Two-Series Factorials

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Screening Experiments (Roth, 2013)

- **Production processes** often involve many factors:
  - material
  - equipment
  - intermediate products (producer, storage, …)
  - conditions (temperature, humidity, pressure)
  - personnel
- Typical questions are:
  - Which factors have an effect on the response?
  - What is the effect of the important factors?
    - main-effects only?
    - what about interaction effects?
- When you have to answer such questions you are basically always confronted with the “side constraint” that you are **not** allowed to run too many experiments.

Screening Experiments (Roth, 2013)

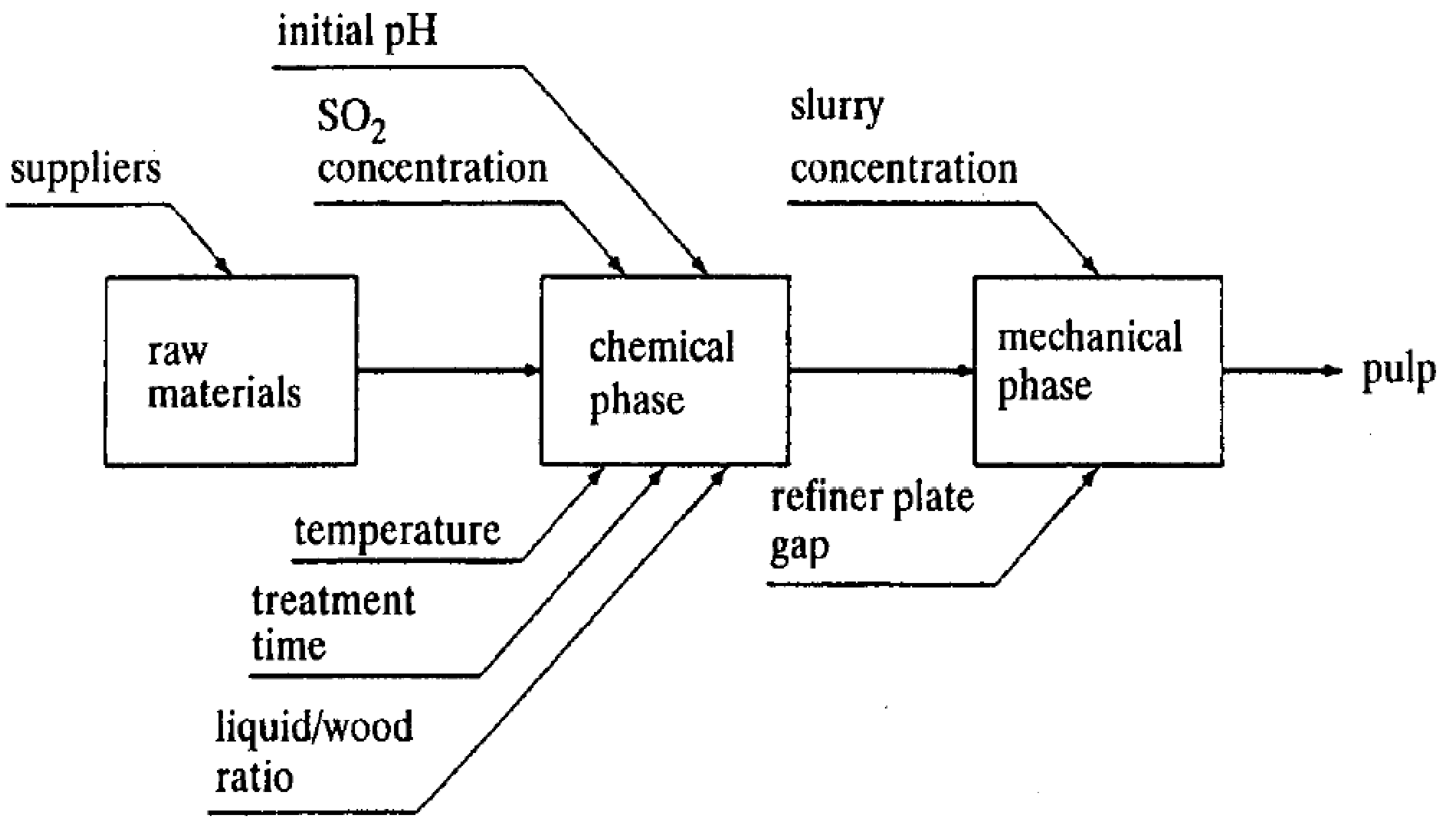


Figure 1.1. Flow Chart, Pulp Manufacturing Process.

Screening Experiments (Roth, 2013)

- E.g., if you have 7 factors with 3 levels each and want to run an experiment for every possible setting a total of $3^7 = 2187$ experiments have to be performed.
- An “easy trick” to **reduce the number of experiments** is to reduce the number of levels per factor. Typical and (minimal) choice is **2 levels**.
- In the previous example it would mean that we “only” have to run $2^7 = 128$ experiments.
- However, we might risk to miss some effects if we make bad choices for the factor levels.

Screening Experiments (Roth, 2013)

- It is **not** advisable to run experiments by varying or optimizing the factors “one by one”.
- Only a factorial experiment where we see **all** (or **many**) possible combinations of factor levels will allow us to say something about possible interactions between the involved factors.

Two-Series Factorials

- A **two-series factorial design** is a factorial design where **all** the factors have just **two levels** that we typically call **“low”** and **“high”**.
- If we have a total of k factors, we call it a $\mathbf{2^k}$ **design**.
- A **complete** or **full** 2^k design is a 2^k design where we observe **all** 2^k possible settings.
- A **fractional** 2^k design is a 2^k design where we only observe a **subset** of all possible combinations.
- A 2^k design is typically the **first step** in the optimization of complex production processes in order to find out the important factors affecting the response (“screening”).

Two-Series Factorials

- We are in a "standard" ANOVA situation with some "historical" specialties with respect to
  - labeling of factor level combinations
  - estimation of effects
  - graphical analysis of effects
- Assume that we have three factors A, B, C with two levels each ("low" and "high").
- A specific factor level combination is typically abbreviated with a **string of lower-case letters**.
- E.g., we denote by acd the **setting** (observation) (**not** the interaction!) where A, C and D are set to the level "high" and B to the level "low".

Two-Series Factorials: 2^3 design

- Hence, in a 2^3 design we have the following $2^3 = 8$ possible configurations.

	A	*B*	*C*
(1)	$-$	$-$	$-$
a	$+$	$-$	$-$
b	$-$	$+$	$-$
ab	$+$	$+$	$-$
c	$-$	$-$	$+$
ac	$+$	$-$	$+$
bc	$-$	$+$	$+$
abc	$+$	$+$	$+$

- Here a "$+$" means "high" and a "$-$" means "low".

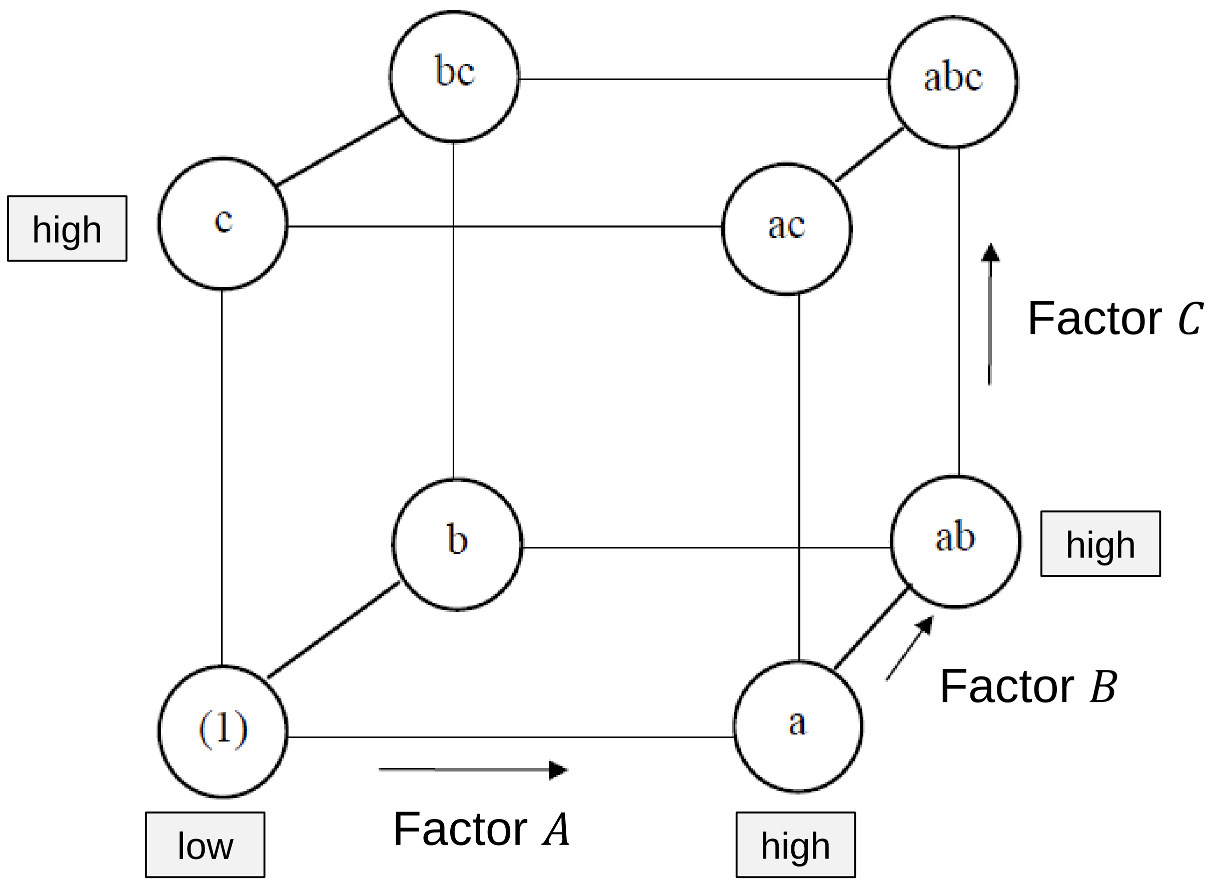
Two-Series Factorials: 2^3 design

- In our “old layout” of a factorial design this would be as follows

	A low	*A high*
B low	(1)	a
B high	b	ab

- Here we dropped the third factor C (or set it to level “low”) for illustrational reasons.

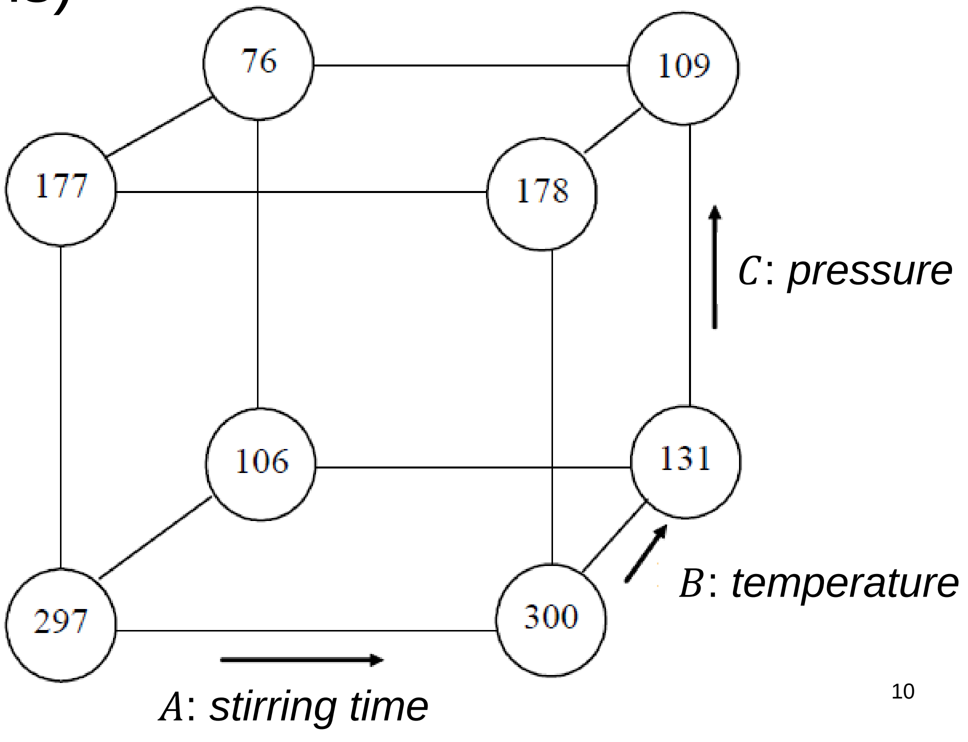
Two-Series Factorials: Visualization of 2^3 design



Example: Cooling Time of Cement (Roth, 2013)

- Response: cooling time of cement [minutes]
- Involved factors with **two levels each**
  - stirring time (A)
  - temperature (B)
  - pressure (C)
- Data (rows are observations)

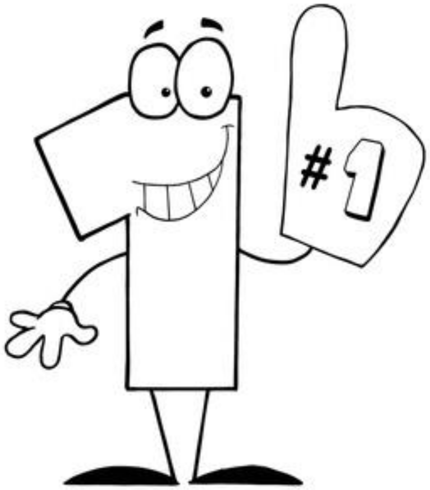
Setting	y
(1)	297
a	300
b	106
ab	131
c	177
ac	178
bc	76
abc	109



Two-Series Factorials: ANOVA Table

- The ANOVA table of a two-series factorial is set up "as usual".
- It has the special property that whatever effect we are looking at, it always has **one** degree of freedom.

Source	*df*
A	1
B	1
C	1
AB	1
AC	1
BC	1
ABC	1



- This means that every effect can be estimated with a **single contrast**.

Two-Series Factorials: Parameter Estimation

- Consider factor A.
- If we use the **sum-to-zero constraint** we have for the corresponding parameter: $\hat{\alpha}_2 = -\hat{\alpha}_1$.
- We call the difference

$$\bar{y}_{2\cdot\cdot} - \bar{y}_{1\cdot\cdot} = \underbrace{(\bar{y}_{2\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})}_{=\hat{\alpha}_2} - \underbrace{(\bar{y}_{1\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})}_{=\hat{\alpha}_1} = \hat{\alpha}_2 - \hat{\alpha}_1 = 2 \cdot \hat{\alpha}_2$$

  the **total effect** of A.
- On the left-hand side we have the average of the response where A is set to "high" minus the average of the response where A is set to "low".
- This is exactly the (weighted) "contrast pattern" that we saw in the table if we interpret "$+$" as 1 and "$-$" as -1.

Two-Series Factorials: Parameter Estimation

- The same holds true for all other main-effects.
- The pattern of the contrasts corresponding to the interaction terms is the **product of the involved patterns** of main-effects, i.e.

	μ	A	B	C	AB	AC	BC	ABC
(1)	$+$	$-$	$-$	$-$	$+$	$+$	$+$	$-$
a	$+$	$+$	$-$	$-$	$-$	$-$	$+$	$+$
b	$+$	$-$	$+$	$-$	$-$	$+$	$-$	$+$
ab	$+$	$+$	$+$	$-$	$+$	$-$	$-$	$-$
c	$+$	$-$	$-$	$+$	$+$	$-$	$-$	$+$
ac	$+$	$+$	$-$	$+$	$-$	$+$	$-$	$-$
bc	$+$	$-$	$+$	$+$	$-$	$-$	$+$	$-$
abc	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$+$
weight	$1/8$	$1/4$	$1/4$	$1/4$	$1/4$	$1/4$	$1/4$	$1/4$
total effect	$\hat{\mu}$	$2 \cdot \hat{\alpha}_2$	$2 \cdot \hat{\beta}_2$	$2 \cdot \hat{\gamma}_2$	$2 \cdot \widehat{(\alpha\beta)}_{22}$	$2 \cdot \widehat{(\alpha\gamma)}_{22}$	$2 \cdot \widehat{(\beta\gamma)}_{22}$	$2 \cdot \widehat{(\alpha\beta\gamma)}_{222}$
estimate	$\mathbf{171.75}$	$\mathbf{15.5}$	$\mathbf{-132.5}$	$\mathbf{-73.5}$	$\mathbf{13.5}$	$\mathbf{1.5}$	$\mathbf{47.5}$	$\mathbf{2.5}$

Two-Series Factorials: Parameter Estimation

- Compare with output of R (see R-file).
- How can we **test** the contrasts (factors) or construct confidence intervals?
- If we have a complete 2^k design and if we assume the standard ANOVA model with an error variance of σ^2 we have for **each** estimated effect (contrast) a variance of

$$\left(\frac{1}{2^{k-1}}\right)^2 2^k \sigma^2 = \frac{\sigma^2}{2^{k-2}}$$

due to weight | due to sum

- In addition, if the true effect is **zero**, the expected value of every estimated effect (contrast) is **zero** too.
- Last but not least, the estimated effects are **normally distributed** and **independent**.

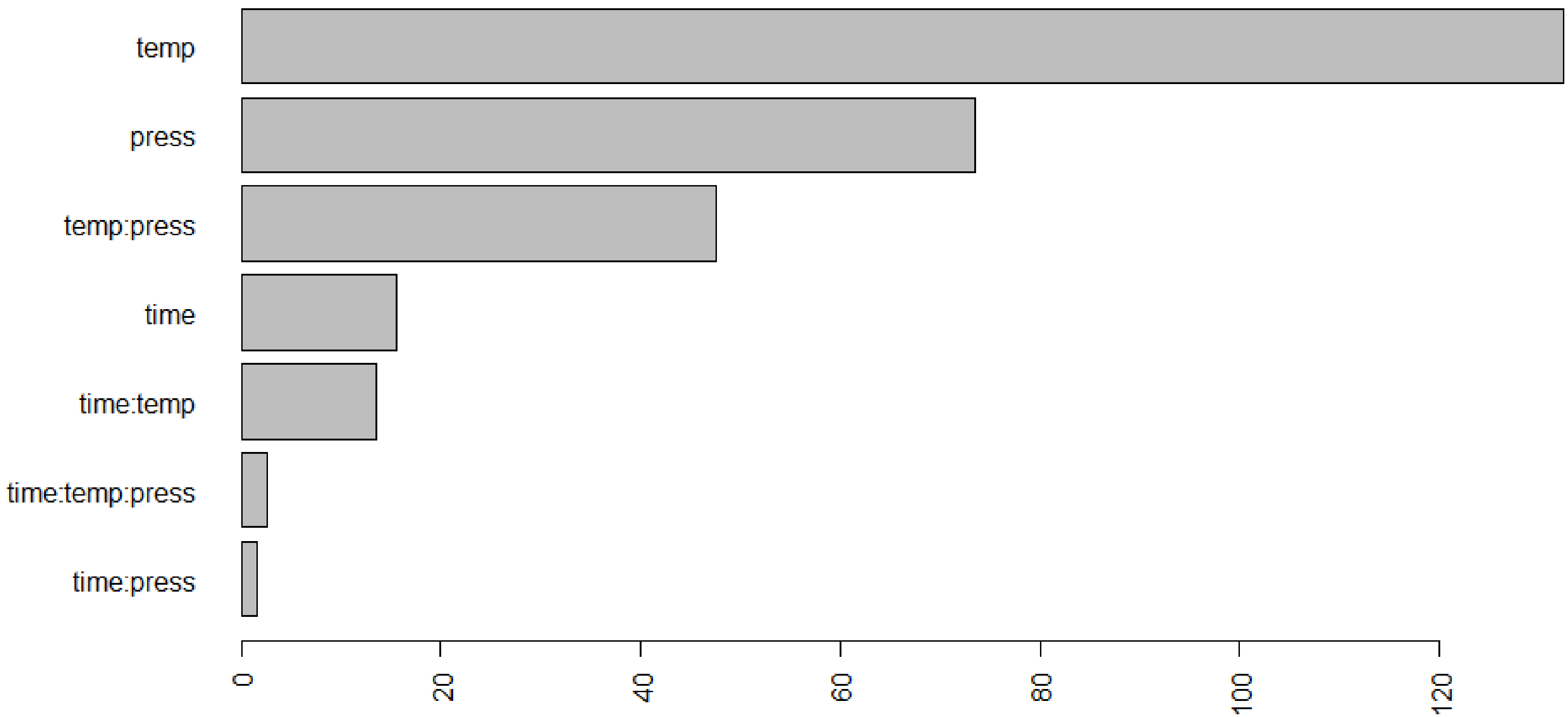
Two-Series Factorials: Inference

- Hence, **estimates corresponding to “null effects”** behave like independent samples from a normal distribution with **mean 0** and **constant variance**.
- If we use the full model (i.e., including all interactions) we do **not** have any df’s left for the error term if we have no replicates.
- However, thanks to the aforementioned properties we can do a **graphical “analysis”** of the effects using
  - pareto chart
  - halfnormal plot

  of the estimated **effects**.

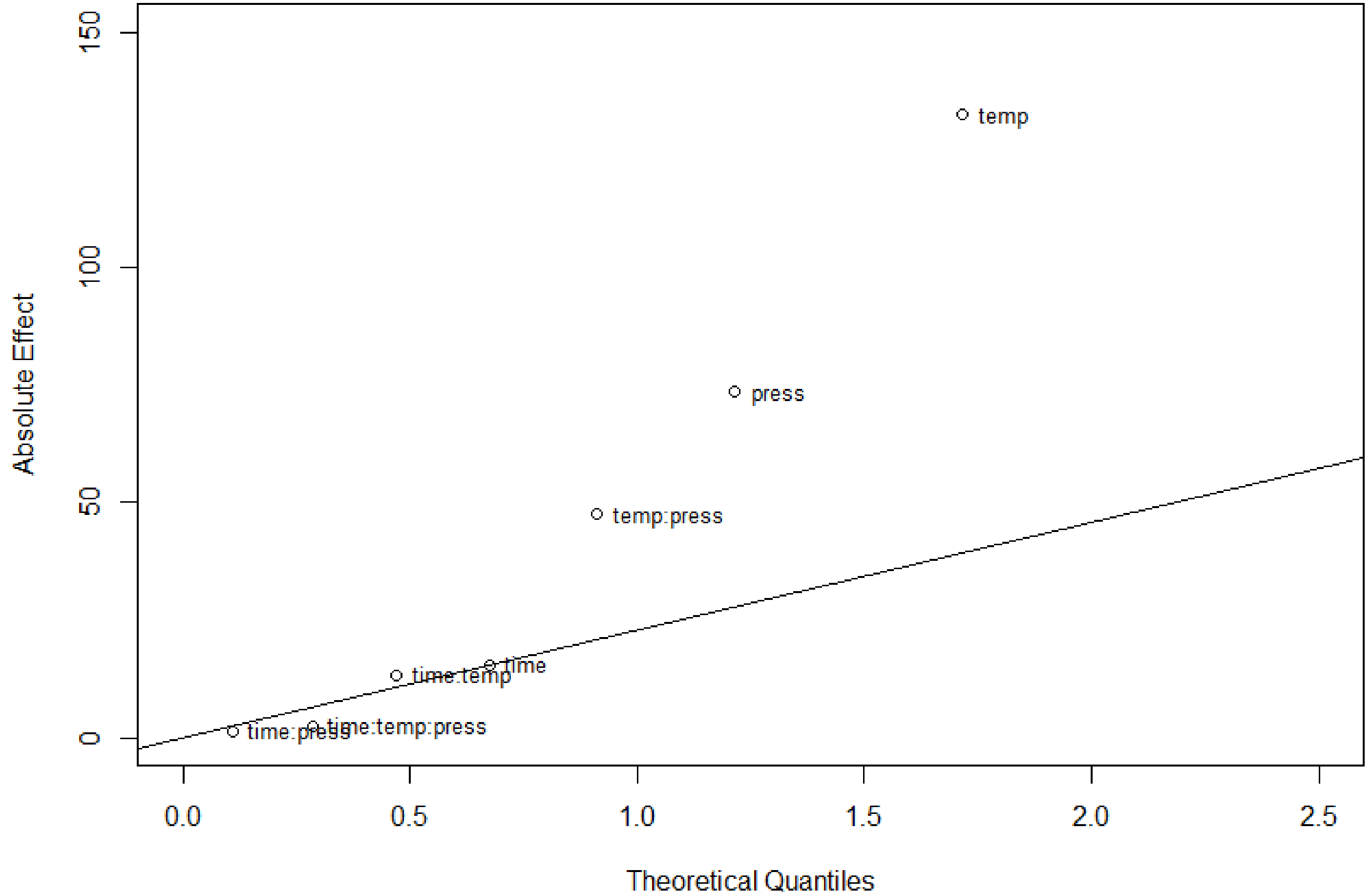
Two-Series Factorials: Pareto Chart

- Barplot of absolute value of estimated effects.
- Can we identify two groups?



Two-Series Factorials: Half-Normal Plot

- Plot sorted absolute effect values against quantiles of **absolute** value of a standard normal distribution.
- Can we detect any outliers?



Two-Series Factorials: Analysis

- If we drop the 3-way interaction we have 1 (!) degree of freedom left for estimating the error variance.
- We can do **tests** in this situation

```
> fit2 <- aov(y ~ (time + temp + press)^2, data = cement)
> summary(fit2)
              Df Sum Sq Mean Sq F value Pr(>F)
time           1    480     480   38.44 0.1018
temp           1  35112   35112 2809.00 0.0120 *
press          1  10804   10804  864.36 0.0216 *
time:temp      1    364     364   29.16 0.1166
time:press     1      5       5    0.36 0.6560
temp:press     1   4512    4512  361.00 0.0335 *
Residuals      1     13      13
```

- This basically confirms the graphical analysis.
- However: effect size is at least as important as statistical significance!

Confounding the Two-Series Factorial

- Assume that we **cannot** do a complete 2^k design in one day but that we are able to do **half** of the settings in one day.
- How should we “distribute” the factor level combinations over the two days?
- We do it by using confounding…

- The idea is to “sacrifice” some effects in order to “protect” the important ones.
- Splitting up the experiment in two blocks means losing efficiency as we have an **incomplete block design** (a day is a **block**).
- The confounded effects are “lost”, while the others are “protected”.

Confounding the Two-Series Factorial

- Example: What happens if we use the following experimental design:

	Day	μ	A	B	C	AB	AC	BC	ABC
(1)	1	+	−	−	−	+	+	+	−
a	2	+	+	−	−	−	−	+	+
b	1	+	−	+	−	−	+	−	+
ab	2	+	+	+	−	+	−	−	−
c	1	+	−	−	+	+	−	−	+
ac	2	+	+	−	+	−	+	−	−
bc	1	+	−	+	+	−	−	+	−
abc	2	+	+	+	+	+	+	+	+

- We are **not** able to distinguish the effect of A from the effect of Day.
- A is confounded with Day in this setup. Hence, this was **not** a good choice because we sacrificed a main-effect!

Confounding the Two-Series Factorial

- We say that we confounded the 2^k design into two blocks of size 2^{k-1}.
- However, our confounding choice was not optimal as we sacrificed a main-effect.
- Better: use a high-order interaction as so called **defining contrast**.
- The idea is to have a look at the column of the defining contrast: all “$+$” go in one block and all “$-$” go in the other block.
- We have completely “lost” the defining contrast as it is confounded with block.

Confounding the Two-Series Factorial

- Hence, if we use the 3-way interaction as defining contrast we get

	Day	μ	A	B	C	AB	AC	BC	ABC
(1)	1	$+$	$-$	$-$	$-$	$+$	$+$	$+$	$-$
a	2	$+$	$+$	$-$	$-$	$-$	$-$	$+$	$+$
b	2	$+$	$-$	$+$	$-$	$-$	$+$	$-$	$+$
ab	1	$+$	$+$	$+$	$-$	$+$	$-$	$-$	$-$
c	2	$+$	$-$	$-$	$+$	$+$	$-$	$-$	$+$
ac	1	$+$	$+$	$-$	$+$	$-$	$+$	$-$	$-$
bc	1	$+$	$-$	$+$	$+$	$-$	$-$	$+$	$-$
abc	2	$+$	$+$	$+$	$+$	$+$	$+$	$+$	$+$

- Here, we would run the configurations $(1), ab, ac, bc$ on day 1 and a, b, c, abc on day 2.

Confounding the Two-Series Factorial

- The block containing (1) is called the **principal block** while the other block is called the **alternate block**.
- What if we want to build **more than two** blocks?
- Say we want to confound a 2^4 design into 4 blocks of size 4 $(4 = 2^2)$.
- Start with **two** defining contrasts, say ABC and BCD.
- Our 4 blocks are built by using as "block assignment" the 4 different combinations of ABC and BCD, that is

ABC	*BCD*	*Block*
$-$	$-$	1
$+$	$+$	2
$+$	$-$	3
$-$	$+$	4

Confounding the Two-Series Factorial

- As we have 4 blocks (i.e., 3 df's) there must be a **third** effect that we are confounding.
- It is the effect that is given by the product of the two effects which is

$$ABC \cdot BCD = AB^2C^2D = AD$$

- The rule is: squared terms are **disappearing**.
- AD is also called the **generalized interaction** of ABC and BCD.
- If we would choose $ABCD$ and BCD as defining contrasts, the generalized interaction would we A, i.e. we would confound the main-effect of A

Analysis of Confounded Two-Series Factorials

- If we have replicates, we can do the "standard" ANOVA as we have an estimate for the error term.
- If we have **no** replicates, we can either pool some of the higher-order interactions into the error term (i.e., not using them in the model) or use the graphical tools presented earlier.
- The difficult part here was the design, **not** the analysis.