$ = individuals, t_k = time periods.

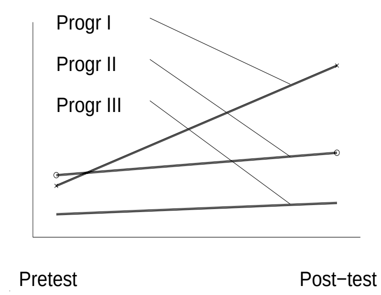
The number of treatments per individual is only 2, so the autocorrelation cannot be distinguished from the treatment effect (and it is most often assumed to be small in this case).

ANOVA under the no-autocorrelation assumption

Model term	EMS ϕ_a	$\sigma^2_{P(a)}$	ϕ_t	ϕ_{at}	$\sigma^2_{PT(a)}$	σ^2_E
a_i	14	2			1	1
$P(a)_{j(i)}$		2			1	1
t_k			21		1	1
at_{ik}				7	1	1
$PT(a)_{jk(i)}$					1	1
$E_{\ell(ijk)}$						1

Source	SSQ	d.f.	s^2	
Program a_i	28.14	2	14.07	$\mathrm{F}_a = 14.07/13.49$
Indiv(progr) $P(a)_{j(i)}$	242.91	18	13.49	
Time t_k	21.26	1	21.26	$\mathrm{F}_t = 21.26/0.117$
Program×Time at_{ik}	12.38	2	6.19	$\mathrm{F}_{at} = 6.19/0.117$
Indiv×Time(progr)	2.10	18	0.117	
Residual	0.00	0		
Total	306.79	41		

Graphical representation of results



Comments on the results found

There is a significant mean effect from participating in a training program. However, the differences between alternative programs are not statistically significant.

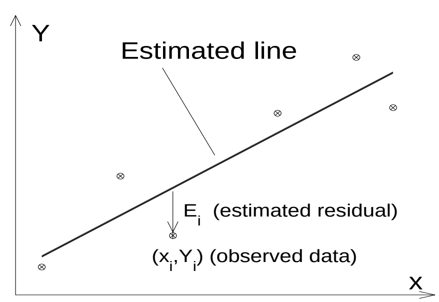
The analysis assumes that complete randomization was applied, but, of course, the factor 'time' cannot be randomized. This is not accounted for in the example.

However the tests used are still reasonable, and the results are understandable.

There is much literature about correct analyses of repeated measures designs.

In designs where 'time' is the factor within individuals there are models which take the time sequence into account using time series analysis methods (autocorrelation for example).

Regression analysis, introduction



$$Y_i = \mu + \alpha \cdot x_i + E_i$$

A linear regression line, the simplest univariate case

Linear regression model and assumptions

$$Y_i = \mu + \alpha \cdot x_i + E_i$$

Assumption : $E_i \in$ Normal$(0, \sigma_E^2)$

Method : Least squares for $\widehat{E}_i = Y_i - \widehat{\mu} - \widehat{\alpha} \cdot x_i$

Solution :

$\widehat{\alpha} = \Sigma_i (Y_i - \overline{Y})(x_i - \overline{x}) / \Sigma_i (x_i - \overline{x})^2$ and $\widehat{\mu} = \overline{Y} - \widehat{\alpha}\overline{x}$

$\widehat{\sigma}_E^2 = [\ Y_i - \widehat{\mu} - \widehat{\alpha} \cdot x_i]^2 / (n-2)$

There is at least one solution.

Some concepts on regression

An estimated regression equation is an empirical model, that is a model based on data.

x_i is value set by the experimenter for the i'th measurement, it is a deterministic quantity chosen by the experimenter without (or with an unimportant) uncertainty.

Y_i is the measured value in case no. i,

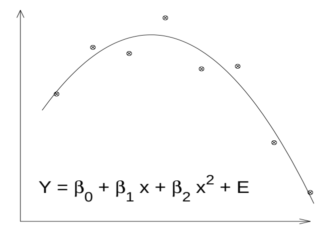
and Y_i is a random variable with

the expectation $\mathsf{E}\{Y_i\} = \mu + \alpha \cdot x_i$ and

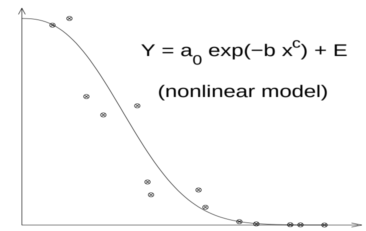
the variance $\mathsf{Var}\{Y_i\} = \mathsf{Var}\{E_i\} = \sigma_E^2$

The errors E_i are assumed to independent with constant variance and (at least approximately) normally distributed.

Two examples of regression equation



Polynomial linear regression estimation

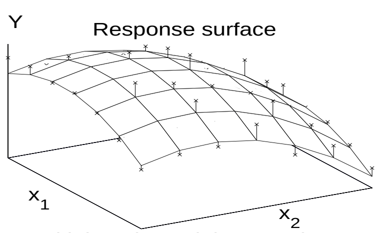


General function estimation

The first example is called a polynomial regression model.

The second example is an example of a non-linear regression model (non-linear in the unknown parameters a_0, b and c).

A regression model often used for optimization of chemical processes



Multiple polynomial regression

$$Y = \alpha + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \gamma_1 \cdot x_1^2 + \gamma_2 \cdot x_2^2 + \delta \cdot x_1 x_2 + E$$

An example of a multiple linear regression model.

Multiple linear regression by an example

Exercise 10-12 and 10-13.

Data and polynomial variables

Y	x_1	x_2	x_1^2	x_2^2	x_1x_2
26	1.0	1.0	1.0	1.0	1.0
24	1.0	1.0	1.0	1.0	1.0
175	1.5	4.0	2.25	16.0	6.0
160	1.5	4.0	2.25	16.0	6.0
163	1.5	4.0	2.25	16.0	6.0
55	0.5	2.0	0.25	4.0	1.0
62	1.5	2.0	2.25	4.0	3.0
100	0.5	3.0	0.25	9.00	1.5
26	1.0	1.5	1.0	2.25	1.5
30	0.5	1.5	0.25	2.25	0.75
70	1.0	2.5	1.0	6.25	2.5
71	0.5	2.5	0.25	6.25	1.25

Determine 2nd order polynomial response function. Linear regression (computer program) yields:

Linear regression estimation

Model	μ	x_1	x_2	x_1^2	x_2^2	x_1x_2
Estimates	24.41	-38.03	0.72	34.98	11.07	-9.98
Standard dev.	26.59	40.45	11.68	21.56	3.16	8.74
t−values	0.92	-0.94	0.06	1.62	3.50	-1.14
p−values (two sided)	0.39	0.38	0.95	0.16	0.01	0.30

Several insignificant coefficients $\Longrightarrow$ reduce model

General regression model test - examples

Layout of the general test

$$\text{Full model} : Y_i = \beta_0 + \beta_1 \cdot x_{i,1} + \ldots + \beta_k \cdot x_{i,k} + E_i$$

$$\text{Reduced model} : Y_i = \beta_0 + \beta_1 \cdot x_{i,1} + \ldots + \beta_m \cdot x_{i,m} + E_i$$

where $m < k$ (fewer independent variables):

The general multiple F-test

Source	SSQ	d.f.	s^2	F-value
Removed terms	SSQ_2=SSQ_0-SSQ_1	f_2=k-m	s_2^2	s_2^2/s_1^2
Residual full model	SSQ_1	f_1=N-k-1	s_1^2	
Reduced model	SSQ_0	f_0=N-m-1		

The table shows a (large) number of reasonable model alternatives:

Model based on	Residual SSQ	d.f.
μ x_1 x_2 x_1^2 x_2^2 x_1x_2	219.07	$12-6=6$
μ x_1 x_2 x_1^2 x_2^2	266.71	$12-5=7$
μ x_1 x_2 x_1^2	787.48	$12-4=8$
μ x_1 x_2 x_2^2	331.89	$12-4=8$
μ x_1 x_1^2	12319.00	$12-3=9$
μ x_2 x_2^2	373.23	$12-3=9$
μ x_1 x_2	809.36	$12-3=9$
μ x_1	23759.67	$12-2=10$
μ x_2	1331.87	$12-2=10$
μ	35311.67	$12-1=11$

Test the term x_1x_2:

Source	SSQ	d.f.	s^2	F-value
x_1x_2	266.71−219.07	1	47.64	1.30
Residual	219.07	6	36.51	
Total	266.71	7		

Test both terms x_1^2 and x_1x_2 in full model:

Source	SSQ	d.f.	s^2	F-value
x_1^2 and x_1x_2	331.89−219.07	2	56.41	1.55
Residual (full model)	219.07	6	36.51	
Total (without x_1^2 and x_1x_2)	331.89	8		

Test if x_1 can be removed from full model:

Source	SSQ	d.f.	s^2	F-value
x_1, x_1^2 and x_1x_2	373.23−219.07	3	51.38	1.41
Residual (full model)	219.07	6	36.51	
Total (without x_1)	373.23	9		

The test shows, that the removal of x_1, x_1^2 and x_1x_2 from the model does not increase the uncertainty significantly, since $F(3,6)_{0.05} = 4.76 >> 1.41$.

An alternative strategy could be (successive testing):

Start by concluding x_1x_2 not significant (no interaction!) and remove it from the full model:

Model based on	Residual SSQ	d.f.
μ x_1 x_2 x_1^2 x_2^2	266.71	$12-5=7$
μ x_1 x_2 x_1^2	787.48	$12-4=8$
μ x_1 x_2 x_2^2	331.89	$12-4=8$
μ x_1 x_1^2	12319.00	$12-3=9$
μ x_2 x_2^2	373.23	$12-3=9$
μ x_1 x_2	809.36	$12-3=9$
μ x_1	23759.67	$12-2=10$
μ x_2	1331.87	$12-2=10$
μ	35311.67	$12-1=11$

The following test(s) can then be based on the residual SSQ 266.71 with 7 d.f.

Conclusion for the example:

The following model could be reasonable to use:

Possible model proposal

Model	μ	x_1	x_2	x_2^2
Estimates	1.74	6.27	6.41	8.09
Standard dev.	16.09	6.28	11.87	2.39
t−values	0.11	1.00	0.54	3.39
p−values (two sided)	0.92	0.35	0.60	0.01

x_2^2 is significant, so x_2 cannot be removed.

x_1 is not significant, but it may be of interest to assess its influence anyhow.

Sometimes it is difficult to find a good model!

The partial F-test

Consider again:

Estimated model

Model	μ	x_1	x_2	x_2^2
Estimates	1.74	6.27	6.41	8.09
Standard dev.	16.09	6.28	11.87	2.39
t−values	0.11	1.00	0.54	$\boxed{3.39}$
p−values (two sided)	0.92	0.35	0.60	0.01

Suppose we want to test x_2^2 separately (however reasonable), based on this model.

Model based on	Residual SSQ	d.f.
μ x_1 x_2 x_2^2	331.89	$12-4=8$
μ x_1 x_2	809.36	$12-3=9$

Test for one parameter - partial F-test				
Source	SSQ	d.f.	s^2	F-value
x_2^2	477.47	1	477.47	$s_2^2/s_1^2 = 11.50 = 3.39^2$
Residual	331.89	8	41.84	Note: F = t^2 here
Reduced model	809.36	9		

The partial F-test is equivalent to the two-sided t-test when d.f. $= 1$.

It is used to remove parameters from the model one-by-one. This method is called 'backwards elimination'.

ANOVA and multiple regression example

Machines				ANOVA model
1	22	36	52	$Y_{ij} = \mu + \alpha_i + \beta_j + E_{ij}$
2	31	missing	59	
Treatments	1	2	3	

Formulation as regression model: $Y = x\theta + E$:

$$\begin{Bmatrix} 22 \\ 36 \\ 52 \\ 31 \\ 59 \end{Bmatrix} = \begin{Bmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{Bmatrix} \begin{Bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{Bmatrix} + \begin{Bmatrix} E_{11} \\ E_{12} \\ E_{13} \\ E_{21} \\ E_{23} \end{Bmatrix}$$

Model is overparametrized: Use two (linear) restrictions!

Result of estimation (use fx: $\alpha_2 = 0$ and $\beta_3 = 0$)

$\widehat{\mu}$	$\widehat{\alpha}_1$	$\widehat{\alpha}_2$	$\widehat{\beta}_1$	$\widehat{\beta}_2$	$\widehat{\beta}_3$
59.5	-8.0	0.0	-29.0	-15.5	0.0

Estimated values are $\widehat{Y}_{ij} = \widehat{\mu} + \widehat{\alpha}_i + \widehat{\beta}_j \quad \Rightarrow \quad \widehat{Y} = \begin{array}{|ccc|} 22.5 & 36.0 & 51.5 \\ 30.5 & \boxed{44.0} & 59.5 \end{array}$

and residuals $\widehat{E} = Y - \widehat{Y} = \begin{array}{|ccc|} -0.5 & 0.0 & 0.5 \\ 0.5 & \text{missing} & -0.5 \end{array}$

$SSQ_{resid} = 1.00$, df=5-(3-1)-(2-1)=1

Test of parameters

Test for row effect: $H_0^\alpha : Y_{ij} = \mu + \beta_j + E_{ij} \Leftrightarrow \{\alpha_1 = \alpha_2 = 0\}$.

Test for column effect: $H_0^\beta : Y_{ij} = \mu + \alpha_i + E_{ij} \Leftrightarrow \{\beta_1 = \beta_2 = \beta_3 = 0\}$.

H_0^α is a hypothetical model <u>without</u> row effect, and H_0^β is a hypothetical model <u>without</u> column effect.

Compute residual SSQ for model H_0^α: $Y_{ij} = \mu + \beta_j + E_{ij}$, : $\rightarrow$ 65.00

ANOVA for H_0^α

Source of variation	SSQ	f	F-value
Rows	64.0	2−1	$\frac{64.0/1}{1.0/1} = 64.00$
Residual	1.0	1	$\sim F(1,1)$
Total under H_0^α	65.0	2	

Compute residual SSQ for model H_0^β: $Y_{ij} = \mu + \alpha_i + E_{ij}$: $\rightarrow$ 842.76

ANOVA for H_0^β

Source of variation	SSQ	f	F-value
Columns	841.67	3−1	$\frac{841.67/2}{1.0/1} = 420.83$
Residual	1.0	1	$\sim F(2,1)$
Total under H_0^β	842.67	3	

The two tables can be collected in one ANOVA table:

Exact ANOVA for H_0^α and H_0^β

Source of variation	SSQ	f	F-value
Rows	64.00	2−1	$\frac{64.0/1}{1.0/1} = 64.00$
Columns	841.67	3−1	$\frac{841.67/2}{1.0/1} = 420.83$
Residual	1.0	1	
Total	925.00	5−1	

It is noted that the two sums of squares for rows and columns show the increase of residual SSQ when the row and column parameters are removed from the full model.

Since the data are not balanced the sums of squares for rows, columns and residual do not sum to the total sum of squares.

Analysis of covariance: ANOVA with covariate

Determination of yield (Y) by addition of a chemical in alternative concentrations: (5%,10%,15%).

A non-controllable factor is degree of purity (x) in raw material. However, we assume that x can be measured.

The results were

5%		10%		15%	
Y	x	Y	x	Y	x
36	20	40	22	35	21
41	25	48	28	37	23
39	24	39	22	42	26
42	25	45	30	34	21
49	32	44	28	32	15

Simple model : $Y_{ij} = \mu + a_i + \epsilon_{ij}$

Model with correction for the covariate x:

$$Y_{ij} = \mu + a_i + \beta \cdot (x_{ij} - \overline{x}_{..}) + E_{ij}$$

or using $\mu^* = \mu - \beta\overline{x}_{..}$

$$Y_{ij} = \mu^* + a_i + \beta \cdot x_{ij} + E_{ij}$$

Which model is the best. What is the risk by using the model neglecting the covariate x ?

How large is Var$\{\epsilon_{ij}\} = \sigma_\epsilon^2$?

$\sigma_\epsilon^2 =$ Var$\{\beta x_{ij} + E_{ij}\} = \beta^2 \cdot$Var$\{x_{ij}\} + \sigma_E^2$

If x_{ij} varies much and β is not very small the residual variance σ_ϵ^2 can be much larger than $\sigma_E^2 \Rightarrow$ The simple model yields less precise estimates and poorer tests.

Mathematical model in general formulation

$$Y = \left\{ \begin{array}{c} 36 \\ 41 \\ 39 \\ 42 \\ 49 \\ 40 \\ 48 \\ 39 \\ 45 \\ 44 \\ 35 \\ 37 \\ 42 \\ 34 \\ 32 \end{array} \right\} \text{ and } x = \left\{ \begin{array}{ccccc} 1 & 1 & 0 & 0 & 20 \\ 1 & 1 & 0 & 0 & 25 \\ 1 & 1 & 0 & 0 & 24 \\ 1 & 1 & 0 & 0 & 25 \\ 1 & 1 & 0 & 0 & 32 \\ 1 & 0 & 1 & 0 & 22 \\ 1 & 0 & 1 & 0 & 28 \\ 1 & 0 & 1 & 0 & 22 \\ 1 & 0 & 1 & 0 & 30 \\ 1 & 0 & 1 & 0 & 28 \\ 1 & 0 & 0 & 1 & 21 \\ 1 & 0 & 0 & 1 & 23 \\ 1 & 0 & 0 & 1 & 26 \\ 1 & 0 & 0 & 1 & 21 \\ 1 & 0 & 0 & 1 & 15 \end{array} \right\}$$

$\theta = \{\mu^*, a_1, a_2, a_3, \beta\}^T$ and $Y = x\theta + E$

Least squares estimation :

$$\widehat{\beta} = \frac{\Sigma_i \Sigma_j (Y_{ij} - \overline{Y}_{i.})(x_{ij} - \overline{x}_{i.})}{\Sigma_i \Sigma_j (x_{ij} - \overline{x}_{i.})^2}$$

$$\widehat{a}_i = \overline{Y}_{i.} - \overline{Y}_{..} - \widehat{\beta}(\overline{x}_{i.} - \overline{x}_{..}) \qquad \widehat{\mu}^* = \overline{Y}_{..} - \beta \overline{x}_{..}$$

If different slopes: $Y_{ij} = \mu + a_i + \beta_i \cdot x_{ij} + E_{ij}$. For balanced data:

$$\widehat{\beta}_i = \frac{\Sigma_j (Y_{ij} - \overline{Y}_{i.})(x_{ij} - \overline{x}_{i.})}{\Sigma_j (x_{ij} - \overline{x}_{i.})^2}$$

$$\widehat{a}_i = \overline{Y}_{i.} - \overline{Y}_{..} - \widehat{\beta}_i \overline{x}_{i.}$$

Start by testing $H_0 : \beta_1 = ... = \beta_k$ (why?)

Test and estimation of example

Model based on	Estimates	Residual SSQ	d.f.
μ^* $\{a_1, a_2, a_3\}$	$\{17.39\}\{-3.82, 3.52, 0.2905\}$		
$\{\beta_1, \beta_2, \beta_3\}$	$\{1.10, 0.86, 0.86\}$	25.25	$15-6=9$
μ^* $\{a_1, a_2, a_3\}$ β	$\{17.18\}\{0.18, 1.32, -1.40\}\{0.9540\}$	27.98	$15-4=11$
μ^* β	$\{14.14\}$ $\{1.0797\}$	41.27	$15-2=13$
μ^* $\{a_1, a_2, a_3\}$	$\{40.20\}\{1.20, 3.00, -4.20\}$	206.00	$15-3=12$
μ^*	$\{40.20\}$	346.40	$15-1=14$

Common slopes: $F_{\beta_1=\beta_2=\beta_3} = \frac{(27.98-25.25)/2}{25.25/9} = 0.49 \sim F(2,9)$

Treatment effect: $F_{treatments} = \frac{(41.27-27.98)/2}{27.98/11} = 2.61 \sim F(2,11)$

Test for purity effect: $F_{purity} = \frac{(206.00-27.98)/1}{27.98/11} = 69.97 \sim F(1,11)$

ANOVA for covariance example - common slope assumed:

ANOVA for covariance model

Source	SSQ	d.f.	s^2	F-value
Concentrations	13.28	2	6.64	2.61
Purity (x)	178.01	1	178.01	69.97
Residual	27.98	11	2.54	
Total	346.40	14		

Conclusion: The treatment effect is not significant. Nevertheless it is (often) of interest to estimate the treatment means under the full model (adjusted means) as well as under the model where the covariate is not taken into account (unadjusted means):

Treatment		5%	10%	15 %
Unadjusted means	$\overline{Y}_{i.}$	41.40	43.20	36.00
Adjusted means	$\overline{Y}_{i.} - \widehat{\beta}(\overline{x}_{i.} - \overline{x}_{..})$	40.38	41.42	38.80

Covariate dependence : $\widehat{\beta}x = 0.9540 \cdot purity$

Residual variance : $\widehat{\sigma}_E^2 = 2.54 = 1.59^2$

Warning: The correct application of the analysis of covariance model assumes, that the covariate (x) does <u>not</u> depend on the treatment

The easy way to EMS in balanced designs - more general

Consider the model:

$$Y_{ijk\ell} = \mu + a_i + B(a)_{j(i)} + C(a)_{k(i)} + BC(a)_{jk(i)} + E_{\ell(ijk)}$$

and suppose $i = \{1, a\}$, $j = \{1, b\}$, $k = \{1, c\}$ and $\ell = \{1, r\}$.

The total number of observations is $N = a \cdot b \cdot c \cdot r$. We want the EMS for the main effect a_i. It will consist of ϕ_a (a_i is a deterministic effect) and all (and only) other *random* terms involving a : $\sigma^2_{B(a)}$, $\sigma^2_{C(a)}$, $\sigma^2_{BC(a)}$, and (of course always) $\sigma^2_E \sim \sigma^2_{E(aBC)}$.

The coefficient corresponding to a term is equal to the number of observations per term in the design. $N = abcr$.

For example consider the term $B(a)_{j(i)}$.

There are $(j = b) \cdot (i = a)$ of these terms and thus $N/(a \cdot b) = c \cdot r$ observations for each $B(a)_{j(i)}$. The coefficient for $\sigma^2_{B(a)}$ is $N/(a \cdot b) = c \cdot r$.

$$\text{EMS}(a) = \text{E}\{S^2_a\} = bcr \cdot \phi_a + cr \cdot \sigma^2_{B(a)} + br \cdot \sigma^2_{C(a)} + r \cdot \sigma^2_{BC(a)} + \sigma^2_E$$

For the term $B(a)_{j(i)}$ the EMS will contain $\sigma^2_{B(a)}$ and $\sigma^2_{BC(a)}$ and σ^2_E (but NOT $\sigma^2_{C(a)}$ because it does not contain $B(a)$).

The easy way to EMS in balanced designs - two more examples

Model : $Y_{ijk\ell} = \mu + a_i + B(a)_{j(i)} + C(a)_{k(i)} + BC(a)_{jk(i)} + E_{\ell(ijk)}$

Term		Expected mean squares				
a_i	:	$\frac{N}{a} \cdot \phi_a +$	$\frac{N}{ab} \cdot \sigma^2_{B(a)} +$	$\frac{N}{ac} \cdot \sigma^2_{C(a)} +$	$\frac{N}{abc} \cdot \sigma^2_{BC(a)} +$	σ^2_E
$B(a)_{j(i)}$	:		$\frac{N}{ab} \cdot \sigma^2_{B(a)} +$		$\frac{N}{abc} \cdot \sigma^2_{BC(a)} +$	σ^2_E
$C(a)_{k(i)}$	:			$\frac{N}{ac} \cdot \sigma^2_{C(a)} +$	$\frac{N}{abc} \cdot \sigma^2_{BC(a)} +$	σ^2_E
$BC(a)_{jk(i)}$	:				$\frac{N}{abc} \cdot \sigma^2_{BC(a)} +$	σ^2_E
$E_{\ell(ijk)}$	:					σ^2_E

where the indices for the components of the variances are the model terms, N is the total number of measurements and 'a', 'b', 'c', etc, are the levels of the factors in the design. Thus fx N=abcr. For the nested index j the number of levels is the number of levels within each (i) - in the usual way.

Note that in the coefficients the numerator is the total number of observations and the denominator is derived directly from the corresponding model term!

Model : $Y_{ijk\ell} = \mu + a_i + b_j + ab_{ij} + C(ab)_{k(ij)} + E_{\ell(ijk)}$

Term		Expected mean squares				
a_i	:	$\frac{N}{a} \cdot \phi_a +$			$\frac{N}{abc} \cdot \sigma^2_{C(ab)} +$	σ^2_E
b_i	:		$\frac{N}{b} \cdot \phi_b +$		$\frac{N}{abc} \cdot \sigma^2_{C(ab)} +$	σ^2_E
ab_{ij}	:			$\frac{N}{ab} \cdot \phi_{ab} +$	$\frac{N}{abc} \cdot \sigma^2_{C(ab)} +$	σ^2_E
$C(ab)_{k(ij)}$	:				$\frac{N}{abc} \cdot \sigma^2_{C(ab)} +$	σ^2_E
$E_{\ell(ijk)}$	:					σ^2_E

For the nested index k the number of levels is the number of levels within each (i, j) combination - again in the usual way. Also note that ϕ_{ab} does not appear in the EMS for neither a_i nor b_j because it is deterministic (fixed). The term $\sigma^2_{C(ab)}$ appears for a_i, b_j and ab_{ij} because it is random and contains all three terms.

Modification: If you have an interaction between a fixed and a random effect, fx between a_i and B_j, the interaction term σ^2_{AB} appears in both EMS(a) and EMS(B) (this corresponds to the 'unrestricted model' page 526). If you only let it appear for the fixed effect a_i, but not for B_j you get the 'restricted model' EMS generally used in 'Montgomery'.

EMS tables for models with three factors

Type I.1 design

$$I.1 : Y_{ijk\ell} = \mu + a_i + b_j + ab_{ij} + c_k + ac_{ik} + bc_{jk} + abc_{ijk} + E_{\ell(ijk)}$$

	a	b	c	r								
	i	j	k	ℓ	ϕ_a	ϕ_b	ϕ_{ab}	ϕ_c	ϕ_{ac}	ϕ_{bc}	ϕ_{abc}	σ_E^2
a_i	0	b	c	r	bcr							1
b_j	a	0	c	r		acr						1
ab_{ij}	0	0	c	r			cr					1
c_k	a	b	0	r				abr				1
ac_{ik}	0	b	0	r					br			1
bc_{jk}	a	0	0	r						ar		1
abc_{ijk}	0	0	0	r							r	1
$E_{\ell(ijk)}$	1	1	1	1								1

The number of factors levels are a, b and c, and r repetitions for each factor combination. The table also correspond to the method shown in supplement VI.

Type I.2 design

$$I.2 : Y_{ijk\ell} = \mu + a_i + b_j + ab_{ij} + C_k + AC_{ik} + BC_{jk} + ABC_{ijk} + E_{\ell(ijk)}$$

	a	b	c	r								
	i	j	k	ℓ	ϕ_a	ϕ_b	ϕ_{ab}	σ_C^2	σ_{AC}^2	σ_{BC}^2	σ_{ABC}^2	σ_E^2
a_i	0	b	c	r	bcr				br		r	1
b_j	a	0	c	r		acr				ar	r	1
ab_{ij}	0	0	c	r			cr				r	1
C_k	a	b	1	r				abr	br	ar	r	1
AC_{ik}	1	b	1	r					br		r	1
BC_{jk}	a	1	1	r						ar	r	1
ABC_{ijk}	1	1	1	r							r	1
$E_{\ell(ijk)}$	1	1	1	1								1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type I.3 design

$$I.3 : Y_{ijk\ell} = \mu + a_i + B_j + AB_{ij} + C_k + AC_{ik} + BC_{jk} + ABC_{ijk} + E_{\ell(ijk)}$$

	a	b	c	r								
	i	j	k	ℓ	ϕ_a	σ_B^2	σ_{AB}^2	σ_C^2	σ_{AC}^2	σ_{BC}^2	σ_{ABC}^2	σ_E^2
a_i	0	b	c	r	bcr		cr		br		r	1
B_j	a	1	c	r		acr	cr			ar	r	1
AB_{ij}	1	1	c	r			cr				r	1
C_k	a	b	1	r				abr	br	ar	r	1
AC_{ik}	1	b	1	r					br		r	1
BC_{jk}	a	1	1	r						ar	r	1
ABC_{ijk}	1	1	1	r							r	1
$E_{\ell(ijk)}$	1	1	1	1								1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type I.4 design

$$I.4 : Y_{ijk\ell} = \mu + A_i + B_j + AB_{ij} + C_k + AC_{ik} + BC_{jk} + ABC_{ijk} + E_{\ell(ijk)}$$

	a	b	c	r								
	i	j	k	ℓ	σ_A^2	σ_B^2	σ_{AB}^2	σ_C^2	σ_{AC}^2	σ_{BC}^2	σ_{ABC}^2	σ_E^2
A_i	1	b	c	r	bcr		cr		br		r	1
B_j	a	1	c	r		acr	cr			ar	r	1
AB_{ij}	1	1	c	r			cr				r	1
C_k	a	b	1	r				abr	br	ar	r	1
AC_{ik}	1	b	1	r					br		r	1
BC_{jk}	a	1	1	r						ar	r	1
ABC_{ijk}	1	1	1	r							r	1
$E_{\ell(ijk)}$	1	1	1	1								1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type II.1 and II.2 designs

$$II.1 : Y_{ijk\ell} = \mu + a_i + B(a)_{j(i)} + C(aB)_{k(ij)} + E_{\ell(ijk)}$$

	a	b	c	r				
	i	j	k	ℓ	ϕ_a	$\sigma^2_{B(a)}$	$\sigma^2_{C(aB)}$	σ^2_E
a_i	0	b	c	r	bcr	cr	r	1
$B(a)_{j(i)}$	1	1	c	r		cr	r	1
$C(aB)_{k(ij)}$	1	1	1	r			r	1
$E_{\ell(ijk)}$	1	1	1	1				1

$$II.2 : Y_{ijk\ell} = \mu + A_i + B(A)_{j(i)} + C(AB)_{k(ij)} + E_{\ell(ijk)}$$

	a	b	c	r				
	i	j	k	ℓ	σ^2_A	$\sigma^2_{B(A)}$	$\sigma^2_{C(AB)}$	σ^2_E
A_i	1	b	c	r	bcr	cr	r	1
$B(A)_{j(i)}$	1	1	c	r		cr	r	1
$C(AB)_{k(ij)}$	1	1	1	r			r	1
$E_{\ell(ijk)}$	1	1	1	1				1

Type III.1 and III.2 designs

$$III.1 : Y_{ijk\ell} = \mu + a_i + b_j + ab_{ij} + C(ab)_{k(ij)} + E_{\ell(ijk)}$$

	a	b	c	r					
	i	j	k	ℓ	ϕ_a	ϕ_b	ϕ_{ab}	$\sigma^2_{C(ab)}$	σ^2_E
a_i	0	b	c	r	bcr			r	1
b_j	a	0	c	r		acr		r	1
ab_{ij}	0	0	c	r			cr	r	1
$C(ab)_{k(ij)}$	1	1	1	r				r	1
$E_{\ell(ijk)}$	1	1	1	1					1

$$III.2 : Y_{ijk\ell} = \mu + a_i + B_j + AB_{ij} + C(aB)_{k(ij)} + E_{\ell(ijk)}$$

	a	b	c	r					
	i	j	k	ℓ	ϕ_a	σ^2_B	σ^2_{AB}	$\sigma^2_{C(aB)}$	σ^2_E
a_i	0	b	c	r	bcr		cr	r	1
B_j	a	1	c	r		acr	cr	r	1
AB_{ij}	1	1	c	r			cr	r	1
$C(aB)_{k(ij)}$	1	1	1	r				r	1
$E_{\ell(ijk)}$	1	1	1	1					1

Type III.3 and IV.1 designs

$$III.3 : Y_{ijk\ell} = \mu + A_i + B_j + AB_{ij} + C(AB)_{k(ij)} + E_{\ell(ijk)}$$

	a	b	c	r					
	i	j	k	ℓ	σ^2_A	σ^2_B	σ^2_{AB}	$\sigma^2_{C(AB)}$	σ^2_E
A_i	1	b	c	r	bcr		cr	r	1
B_j	a	1	c	r		acr	cr	r	1
AB_{ij}	1	1	c	r			cr	r	1
$C(AB)_{k(ij)}$	1	1	1	r				r	1
$E_{\ell(ijk)}$	1	1	1	1					1

$$IV.1 : Y_{ijk\ell} = \mu + a_i + B(a)_{j(i)} + C(a)_{k(i)} + BC(a)_{jk(i)} + E_{\ell(ijk)}$$

	a	b	c	r					
	i	j	k	ℓ	ϕ_a	$\sigma^2_{B(a)}$	$\sigma^2_{C(a)}$	$\sigma^2_{BC(a)}$	σ^2_E
a_i	0	b	c	r	bcr	cr	br	r	1
$B(a)_{j(i)}$	1	1	c	r		cr		r	1
$C(a)_{k(i)}$	1	b	1	r			br	r	1
$BC(a)_{jk(i)}$	1	1	1	r				r	1
$E_{\ell(ijk)}$	1	1	1	1					1

Type IV.2 design

$$IV.2 : Y_{ijk\ell} = \mu + A_i + B(A)_{j(i)} + C(A)_{k(i)} + BC(A)_{jk(i)} + E_{\ell(ijk)}$$

	a	b	c	r					
	i	j	k	ℓ	σ^2_A	$\sigma^2_{B(A)}$	$\sigma^2_{C(A)}$	$\sigma^2_{BC(A)}$	σ^2_E
A_i	1	b	c	r	bcr	cr	br	r	1
$B(A)_{j(i)}$	1	1	c	r		cr		r	1
$C(A)_{k(i)}$	1	b	1	r			br	r	1
$BC(A)_{jk(i)}$	1	1	1	r				r	1
$E_{\ell(ijk)}$	1	1	1	1					1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type V.1 design

$$V.1: Y_{ijk\ell} = \mu + a_i + b_j + ab_{ij} + C(a)_{k(i)} + BC(a)_{jk(i)} + E_{\ell(ijk)}$$

	a	b	c	r						
	i	j	k	ℓ	ϕ_a	ϕ_b	ϕ_{ab}	$\sigma^2_{C(a)}$	$\sigma^2_{BC(a)}$	σ^2_E
a_i	0	b	c	r	bcr			br	r	1
b_j	a	0	c	r		acr			r	1
ab_{ij}	0	0	c	r			cr		r	1
$C(a)_{k(i)}$	1	b	1	r				br	r	1
$BC(a)_{jk(i)}$	1	1	1	r					r	1
$E_{\ell(ijk)}$	1	1	1	1						1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type V.2 design

$$V.2: Y_{ijk\ell} = \mu + a_i + B_j + AB_{ij} + C(a)_{k(i)} + BC(a)_{jk(i)} + E_{\ell(ijk)}$$

	a	b	c	r						
	i	j	k	ℓ	ϕ_a	σ^2_B	σ^2_{AB}	$\sigma^2_{C(a)}$	$\sigma^2_{BC(a)}$	σ^2_E
a_i	0	b	c	r	bcr		cr	br	r	1
B_j	a	1	c	r		acr	cr		r	1
AB_{ij}	1	1	c	r			cr		r	1
$C(a)_{k(i)}$	1	b	1	r				br	r	1
$BC(a)_{jk(i)}$	1	1	1	r					r	1
$E_{\ell(ijk)}$	1	1	1	1						1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type V.3 design

$$V.3: Y_{ijk\ell} = \mu + a_i + B_j + AB_{ij} + C(B)_{k(j)} + AC(B)_{ik(j)} + E_{\ell(ijk)}$$

	a	b	c	r						
	i	j	k	ℓ	ϕ_a	σ^2_B	σ^2_{AB}	$\sigma^2_{C(B)}$	$\sigma^2_{AC(B)}$	σ^2_E
a_i	0	b	c	r	bcr		cr		r	1
B_j	a	1	c	r		acr	cr	ar	r	1
AB_{ij}	1	1	c	r			cr		r	1
$C(B)_{k(j)}$	a	1	1	r				ar	r	1
$AC(B)_{ik(j)}$	1	1	1	r					r	1
$E_{\ell(ijk)}$	1	1	1	1						1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Type V.4 design

$$V.4: Y_{ijk\ell} = \mu + A_i + B_j + AB_{ij} + C(A)_{k(i)} + BC(A)_{jk(i)} + E_{\ell(ijk)}$$

	a	b	c	r						
	i	j	k	ℓ	σ^2_A	σ^2_B	σ^2_{AB}	$\sigma^2_{C(A)}$	$\sigma^2_{BC(A)}$	σ^2_E
A_i	1	b	c	r	bcr		cr	br	r	1
B_j	a	1	c	r		acr	cr		r	1
AB_{ij}	1	1	c	r			cr		r	1
$C(A)_{k(i)}$	1	b	1	r				br	r	1
$BC(A)_{jk(i)}$	1	1	1	r					r	1
$E_{\ell(ijk)}$	1	1	1	1						1

The number of levels for the factors are a, b and c, and r repetitions are made for each factor combination.

Supplement VI.1

$\boxed{\text{Montgomery's method for computing EMS-values - simple version}}$

The method is illustrated by the EMS-tables shown in supplement V and in the tables shown in slides 14.1 to 14.5, for example.

1.19.

Construct correct model fx:

$$Y_{ijk} = \mu + a_i + B_j + AB_{ij} + E_{k(ij)}$$

Model	Type	a	b	n	Coefficients to			
term	of term	i	j	k	ϕ_a	σ_B^2	σ_{AB}^2	σ_E^2
a_i	determ.	$\boxed{0}$	b	n	b·n		n	1
B_j	random	a	$\boxed{1}$	n		a·n	n	1
AB_{ij}	random	$\boxed{1}$	$\boxed{1}$	n			n	1
$E_{k(ij)}$	random	1	1	$\boxed{1}$				1

1: Write 1 under all indices in parentheses

2: Write $\boxed{0}$ or $\boxed{1}$ under all index coincidences: $\boxed{0}$ for deterministic effect terms and

$\boxed{1}$ for random effect terms

Supplement VI.2

3: Write the number of levels for the indices in the columns at the remaining positions (a, b or n in the example)

4: For each term cover the columns for the indices of the term. Look up all rows with terms having index as the term considered or the same plus more indices.

5: The product of the numbers in the row (except the covered one(s)) is the coefficient to the corresponding component. Fx the term a_i will get contributions from the rows with a_i, AB_{ij} and $E_{k(ij)}$, i.e. components ϕ_a, σ_{AB}^2 and σ_E^2 (the 'i'-column covered)

For mixed models the method corresponds to the 'Unrestricted Mixed Model', as in the present example – see Montgomery p. 504.

Supplement VII.1

$\boxed{\text{Multiple linear regression in general formulation}}$

$$Y = \begin{Bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_N \end{Bmatrix}, \quad x = \begin{Bmatrix} 1 & x_{1,1} & x_{1,2} & \ldots & x_{1,k} \\ 1 & x_{2,1} & x_{2,2} & \ldots & x_{2,k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N,1} & x_{N,2} & \ldots & x_{N,k} \end{Bmatrix}, \quad \beta = \begin{Bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{Bmatrix} \text{ and } E = \begin{Bmatrix} E_1 \\ E_2 \\ \vdots \\ E_N \end{Bmatrix}$$

$\boxed{\text{Matrix notation model : } Y = x\beta + E}$

$\boxed{\text{Least squares condition: } (x'x)\beta = x'Y}$

Simplest solution: $\beta = (x'x)^{-1}x'Y$ if $(x'x)^{-1}$ exists.

Supplement VII.2

General model reduction test

$$x = \left\{\begin{matrix} 1 & x_{1,1} & \dots & x_{1,m} & x_{1,m+1} & \dots & x_{1,k} \\ 1 & x_{2,1} & \dots & x_{2,m} & x_{2,m+1} & \dots & x_{2,k} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N,1} & \dots & x_{N,m} & x_{N,m+1} & \dots & x_{N,k} \end{matrix}\right\} = \{x_0 \mid x_1\}$$

Model $Y = x\beta + E = x_0\beta_0 + x_1\beta_1 + E$

where x_0 corresponds to x's that are not to be tested, while x_1 corresponds to x's that are to be testet. Formally:

Hypothesis : $\beta_1 = 0 \Longleftrightarrow Y = x_0\beta_0 + E$ versus $\beta_1 \neq 0$

Supplement VII.3

Method:

Solve $(x^T x)\widehat{\beta} = x^T Y$ and $(x_0^T x_0)\widehat{\beta}_0 = x_0^T Y$

Compute

$SSQ_1 = (Y - x\widehat{\beta})^T(Y - x\widehat{\beta})$ and $f_1 =$ N-k-1 (Residual SSQ full model)

$SSQ_0 = (Y - x_0\widehat{\beta}_0)^T(Y - x_0\widehat{\beta}_0)$ and $f_0 =$ N-m-1 (Residual SSQ reduced model

$SSQ_2 = SSQ_0 - SSQ_1$ and $f_2 = f_0 - f_1 =$ k-m (Increase of SSQ for $\beta_1 = 0$)

The general multiple F-test. see also slide 17.8

Source	SSQ	d.f.	s^2	F-value
Removed terms	SSQ_2	f_2=k-m	s_2^2	s_2^2/s_1^2
Residual full model	SSQ_1	f_1=N-k-1	s_1^2	
Reduced model	SSQ_0	f_0=N-m-1		

Critical 5% F-value $= F$(k-m,N-k-1)$_{0.05}$

variable.

In the present example the purity must not depend on the concentration of the additive. The purity should therefore , for example, be measured before the treatment is applied.

After the analysis the covariate (x) should generally be analyzed in relation to the treatments (ANOVA, plots etc.)