STAT 850 Notes

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1 Randomized Block Design

Problem Setting:

- One block factor with b levels. and one treatment factor with t levels.
- Treatments randomized with blocks.
- No replicate observations. Our observed data y_{ij} represents the data in ith block with jth factor.

	Treatment				
	A	B	C	D	Mean
Block 1	89	88	97	94	92
Block 2	84	77	92	79	83
Block 3	81	87	87	85	85
Block 4	87	92	89	84	88
Block 5	79	81	80	88	82
Mean	84	85	89	86	86

Table 1.

Model without block-treatment interactions:

$$y_{ij} = \mu + b_i + t_j + \epsilon_{ij} \quad i \in 1{:}B, j = 1{:}T$$

with $\epsilon_{ij} \overset{\text{iid}}{\sim} N(0, \sigma^2)$ and $\sum_j t_j = 0$. b_is and t_js indicate block and factor effects.

There are two settings for the block effects in the model:

- **Fixed block effects:** $\sum_{i=1}^{N} b_i = 0$ (sum to zero constraint for block effects)
- **Random block effects:** $b_1, \ldots, b_B \overset{\text{iid}}{\sim} N(0, \sigma_B^2)$

Data decomposition: the observed data can be decomposed to a summation of the (estimated) effects:

$$\begin{aligned} y_{ij} &= y_{\cdot\cdot} + (y_{i\cdot} - y_{\cdot\cdot}) + (y_{\cdot j} - y_{\cdot\cdot}) + (y_{ij} - y_{i\cdot} - y_{\cdot j} + y_{\cdot\cdot}) \\ &= \hat{\mu} + \hat{b}_i + \hat{t}_j + \hat{\epsilon}_{ij} \end{aligned}$$

ANOVA decomposition: the total sum of squares can be decomposed to:

$$\underbrace{\sum_i \sum_j (y_{ij} - y_{\cdot\cdot})^2}_{\text{Total sum of squares}} = \underbrace{t \sum_i (y_i - y_{\cdot\cdot})^2}_{\text{Blocks}} + \underbrace{b \sum_j (y_{\cdot j} - y_{\cdot\cdot})^2}_{\text{Treatments}} + \underbrace{\sum_i \sum_j (y_{ij} - y_{i\cdot} - y_{\cdot j} + y_{\cdot\cdot})^2}_{\text{Errors}}$$

Source	SS	df	$\mathbb{E}(\text{MS} = \text{SS/df})$
	Fixed block effects		
Blocks	$t\sum_i (y_{i.} - y_{..})^2$	$b-1$	$\sigma^2 + t\,(b-1)^{-1}\sum_i b_i^2$
Treatments	$b\sum_j (y_{.j} - y_{..})^2$	$t-1$	$\sigma^2 + b\,(t-1)^{-1}\sum_j t_j^2$
Error	$\sum_{ij} (y_{ij} - y_{i.} - y_{.j} + y_{..})^2$	$(b-1)\,(t-1)$	σ^2
Total	$\sum_{ij} (y_{ij} - y_{..})^2$	$bt-1$	
	Random block effects		
Blocks	$t\sum_i (y_{i.} - y_{..})^2$	$b-1$	$\sigma^2 + t\,\sigma_b^2$
Treatments	$b\sum_j (y_{.j} - y_{..})^2$	$t-1$	$\sigma^2 + b\,(t-1)^{-1}\sum_j t_j^2$
Error	$\sum_{ij} (y_{ij} - y_{i.} - y_{.j} + y_{..})^2$	$(b-1)\,(t-1)$	σ^2
Total	$\sum_{ij} (y_{ij} - y_{..})^2$	$bt-1$	

Table 2. ANOVA table for Randomized Block Design

2 Factorial Treatment Structure

2.1 Model Setting

Consider an experiment with two factors P and Q (***P* and *Q* may have interactions**) with levels $j = 1, 2, \ldots, p$, and $k = 1, 2, \ldots, q$, replicated r times ($l = 1, 2, \ldots, r$), with model

$$y_{jkl} = \mu_{jk} + \epsilon_{jkl}$$

Group effect parameters:

- Grand mean: $\mu_{..} = (pq)^{-1}\sum_j \sum_k \mu_{jk}$
- Group means for factor P: $\mu_{j.} = q^{-1}\sum_k \mu_{jk}$
- Group means for factor Q: $\mu_{.k} = p^{-1}\sum_j \mu_{jk}$
- Effect of factor P: $p_j = \mu_{j.} - \mu_{..}$
- Effect of factor Q: $q_k = \mu_{.k} - \mu_{..}$

We have sum to zero constrains under this setting:

$$\sum_j p_j = 0, \quad \sum_k q_k = 0$$

Interaction effect parameters:

$$(pq)_{jk} = \mu_{jk} - (\mu_{..} + p_j + q_k) = (\mu_{jk} - \mu_{.k}) - (\mu_{j.} - \mu_{..})$$

Also, we have

$$\sum_j (pq)_{jk} = 0 \quad \text{for all } k, \quad \sum_k (pq)_{jk} = 0 \quad \text{for all } j$$

Then the model can be expand as:

$$\mu_{jk} = \mu_{..} + p_j + q_k + (pq)_{jk}. \tag{1}$$

Remark 1. p and q without subscripts denote the number of levels for fator P and Q, while p_i and q_j denote the effect parameter for each level.

Example 1. (4×4 Design)

	μ_{jk}				$\mu_{j.}$	p_j	$(p\,q)_{jk}$			
	4	10	20	30	16	-6	-3	-4	1	6
	14	20	40	50	31	9	-8	-9	6	11
	14	20	10	20	16	-6	7	6	-9	-4
	20	30	30	20	25	3	4	7	2	-13
$\mu_{.k}$	13	20	25	30	22					
q_k	-9	-2	3	8						

Table 3. 4×4 design data table

2.2 Compare differences between treatments

To compare differences between treatments, we define **contrast** and **interaction contrast**:

Definition 1. *A contrast for the main effects of factor P is defined as*

$$C_P = \sum_{j=1}^{p} l_j \mu_{j.},$$

where $l_1, \ldots, l_p$ are coefficients with $\sum_{j=1}^{p} l_j = 0$.

Example 2. (Simple Pairwise Comparison)

$$C_P = \mu_{1.} - \mu_{2.}$$

Definition 2. *An interaction contrast is defined as:*

$$C_{PQ} = \sum_{j=1}^{p} \sum_{k=1}^{q} l_j m_k \mu_{jk},$$

where $m_1, \ldots, m_q$ are also coefficients with $\sum_{k=1}^{q} m_k = 0$.

Example 3. Test whether the difference between levels of P depends on the level of Q.

$$C_{\mathrm{PQ}} = (\mu_{11} - \mu_{12}) - (\mu_{21} - \mu_{22})$$

Interpretation of main and interaction effects:

1. **Always start by checking main effects.** Interactions modify these effects and only make sense in that context.

2. **If interactions are negligible,** simplify the interpretation and focus on main effects**.**

3. **If 3 or higher order interactions are negligible**, but second-order interactions are significant, then we should focus on both main effects and second-order interactions.

4. If a two-factor interaction is **very important**, and its **mean square (MS) value is similar to the MS values for main effects**, then the best way to interpret results is by **looking at the mean values for two-factor combinations** rather than just reporting main effects.

5. If ar **two-factor interaction is significant**, but **one or both main effects are much larger than the interaction**, then the interpretation should consider main effects first, with adjustments for interaction effects.

2.3 Least-squares estimation for an unreplicated 2×3 design

Consider a two-way factorial design with $p=2$ and $q=3$

$$\mu_{jk} = \mu_{..} + p_j + q_k + (p\,q)_{jk}$$

	1	2	3
1	y_{11}	y_{12}	y_{13}
2	y_{21}	y_{22}	y_{23}

Table 4.

$$\mathbf{y}=\begin{pmatrix} y_{11} \\ y_{12} \\ y_{13} \\ y_{21} \\ y_{22} \\ y_{23} \end{pmatrix} = \mathbf{X}\beta = \begin{pmatrix} 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 0 & -1 & 0 \\ 1 & -1 & 0 & 1 & 0 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \mu.. \\ p_1 \\ q_1 \\ q_2 \\ (p\,q)_{11} \\ (p\,q)_{12} \end{pmatrix} + \epsilon$$

The columns of $\mathbf{X}$ w.r.t. different parameter groups are orthogonal. In this case, the columns with respect to p and columns with respect to q are orthogonal. Also, they are orthogonal to the columns w.r.t. pq. Therefore, $\mathbf{X}^T\mathbf{X}$ appears to be block diagonal:

$$\mathbf{X}'\mathbf{X}=\begin{pmatrix} 6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 2 & 0 & 0 \\ 0 & 0 & 2 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & 0 & 2 & 4 \end{pmatrix}$$

$$(\mathbf{X}'\mathbf{X})^{-1}=\begin{pmatrix} 1/6 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & -1/6 & 0 & 0 \\ 0 & 0 & -1/6 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & -1/6 \\ 0 & 0 & 0 & 0 & -1/6 & 1/3 \end{pmatrix}$$

The least square solution gives

$$\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}=\begin{pmatrix} y.. \\ y_{1.} - y.. \\ y_{.1} - y.. \\ y_{.2} - y.. \\ y_{11} - y_{1.} - y_{.1} + y.. \\ y_{12} - y_{1.} - y_{.2} + y.. \end{pmatrix}.$$

Note that the number of parameter equals to the number of observations, $\mathbf{X}$ is invertible, $\hat{\beta}$ is the solution to $\mathbf{X}\beta = \mathbf{y}$.

Now we consider an additive model without interactions:

$$\mu_{jk} = \mu_{..} + p_j + q_k,$$

the least square solution gives:

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}\mathbf{y} = (\ y_{..}\ \ y_{1\cdot} - y_{..}\ \ y_{\cdot 1} - y_{..}\ \ y_{\cdot 2} - y_{..}\ )^T,$$

which align with the solution of the model with interactions. This is due to the orthogonality.

2.4 Experiment with Replication

The model for an experiment with replication can be written as:

$$y_{jkl} = \mu + p_j + q_k + (pq)_{jk} + \epsilon_{jkl}, j = 1, \ldots, p; k = 1, \ldots q, l = 1, \ldots r,$$

where ϵ_{jkl} are i.i.d. $\mathcal{N}(0, \sigma^2)$. We can decompose data as:

$$\begin{aligned} y_{jkl} &= \hat{\mu} + \hat{p}_j + \hat{q}_k + \widehat{(p\,q)}_{jk} + \hat{\epsilon}_{jkl} \\ &= y_{...} + (y_{j\cdot\cdot} - y_{...}) + (y_{\cdot k\cdot} - y_{...}) + (y_{jk\cdot} - y_{j\cdot\cdot} - y_{\cdot k\cdot} + y_{...}) + (y_{jkl} - y_{jk\cdot}). \end{aligned}$$

The sum of squares are defined as:

$$\begin{aligned} S_P &= q\,r \sum_j (y_{j\cdot\cdot} - y_{...})^2 \\ S_Q &= p\,r \sum_k (y_{\cdot k\cdot} - y_{...})^2 \\ S_{PQ} &= r \sum_j \sum_k (y_{jk\cdot} - y_{j\cdot\cdot} - y_{\cdot k\cdot} + y_{...})^2 \\ S_R &= \sum_j \sum_k \sum_l (y_{jkl} - y_{jk\cdot})^2 \\ S_D &= \sum_j \sum_k \sum_l (y_{jkl} - y_{...})^2 \end{aligned}$$

Source	SS	df	MS	Ratio
Factor P	$S_P = 1.03301$	$p - 1 = 2$	$s_P^2 = 0.51651$	$s_P^2 / s_R^2 = 23.22$
Factor Q	$S_B = 0.92121$	$q - 1 = 3$	$s_Q^2 = 0.30707$	$s_Q^2 / s_R^2 = 13.81$
Interaction	$S_{PQ} = 0.25014$	$(p-1)(q-1) = 6$	$s_{PQ}^2 = 0.04169$	$s_{PQ}^2 / s_R^2 = 1.87$
Residual	$S_R = 0.80073$	$p\,q\,(r-1) = 36$	$s_R^2 = 0.02224$	
Total	$S_D = 3.00508$	$p\,q\,r - 1 = 47$		

Table 5. ANOVA table for two factors experiments with replications

2.5 Model Checking

1. Define the estimated value of μ_{jk} under the full model as $\hat{\mu}_{\mathrm{jk}} = y_{\mathrm{jk}\cdot}$. Let $\tilde{\mu}_{jk} = y_{j\cdot\cdot} + y_{\cdot k\cdot} - y_{...}$ denote the estimated value of μ_{jk} assuming no interactions.

2. To assess the homogeneity of variance in interactions, create a plot of the residuals $y_{jkl} - \hat{\mu}_{\text{jk}}$ against the fitted values $\hat{\mu}_{\text{jk}}$. A consistent spread of residuals across different values of $\hat{\mu}_{\text{jk}}$ suggests homogeneity, while a pattern or funnel shape may indicate variance issues.

3. To detect possible nonadditivity, plot $y_{jk} - \tilde{\mu}_{jk}$ against $\tilde{\mu}_{jk}$. If the plot exhibits a curvilinear pattern, this suggests the presence of transformable nonadditivity, meaning that a transformation of the response variable may be necessary for a better model fit.

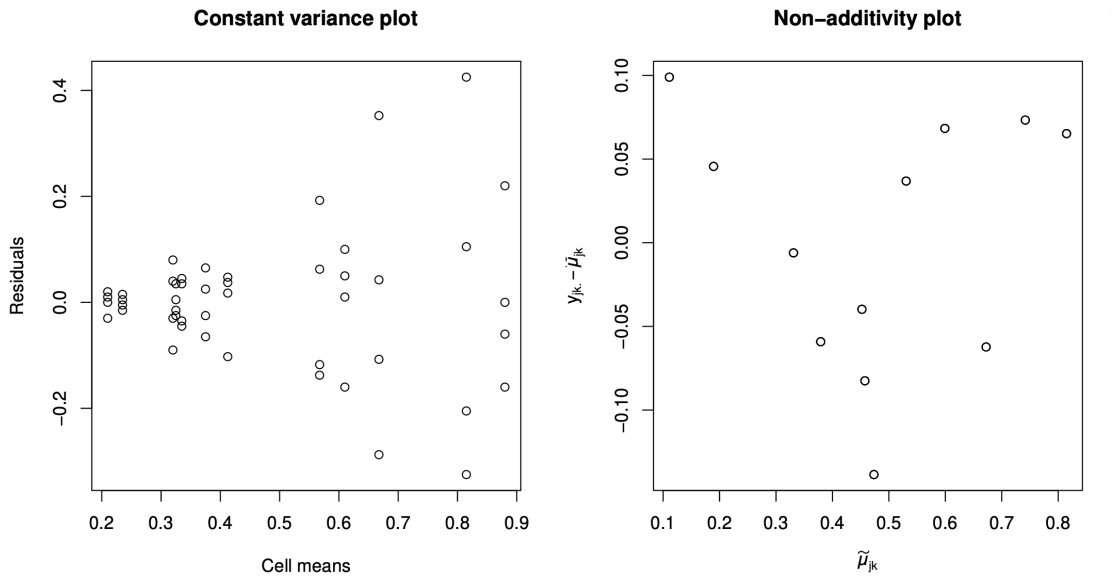

Figure 1. Model checking plots suggesting heteroscedasticity and non-additivity

2.6 Transformations

2.6.1 Taylor Power Transformation

Consider heterogeneous data $\text{Var}(y_{jkl}) = \sigma_{jk}^2$ and assume that $\sigma_{jk}^2 \propto \mu_{jk}^{\beta}$ for some β. We can use **Taylor power transformation** to deal with the heteroscedasticity (Assume $y_{jk\cdot} > 0$).

1. Calculate the sample mean $y_{jk\cdot}$ and sample standard deviation s_{jk} for each (j,k) cell.

2. Fit a linear regression on $\log s_{jk} \sim \log y_{jk\cdot}$.

3. The fitted slope $\hat{\beta}$ is an estimate of β.

4. Use the transformation $(y^{\lambda} - 1)/\lambda$ with $\lambda := 1 - \hat{\beta}$.

5. If $\lambda = 0$, apply the log transformation $y_{jkl}^{*} = \log(y_{jkl})$.

Remark 2. Simple power transformation uses y^{λ}, which doesn't smoothly transit to $\log y$ as $\lambda \to 0$.

Justification for the method:

Define

$$z = f_{\lambda}(y) = \begin{cases} (y^{\lambda} - 1)/\lambda, & \lambda \neq 0 \\ \log y, & \lambda = 0 \end{cases} \tag{2}$$

By Taylor expansion:

$$z_{jkl} = f_\lambda(y_{jkl}) \approx f_\lambda(\mu_{jk}) + f'_\lambda(\mu_{jk})\,(y_{jkl} - \mu_{jk}).$$

Since $f'(y) = y^{\lambda-1}$,

$$\begin{aligned}\mathrm{Var}(z_{jkl}) \approx & (f'_\lambda(\mu_{jk}))^2 \mathrm{Var}(y_{jkl}) \\ = & \mu_{jk}^{2(\lambda-1)}\,\sigma_{jk}^2 \\ \propto & \mu_{jk}^{2(\lambda-1)}\,\mu_{jk}^{2\beta} \\ = & \mu_{jk}^{2(\lambda-1+\beta)},\end{aligned}$$

and $\mathrm{Var}(z_{jkl})$ becomes a constant if $\lambda = 1 - \beta$.

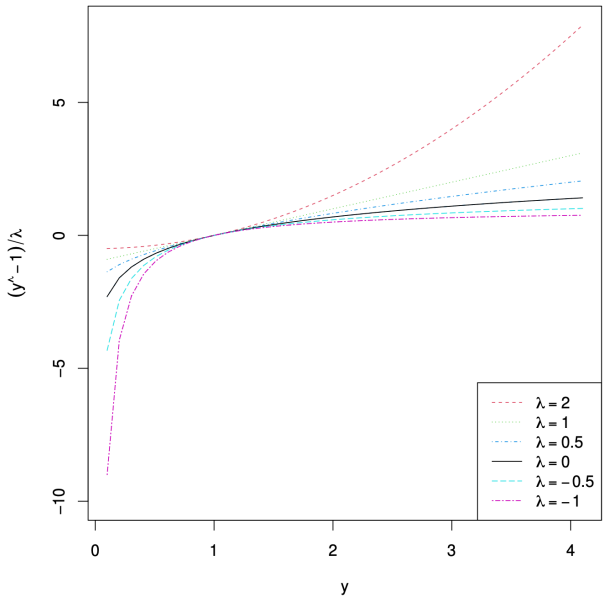

Figure 2. Power transformations

2.6.2 Box-Cox Transformation

Assumptions: There exists a λ such that $\{f_\lambda(y_i)\}_{i=1}^n$:

- are mutually independent
- are normally distributed
- have constant variance
- satisfy a linear model $f_\lambda(\mathbf{y}) = \mathbf{X}\beta + \boldsymbol{\epsilon}$

2.6.3 Maximum Likelihood Estimation of Box-Cox $\boldsymbol{\lambda}$

Assume $\mathbf{y}^{(\lambda)} = f_\lambda(\mathbf{y}) = \mathbf{X}\beta + \boldsymbol{\epsilon}$ where f_λ is defined in (2) with $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2\mathbf{I})$ for some λ. Then the likelihood function for the untransformed data follows:

$$L(\lambda, \beta, \sigma) = \frac{1}{(2\,\pi\,\sigma^2)^{n/2}} \exp\left\{-\frac{(\mathbf{y}^{(\lambda)} - \mathbf{X}\boldsymbol{\beta})^T\,(\mathbf{y}^{(\lambda)} - \mathbf{X}\boldsymbol{\beta})}{2\,\sigma^2}\right\} J(\lambda, \mathbf{y})$$

with Jacobian

$$J(\lambda, y) = \prod_{i=1}^{n} y_i^{\lambda-1}$$

We first find the LSEs of β and σ_λ for fixed λ:

$$\hat{\beta}_\lambda = (X^T X)^{-1} X^T \mathbf{y}^{(\lambda)}, \quad \hat{\sigma}_\lambda = \frac{(\mathbf{y}^{(\lambda)} - \mathbf{X}\hat{\boldsymbol{\beta}}_\lambda)^T (\mathbf{y}^{(\lambda)} - \mathbf{X}\hat{\boldsymbol{\beta}}_\lambda)}{n-p-1},$$

then we have

$$\begin{aligned} \ell(\lambda, \hat{\boldsymbol{\beta}}_\lambda, \hat{\sigma}_\lambda) &= \frac{\exp\left(-(n-p-1)/2\right)}{(2\pi)^{n/2}\hat{\sigma}_\lambda^n} J(\lambda, \mathbf{y}) \\ &= \hat{\sigma}_\lambda^{-n} \prod_{i=1}^{n} y_i^{\lambda-1} \frac{\exp\left(-(n-p-1)/2\right)}{(2\pi)^{n/2}} \end{aligned}$$

Let $\ell(\lambda) = \log L(\lambda, \hat{\beta}_\lambda, \hat{\sigma}_\lambda)$, and find the MLE $\hat{\lambda}$ that maximizes $\ell(\lambda)$.

The **confidence interval** follows from the standard result that the log-likelihood ratio statistic follows a chi-square distribution with 1 degree of freedom

$$2(\ell(\hat{\lambda}) - \ell(\lambda)) \sim \chi_1^2.$$

Then the confidence interval is the root for $\ell(\lambda) = \ell(\hat{\lambda}) - 0.5\chi_{1,\alpha}^2$.

Remark 3. The `boxcox` function in `MASS` library gives the MLE of λ.

```
library(MASS)
bc <- boxcox(y ~ p+q)
title(paste("Without interaction, lambda =",round(bc$x[which.max(bc$y)],2)))
bc <- boxcox(y ~ p*q)
title(paste("With interaction, lambda =",round(bc$x[which.max(bc$y)],2)))
```

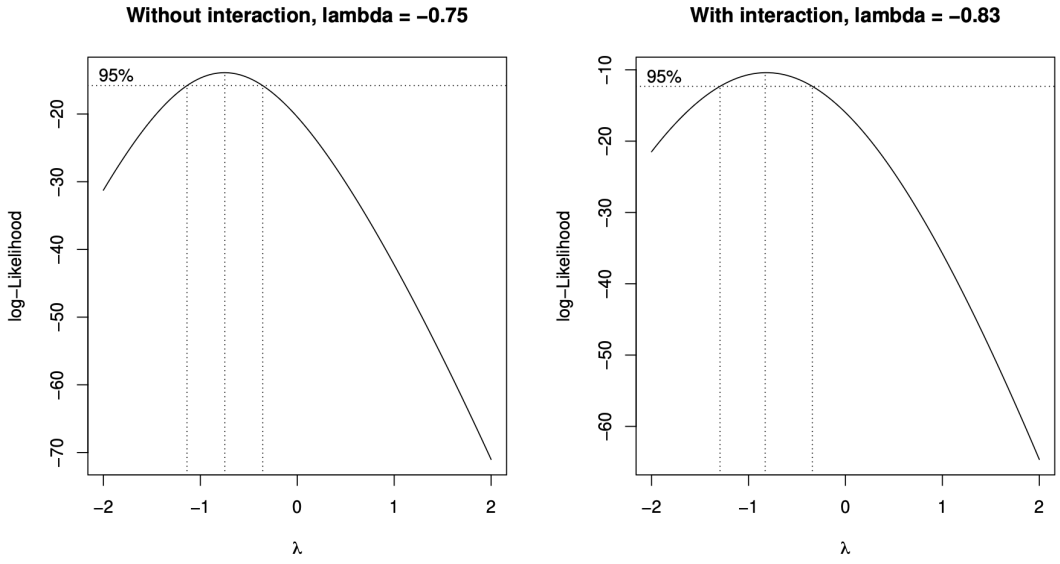

Figure 3. Likelihood of Box-Cox Transformation

Example 4. For the Poison data, we present the ANOVA table after the two transformations.

	Df	Sum Sq	Mean Sq	F value	P-value
Poison	2	34.877	17.4386	70.6302	5.17e−13
Treatment	3	20.414	6.8048	27.5610	2.48e−09
Interaction	6	1.571	0.2618	1.0603	0.4046
Residuals	35	8.643	0.2469		
Poison	2	11.926	5.9631	66.5525	1.18e−12
Treatment	3	7.158	2.3860	26.6295	3.76e−09
Interaction	6	0.486	0.0810	0.9040	0.5032
Residuals	35	3.136	0.0896		

Table 6. ANOVA table after simple Taylor power transformation ($y^{(\lambda)} = y^{\lambda}$ with $\lambda = -1$) (above) and Box-Cox transformation (below).

Remark 4. The residual Df is reduced by 1 to compensate for the estimation of λ.

2.7 Confidence Intervals

2.7.1 When interactions are not significant

Let $u_j = \mu + p_j$ and $v_k = \mu + q_k$. Let the unbiased estimators be $\hat{u}_j = y_{j\cdot}$ and $\hat{v}_k = y_{\cdot k}$ with $\mathrm{Var}(\hat{u}_j) = \sigma^2/(pr)$, $\mathrm{Var}(\hat{v}_k) = \sigma^2/(qr)$. The sample standard deviation is

$$s(\hat{u}_j) = S_R/\sqrt{pr}, s(\hat{v}_k) = S_R/\sqrt{qr}.$$

Then $100(1-\alpha)\%$ confidence interval for u_j is $\hat{u}_j \pm t_{\nu_R;\alpha/2} \times \mathrm{se}(\hat{u}_j)$, where $\nu_R = pq(r-1)$ is the degree of freedom for S_R.

For simultaneous confidence intervals, we define the contrast of interest be

$$L = \sum_{j=1}^{p} c_j u_j, \quad \text{where } \sum_{j=1}^{p} c_j = 0$$

with its estimator

$$\hat{L} = \sum_{j=1}^{p} c_j y_{j\cdot} \quad \text{with} \quad s(\hat{L}) = S_R \sqrt{(qr)^{-1} \sum_{j=1}^{p} c_j^2}$$

Then a $100(1-\alpha)\%$ simultaneous confidence interval for L takes the form:

$$\hat{L} \pm T s(\hat{L}),$$

where T is a multiplier that depends on the type of the inference method used.

1. **Tukey's Method (Pairwise Comparisons):** Tukey's method is designed for simultaneous confidence intervals when comparing all possible pairwise differences between group means. The multiplier is:

$$T = \frac{q(p, \nu_R; \alpha)}{\sqrt{2}}$$

where $q(p, \nu_R; \alpha)$ is the studentized range statistic for p groups and residual degrees of freedom ν_R.

When comparing all pairs, each pairwise difference is a contrast (with coefficients $c_j = 1$ for one group and $c_j = -1$ for the other, and 0 elsewhere). Each interval is given by:

$$\text{CI for } (u_j - u_k)\text{: } AC \quad (y_{j\cdot\cdot} - y_k) \pm \frac{q\,(p, \nu_R; \alpha)}{\sqrt{2}}\, s_R \sqrt{\frac{1^2 + (-1)^2}{q\,r}}$$

Here, the multiplier $\frac{q\,(p, \nu_R; \alpha)}{\sqrt{2}}$ is applied to each pairwise contrast.

2. **Scheffé's Method (All Contrasts):** Scheffés method is more conservative and applies to all possible contrasts, not just pairwise comparisons. The multiplier is:

$$T = \sqrt{(p-1)\, F_{(p-1),\nu_R;\alpha}}$$

where $F_{(p-1),\nu_R;\alpha}$ is the critical value from the F-distribution with $p-1$ and ν_R degrees of freedom.

For any contrast $L = \sum_j c_j\, u_j$, the simultaneous confidence interval is:

$$\hat{L} \pm \sqrt{(p-1)\, F_{(p-1),\nu_R;\alpha}}\, S_R \sqrt{\frac{1}{q\,r} \sum_j c_j^2}$$

This interval applies to every possible contrast you might form.

3. **Bonferroni's Method (For g Comparisons):** The Bonferroni method controls the familywise error rate by adjusting the significance level for multiple comparisons. For any set of g comparisons, the multiplier is:

$$T = t_{\nu_R;\alpha/(2g)}$$

where $t_{\nu_R;\alpha/(2g)}$ is the t-distribution critical value with residual degrees of freedom ν_R and a Bonferroni-adjusted significance level of $\alpha\,/\,(2\,g)$.

If you have a specific set of g comparisons (contrasts) you plan to test, each interval is:

$$\hat{L} \pm t_{\nu_R;\alpha/(2g)}\, S_R \sqrt{\frac{1}{q\,r} \sum_j c_j^2}.$$

Each of the g contrasts gets its own interval, with the critical value adjusted by dividing α by $2\,g$.

2.7.2 When interactions are significant

In this case, each combination of factor levels has its own mean:

$$\mu_{jk} = \mu + p_j + q_k + (pq)_{jk}$$

If we are interested in comparing the means of two specific treatment combinations, say $\mu_{j_1k_1}$ and $\mu_{j_2k_2}$, we are comparing two of the pq treatments.

1. **Tukey's Method:** for all possible pairs of treatment means,

$$(\hat{\mu}_{j_1k_1} - \hat{\mu}_{j_2k_2}) \pm \frac{q(p\,q, \nu_R; \alpha)}{\sqrt{2}}\, S_R \sqrt{\frac{2}{r}}$$

   where $q(pq, \nu_R; \alpha)$ is the quantile of the studentized range statistic for pq treatments and ν_R is the residual degrees of freedom.

2. **Bonferroni's Method:** for g pairs of comparisons,

$$(\hat{\mu}_{j_1k_1} - \hat{\mu}_{j_2k_2}) \pm t_{\nu_R;\alpha/(2g)}\, s_R \sqrt{\frac{2}{r}},$$

   where $t_{\nu_R;\alpha/(2g)}$ is the quantile from t-distribution.

3. **Scheffé's Method for General Contrasts**: the contrast takes the form:

$$L = \sum_{j=1}^{p} \sum_{k=1}^{q} c_{jk}\, \mu_{jk}, \quad \text{with} \quad \sum_{j,k} c_{jk} = 0$$

   The confidence interval for the contrast L is given by:

$$\hat{L} \pm \sqrt{(p\,q-1)\, F_{(pq-1),\nu_R;\alpha}}\, s(\hat{L})$$

   where:

   - $\hat{L} = \sum_{j,k} c_{jk} \hat{\mu}_{jk}$,
   - $s(\hat{L}) = s_R \sqrt{\sum_{j,k} \frac{c_{jk}^2}{r}}$ (assuming balanced replication),
   - $F_{(pq-1),\nu_R;\alpha}$ris the critical value from the F-distribution with $pq-1$ and ν_R degrees of freedom.

2.8 Two-way Factorial with Blocks

2.8.1 No Replicates Within Blocks

Model:

$$y_{ijk} = \mu + b_i + t_{jk} + \varepsilon_{ijk} = \mu + b_i + p_j + q_k + (pq)_{jk} + \varepsilon_{ijk}$$

for $i = 1, \ldots, b$, $j = 1, \ldots, p$, and $k = 1, \ldots, q$, with sum-to-zero constrains:

$$\sum_i b_i = \sum_j p_j = \sum_k q_k = 0.$$

Data decomposition:

$$\begin{aligned} y_{ijk} &= y_{...} + (y_{i..} - y_{...}) + (y_{.jk} - y_{...}) + (y_{ijk} - y_{i..} - y_{.jk} + y_{...}) \\ &= y_{...} + (y_{i..} - y_{...}) + (y_{.j.} - y) + (y_{..k} - y_{...}) \\ &+ (y_{.jk} - y_{.j.} - y_{..k} + y_{...}) + (y_{ijk} - y_{i..} - y_{.jk} + y_{...}) \end{aligned}$$

Source	SS	df
Blocks	$p\,q\sum_i (y_{i..} - y_{...})^2$	$b-1$
P	$b\,q\sum_j (y_{.j.} - y_{...})^2$	$p-1$
Q	$b\,p\sum_k (y_{..k} - y_{...})^2$	$q-1$
PQ	$b\sum_j\sum_k (y_{.jk} - y_{.j.} - y_{..k} + y_{...})^2$	$(p-1)\,(q-1)$
Residual	$\sum_i\sum_j\sum_k (y_{ijk} - y_{i..} - y_{.jk} + y_{...})^2$	$(b-1)\,(p\,q-1)$
Total	$\sum_i\sum_j\sum_k (y_{ijk} - y_{...})^2$	$b\,p\,q-1$

Table 7. ANOVA table for two-way factorial with blocks and without replicates

2.8.2 With Replicates Within Blocks

Model:

$$y_{ijkl} = \mu + b_i + t_{jk} + \varepsilon_{ijk} = \mu + b_i + p_j + q_k + (pq)_{jk} + \varepsilon_{ijkl}$$

or $i = 1, \ldots, b$, $j = 1, \ldots, p$, $l = 1, \ldots, r$, and $k = 1, \ldots, q$, with sum-to-zero constrains:

$$\sum_i b_i = \sum_j p_j = \sum_k q_k = 0.$$

Data decomposition:

$$\begin{aligned} y_{ijkl} &= y_{....} + (y_{i...} - y_{....}) + (y_{.j..} - y_{....}) + (y_{..k.} - y_{....}) \\ &+ (y_{.jk.} - y_{.j..} - y_{...k} + y_{....}) + (y_{ijkl} - y_{i...} - y_{.jk.} + y_{....}) \end{aligned}$$

Source	SS	df
Blocks	$p\,qr\sum_i (y_{i...} - y_{....})^2$	$b-1$
P	$b\,qr\sum_j (y_{.j..} - y_{....})^2$	$p-1$
Q	$b\,pr\sum_k (y_{..k.} - y_{....})^2$	$q-1$
PQ	$b\sum_j\sum_k (y_{.jk.} - y_{.j..} - y_{..k.} + y_{....})^2$	$(p-1)\,(q-1)$
Residual	$\sum_i\sum_j\sum_k\sum_l (y_{ijkl} - y_{i...} - y_{.jk.} + y_{....})^2$	$bpqr - b - pq + 1$
Total	$\sum_i\sum_j\sum_k\sum_l (y_{ijkl} - y_{....})^2$	$b\,p\,qr-1$

Table 8.

2.8.3 Advantages of Two-level Factorial Designs

1. **Efficiency in runs:** They require only a few experimental runs per factor, making them cost-effective and time-saving even when several factors are under study.

   Two-level factorial designs use only two settings per factor, which are chosen to maximize the contrast between high and low values. This strong contrast helps in estimating the main effects with greater clarity.

2. **Identifying Major Trends:** While they don't cover the entire range of possible factor values, these designs help reveal the main effects and trends, pointing toward areas that merit further investigation.

3. **Flexible Augmentation:** If more detailed local analysis is needed later, two-level designs can be expanded or combined with additional points (composite designs) to explore the factor space more thoroughly.

4. **Modular Design Building:** They serve as building blocks. By combining them appropriately, you can tailor the complexity of the experimental design to match the sophistication of the problem at hand.

5. **Precision in Effect Estimation:** With fewer runs and a clear structure, the estimates of the main effects of factors are generally precise.

6. They form the basis for two-level fractional factorial designs.

3 Factorial Design

3.1 Comparison of designs

3.1.1 OFAT v.s. Factorial

OFAT Experiments: An experimental approach in which only **one factor (independent variable)** is varied at a time while keeping all other factors constant. The goal is to observe the effect of that single factor on the response variable.

2^2 Factorial Design: an experimental design where there are **two factors**, each with **two levels** (e.g., "low" and "high"). This results in **$2^2 = 4$ experimental runs**, covering all possible combinations of factor levels.

Example 5. OFAT Design: An engineer designed an experiment to compare a standard and a new gas anneal process by varying pressure and temperature across three runs:

1. Standard pressure & standard temperature
2. Standard pressure & new temperature
3. New pressure & new temperature

A single lot of 48 wafers was used, with 16 wafers assigned to each run.

	Temperature	
Pressure	Standard	New
Standard	16 wafers	16 wafers
New	-	16 wafers

Table 9. OFAT Design

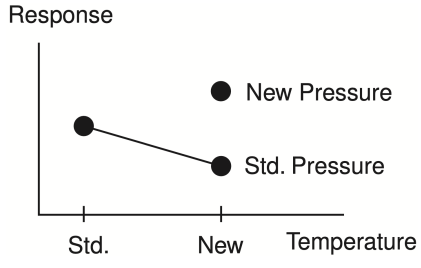

Figure 4. OFAT Design

2^2 Factorial Design:

	Temperature	
Pressure	Standard	New
Standard	12 wafers	12 wafers
New	12 wafers	12 wafers

Table 10. 2^2 Factorial Design

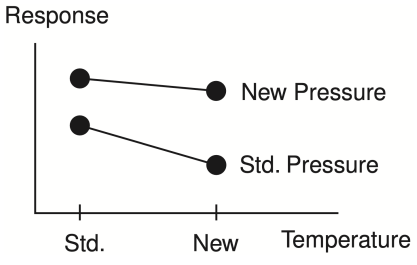

Figure 5. 2^2 Factorial Design

Advantages of 2^2 Factorial Design:

1. Estimates of the factor effects are more precise (all 48 wafers are used, while only 32 wafers in the OFAT design)
    a. Variance of each effect is $\sigma^2/12$ for the 2^2 design.
    b. Variance of each factor effect for the OFAT is $\sigma^2/8$(50% more).
2. Interaction effect can be estimated.
3. 2^2 design provides data over a broader factor space.

3.1.2 Central Composite Design

Example 6. Two engineers planned an experiment for a rapid thermal anneal process. They wanted to study the sensitivity of the response sheet resistance to two factors—time and temperature. The followings are 3 different designs

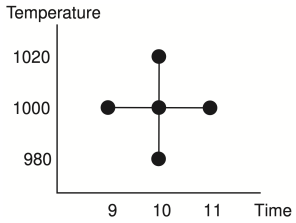

Figure 6. OFAT Design

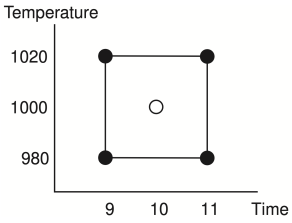

Figure 7. 2^2 Design

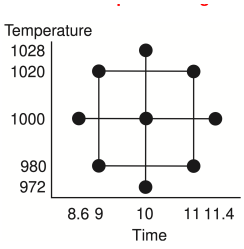

Figure 8. Central Composite

Central Composite Design (CCD): is a type of **Response Surface Methodology (RSM)** used for building a quadratic model in experimental designs. It helps **optimize processes** by exploring both linear and interaction effects, as well as curvature in factor responses. It contains the following components:

- **Factorial Points**: A full or fractional factorial design that represents the main effects and interactions.
- **Axial (Star) Points**: Points placed outside the factorial design to capture curvature and quadratic effects.
- **Center Points**: Replicated runs at the center of the design space to improve model accuracy and detect pure error.

Type	X_1	X_2
Factorial Points	$-1, +1$	$-1, +1$
Axial Points	$\pm\alpha$	$\pm\alpha$
Center Points	0	0

Table 11. Example of CCD with two factors

Advantages of Central Composite Design:

1. Estimates of factor effects are more precise

2. Interactions can be estimated

3. Curvature can be estimated in the entire space

4. Optimization is possible for the entire space

5. If center point is replicated 4 times, the design is rotatable, i.e., equal precision in estimation at all points equidistant from the center

3.1.3 2^3 Design

Example 7. 3-factor OFAT design & 2^3 experiment

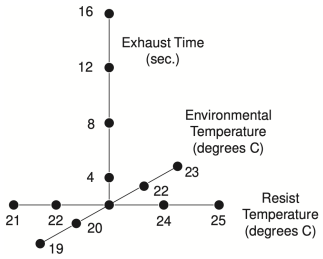

Figure 9. 3-factor OFAT in 15 runs

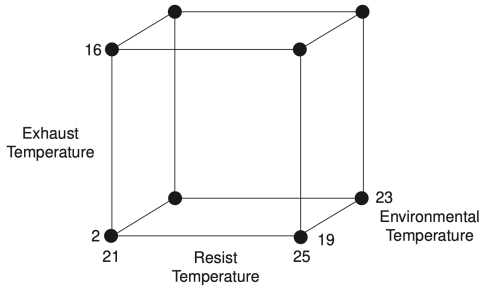

Figure 10. 2^3 experiment in 8 runs

Advantages of the 2^3 design:

1. Requires less resources: 8 runs instead of 15.

2. Estimates of factor effects are more accurate: all 8 runs are used in each estimate. But in OFAT, only 5 runs are used in each estimate.

3. Interaction effects can be estimated.

4. 2^3 design yields information over a larger region of the factor space

3.1.4 Box-Behnken design

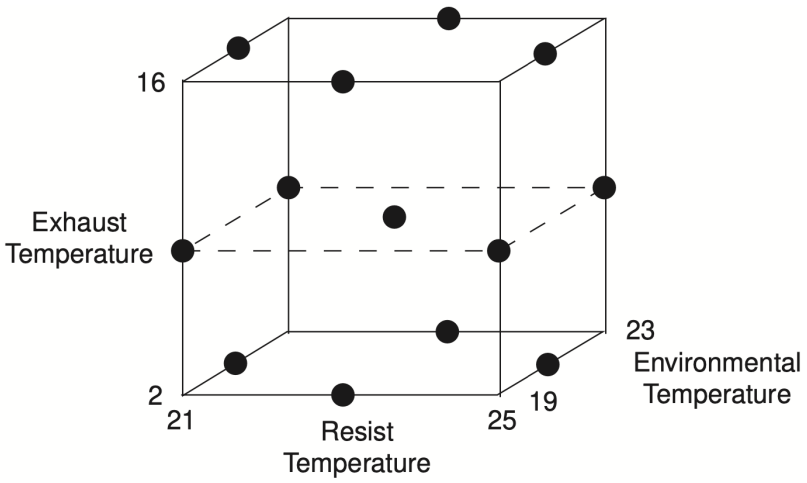

Figure 11. Box-Behnken design in 15 runs

Advantages of Box-Behnken Design:

1. Interactions can be estimated in Box-Behnken design.
2. Runs are more evenly spread out—hence more accurate predictions while OFAT can estimate curvature along 3 lines only.
3. Box-Behnken can estimate curvature in entire experimental region.
4. Box-Behnken design can be optimized over entire factor space while OFAT can be optimized along 3 lines only.

3.2 Analysis of Factorial Design

3.2.1 2^2 Design

Notation 1. *We use the following notations to represent factors and interactions in a* 2^2 *design:*

- *Two factors* A *and* B*, each at two levels.*
- *4 sets of experimental conditions. "Low" indicated by "−" and "high" indicated by "+".*
- *Use notation* (1)*, a, b, ab to denote the mean responses at the treatment combinations listed in figure 12.*

Run	A	B	Symbol
1	-	-	(1)
2	+	-	a
3	-	+	b
4	+	+	ab

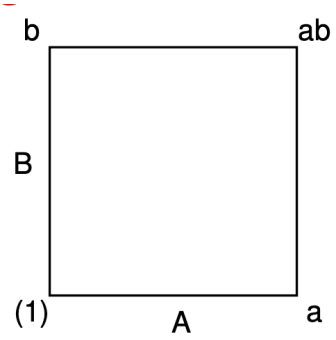

Figure 12. Notations in a 2^2 design

Model:

$$y_{ijk} = \eta + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk} \tag{3}$$

with sum-to-zero constrains:

$$\alpha_1 + \alpha_2 = \beta_1 + \beta_2 = (\alpha\,\beta)_{11} + (\alpha\,\beta)_{12} = (\alpha\,\beta)_{21} + (\alpha\,\beta)_{22} = (\alpha\,\beta)_{11} + (\alpha\,\beta)_{21} = 0.$$

Define $\alpha_2 = \alpha$, $\beta_2 = \beta$, then we can write

$$\alpha_1 = -\alpha, \beta_1 = -\beta, (\alpha\,\beta)_{21} = -(\alpha\,\beta), (\alpha\,\beta)_{11} = (\alpha\,\beta), (\alpha\,\beta)_{12} = -(\alpha\,\beta)$$

i	j	A	B	Observation	Without constraints	With constraints
1	1	-	-	(1)	$\eta+\alpha_1+\beta_1+(\alpha\,\beta)_{11}$	$\eta-\alpha-\beta+(\alpha\,\beta)$
2	1	+	-	a	$\eta+\alpha_2+\beta_1+(\alpha\,\beta)_{21}$	$\eta+\alpha-\beta-(\alpha\,\beta)$
1	2	-	+	b	$\eta+\alpha_1+\beta_2+(\alpha\,\beta)_{12}$	$\eta-\alpha+\beta-(\alpha\,\beta)$
2	2	+	+	ab	$\eta+\alpha_2+\beta_2+(\alpha\,\beta)_{22}$	$\eta+\alpha+\beta+(\alpha\,\beta)$

Table 12. Summary of 2^2 design model

Then we have the least square estimates of the parameters:

$$\begin{aligned}\hat{\eta}&=[a\,b+a+b+(1)]/4=y...\\ \hat{\alpha}&=[a\,b+a-b-(1)]/4\\ \hat{\beta}&=[a\,b-a+b-(1)]/4\\ \widehat{(\alpha\,\beta)}&=[a\,b-a-b+(1)]/4\end{aligned}$$

Remark 5. The interaction coefficients cancel out because of the sum-to-zero constrains.

The **main effect of A** is defined as:

$$\begin{aligned}A&=2\,\hat{\alpha}=[a\,b+a-b-(1)]/2\\ &=[a\,b+a]/2-[b+(1)]/2\\ &=(1/2)\,\{[a\,b-b]+[a-(1)]\}\end{aligned}$$

The **interaction effect** is defined as:

$$\begin{aligned}A\,B&=2\,\widehat{(\alpha\,\beta)}\\ &=[a\,b-a-b+(1)]/2\\ &=(1/2)\,\{[a\,b-b]-[a-(1)]\}\\ &=(1/2)\,\{[a\,b-a]-[b-(1)]\}\end{aligned}$$

Notation 2. *We use upraight letters to denote the factors, and use italic letters to denote the effects defined above.*

3.2.2 Generalization to 2^3 Design

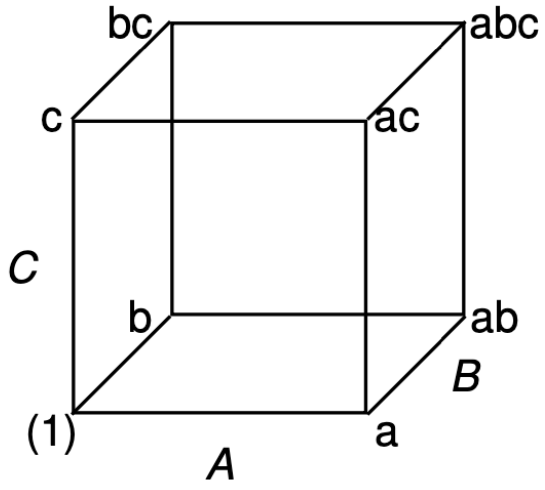

Figure 13. 2^3 design

Mean effect of A:

$$\begin{aligned}
A =& (a + a\,b + a\,c + a\,b\,c)/4 - ((1) + b + c + b\,c)/4 \\
=& \text{mean of high A} - \text{mean of low A} \\
=& (1/4)\,\{(a - (1)) + (a\,b - b) + (a\,c - c) + (a\,b\,c - b\,c)\} \\
=& \text{mean of 4univariate A effects} \\
=& (1/2)\,[\{a\,b\,c + a\,c - b\,c - c\}/2 + \{a\,b + a - b - (1)\}/2] \\
=& (1/2)\,\{\text{Effect in A-B design at high C+Aeffect in A-B design at low C}\}
\end{aligned}$$

Interaction Effects:

- The 2^3 consists of two 2^2 designs: one at high C and one at low C
- AB interaction at low C is $A\,B_1 = (a\,b + (1) - a - b)/2$
- AB interaction at high C is $A\,B_2 = (a\,b\,c + c - a\,c - b\,c)/2$
- $A\,B$ and $A\,B\,C$ effects for 2^3 are defined as

$$\begin{aligned}
A\,B &= (1/2)\,(A\,B_2 + A\,B_1) = (1/4)\,(a\,b\,c + c - a\,c - b\,c + a\,b + (1) - a - b) \\
A\,B\,C &= (1/2)\,(A\,B_2 - A\,B_1) = (1/4)\,(a\,b\,c + c - a\,c - b\,c - a\,b - (1) + a + b)
\end{aligned}$$

Alternative Expressions:

The LSEs

$$\begin{aligned}
\hat{\eta} &= [a\,b\,c + a\,b + a\,c + b\,c + a + b + c + (1)]/8 \\
A &= [a\,b\,c + a\,b + a\,c + a - b\,c - b - c - (1)]/4 \\
A\,B &= [a\,b\,c + a\,b - a\,c - b\,c - a - b + c + (1)]/4 \\
A\,B\,C &= [a\,b\,c - b\,c - a\,c - a\,b + a + b + c - (1)]/4
\end{aligned}$$

Combining the expressions, we have:

$$\begin{aligned}
\hat{\eta} &= (a+1)\,(b+1)\,(c+1)/8 \\
A &= (a-1)\,(b+1)\,(c+1)/4 \\
A\,B &= (a-1)\,(b-1)\,(c+1)/4 \\
A\,B\,C &= (a-1)\,(b-1)\,(c-1)/4
\end{aligned}$$

- Variance of any effect estimation is var(effect) $= 4\,N^{-1}\,\sigma^2$, where N is total number of observations and $\sigma^2 = \text{var}(\epsilon)$
- Let s_i^2 be the estimate of σ^2 at the i th treatment combination ($i = 1, 2, \ldots, g$). Let $\nu_i = r_i - 1$ be the degrees of freedom for s_i^2, where r_i is the number of replicates in rth combination. Then the pooled estimate of σ^2 is:

$$s^2 = \frac{\nu_1\,s_1^2 + \cdots + \nu_g\,s_g^2}{\nu_1 + \cdots + \nu_g}$$

- Confidence intervals for estimated effects may be obtained using the Bonferroni method.

- Hidden replication property: When estimating the effect of a single factor (say, A) in a 2^3 design (with factorsr$A$, B, and C), the precision of the estimate for A is the same as it would be if you had conducted an experiment with only A at two levels with the same number of replications (for example, 4 runs at low A and 4 runs at high A).

We may use a **table of contrast** to summary the result of a 2^3 design. The "Dot product" in this table refers to the inner product between each column (e.g. A) and the response vector $\mathbf{y}$, and Dividing it by $N/2$ gives the estimate of the corresponding effect.

	A	B	C	AB	AC	BC	ABC	y
	-1	-1	-1	1	1	1	-1	60
	1	-1	-1	-1	-1	1	1	72
	-1	1	-1	-1	1	-1	1	54
	1	1	-1	1	-1	-1	-1	68
	-1	-1	1	1	-1	-1	1	52
	1	-1	1	-1	1	-1	-1	83
	-1	1	1	-1	-1	1	-1	45
	1	1	1	1	1	1	1	80
Dot product	92	-20	6.0	6.0	40	0	2.0	
Division by $N/2$	23	-5	1.5	1.5	10	0	0.5	

Table 13. Table of contrast example

Notation 3. ***(Notation summary)*** *We use upright letters (e.g.* A, AB*) to represent the factor or the corresponding columns in the table of contrast, and use italic letters (e.g. A, AB) to represent the corresponding effects defined in section 3.2.1.*

3.2.3 Regression Formulation

The model of 2^3 design can be written as:

$$\mathbb{E}(y_{ijk}) = \eta + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk}$$

For an observation y_l, Let $x_{il} = 1$ indicate the ith factor is at its high level and $x_{il} = -1$ indicate the ith factor is at its low level. Then we can write

$$\mathbb{E}(y_l) = \beta_0 + \beta_1 x_{1l} + \beta_2 x_{2l} + \beta_3 x_{3l} + \beta_{12} x_{1l} x_{2l} + \beta_{13} x_{1l} x_{3l} + \beta_{23} x_{2l} x_{3l} + \beta_{123} x_{1l} x_{2l} x_{3l}.$$

The LSEs are:

$$\begin{aligned}
\hat{\eta} = \hat{\beta}_0 &= [abc + ab + ac + bc + a + b + c + (1)]/8 \\
A = 2\,\hat{\beta}_1 &= [abc + ab + ac + a - bc - b - c - (1)]/4 \\
AB = 2\,\hat{\beta}_{12} &= [abc + ab - ac - bc - a - b + c + (1)]/4 \\
ABC = 2\,\hat{\beta}_{123} &= [abc - bc - ac - ab + a + b + c - (1)]/4, \text{etc.}
\end{aligned}$$

The general 2^k design model can be written in a matrix form:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\mathbf{y}$ is the vector of observations and when $k=3$:

$$\mathbf{X}=\left(\begin{array}{c|ccc|ccc|c} 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{array}\right), \quad \boldsymbol{\beta}=\left(\begin{array}{c} \eta \\ \alpha \\ \beta \\ \gamma \\ (\alpha\,\beta) \\ (\alpha\,\gamma) \\ (\beta\gamma) \\ (\alpha\,\beta\gamma) \end{array}\right)$$

Note that $\mathbf{X}$ is an orthogonal matrix, then $\mathbf{X}^T\mathbf{X}=2^k\mathbf{I}$ is an diagonal matrix, and we have

$$\hat{\boldsymbol{\beta}}=2^{-k}\mathbf{X}^T\mathbf{y}.$$

3.3 Yates Algorithm for 2^k Experiments

Yates algorithm is a systematic computational procedure used to analyze data from a full 2^k factorial experiment. In these experiments, you have k factors, each at two levels (often labeled as "low" and "high"). The algorithm helps you calculate the main effects and interaction effects quickly and efficiently.

1. **Order the Data:**
   List the experimental data in the standard order (the order shown in the 1st column of table 14).

2. **Construct k New Columns:**
   For each new column (starting from the first column of responses), perform the following:

   - **Addition (First Half):**
     For the first 2^{k-1} entries, form each new entry by adding pairs of consecutive entries from the previous column. That is, for row$i$, compute:

     $$\text{New entry}=(\text{entry in row } 2\,i-1)+(\text{entry in row } 2\,i).$$

   - **Subtraction (Second Half):**
     For the remaining 2^{k-1} entries, compute each new entry by subtracting the entry in row $2i-1$ from the entry in row $2i$ in the previous column:

     $$\text{New entry}=(\text{entry in row } 2\,i)-(\text{entry in row } 2\,i-1).$$

3. **Create a Scaling Column:**
   Add an additional column (the $(k+1)$th column) where all entries are 2^{k-1}, except the first entry, which is 2^k.

4. **Compute the Estimates:**
   Obtain the effect estimates by dividing the entries in the kth column by the corresponding entries in the $(k+1)$th (scaling) column.

5. **Identify the Effects:**
   Determine the identity of each effect by inspecting the signs of the factors along each row in the table.

A	B	C	y	(1)	(2)	(3)	Div.	Est.	Effect
-1	-1	-1	60	132	254	514	8	64.25	$\bar{y}$
1	-1	-1	72	122	260	92	4	23.00	A
-1	1	-1	54	135	26	-20	4	-5.00	B
1	1	-1	68	125	66	6	4	1.50	AB
-1	-1	1	52	12	-10	6	4	1.50	C
1	-1	1	83	14	-10	40	4	10.00	AC
-1	1	1	45	31	2	0	4	0.00	BC
1	1	1	80	35	4	2	4	0.50	ABC

Table 14. Example of data table created by Yates algorithm

3.4 Factorial Design with blocks

3.4.1 2^2 Design in 2 Blocks of Size 2

Let $x_1, x_2, z \in \{-1, 1\}$, where x_1, x_2 indicates levels of A and B and z indicates the block variables. The model is defined as

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \delta z + \varepsilon$$

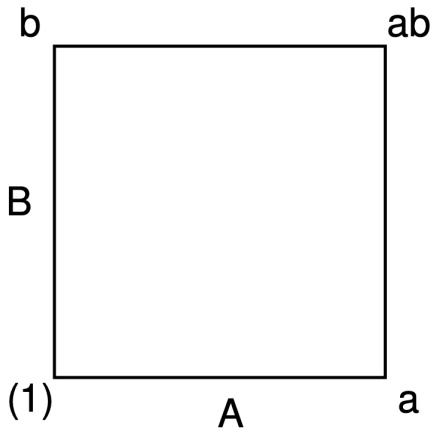

Figure 14. 2^2 design with blocks

Consider 3 possible designs:

- D1. (1), a in block 1; b, ab in block 2
- D2. (1), b in block 1; a, ab in block 2
- D3. (1), ab in block 1; a, b in block 2

In D1, B is confounded by the block effect because $z = x_2$ leads to:

$$\mathbb{E}(ab + b - a - (1)) = 4\beta_2 + 4\delta,$$

while A and AB are not confounded.

3.4.2 2^3 in 2 Blocks of Size 4

OFAT Block Design:

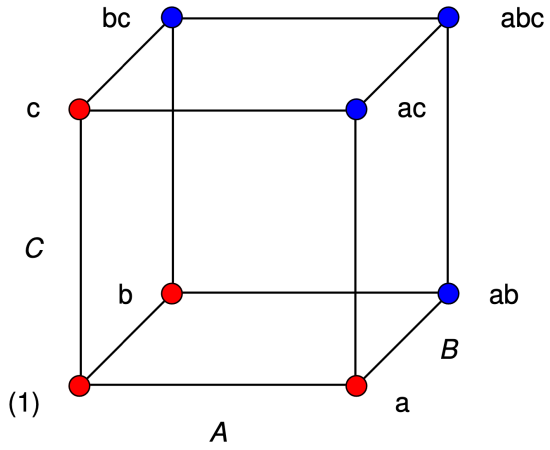

Figure 15. OFAT block design. Different colors indicate the experiment is conducted in different blocks.

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

Table 15. Treatment table of OFAT block design

The corresponding model is:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 + \delta z + \epsilon \tag{4}$$

A is confounded in the design shown in Figure 15 and Table 15 because the expression

$$A = [a\,b\,c + a\,b + a\,c + a - b\,c - b - c - (1)]\,/\,4$$

cannot eliminate δ if we plug in (4).

We may change the design of the experiment to make the parameters of interest unfounded while some other parameters confounded. As shown in table 16, we can make the assignment of blocks exactly the same as the assignment of the 3-way interaction ABC. By doing this, only ABC is confounded in our data. However, we can never make all the parameters unconfounded if we have to impose 2 blocks of size 4.

	A	B	C	AB	AC	BC	ABC	Block
(1)	-	-	-	+	+	+	-	-
a	+	-	-	-	-	+	+	+
b	-	+	-	-	+	-	+	+
ab	+	+	-	+	-	-	-	-
c	-	-	+	+	-	-	+	+
ac	+	-	+	-	+	-	-	-
bc	-	+	+	-	-	+	-	-
abc	+	+	+	+	+	+	+	+

Table 16. Experimental design such that only ABC is confounded.

Remark 6. In a 2^k design in 2 blocks, we usually use the largest-order interaction column to define the assignment of blocks such that only the highest order interaction is confounded.

3.4.3 2^3 in 4 Blocks of Size 2

If we have 4 blocks, we need two block variables $X, Y \in \{-1, 1\}$ to represent the block combinations in the table.

	A	B	C	AB	AC	BC	ABC	X	Y
(1)	-	-	-	+	+	+	-	+	+
a	+	-	-	-	-	+	+	-	+
b	-	+	-	-	+	-	+	-	-
ab	+	+	-	+	-	-	-	+	-
c	-	-	+	+	-	-	+	+	-
ac	+	-	+	-	+	-	-	-	-
bc	-	+	+	-	-	+	-	-	+
abc	+	+	+	+	+	+	+	+	+

Table 17. 2^3 design with blocks of size 2

If we put the columns $X = AB, Y = \text{BC}$, then **all** the two-way interactions are confounded while the other parameters are not.

3.4.4 2^4 in 4 blocks

A	B	C	D	ABC	ABD	CD	Block
-	-	-	-	-	-	+	1
+	-	-	-	+	+	+	4
-	+	-	-	+	+	+	4
+	+	-	-	-	-	+	1
-	-	+	-	+	-	-	3
+	-	+	-	-	+	-	2
-	+	+	-	-	+	-	2
+	+	+	-	+	-	-	3
-	-	-	+	-	+	-	2
+	-	-	+	+	-	-	3
-	+	-	+	+	-	-	3
+	+	-	+	-	+	-	2
-	-	+	+	+	+	+	4
+	-	+	+	-	-	+	1
-	+	+	+	-	-	+	1
+	+	+	+	+	+	+	4

Table 18. 2^4 design with blocks of size 2

Use ABC and ABD to define blocks as shown in figure 18, then CD is confounded as well since $\text{ABC} \times \text{ABD} = \text{CD}$.

3.4.5 Partial Confounding

4 Fractional two-level designs

2^k designs include too many interactions and variables when k is large. But in most cases we are only interested in few of them. **Fractional factorial design** reduce the number of experiments by assuming many higher-order interactions are negligible and we only care about main effects and two-factor interactions.

4.1 Half-fraction of 2^3

Assume that all interactions are negligible, then the model can be written as

$$y = \mu + \alpha x_1 + \beta x_2 + \gamma x_3 + \varepsilon, \quad x_1, x_2, x_3 = \pm 1 \tag{5}$$

Now we investigate different experimental designs.

1. **Design 1 (OFAT):** Using runs (1), a, b and c, i.e. using the design matrix:

$$X = \begin{pmatrix} 1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

   and the covariance matrix for the estimation is:

$$\sigma^2(X^TX)^{-1} = \sigma^2 \begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & 1/4 & 1/4 \\ 1/2 & 1/4 & 1/2 & 1/4 \\ 1/2 & 1/4 & 1/4 & 1/2 \end{pmatrix}$$

2. **Design 2:** Using runs a, b, c, and abc, i.e. using the design matrix:

$$X = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},$$

   and the covariance matrix for the estimation is

$$\sigma^2(X^TX)^{-1} = \sigma^2 \begin{pmatrix} 1/4 & 0 & 0 & 0 \\ 0 & 1/4 & 0 & 0 \\ 0 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 1/4 \end{pmatrix}$$

4.2 Construction of 2^{5-1} design

1. Write a full 2^4 design in variables A, B, C and D

2. Add a column of signs for factor E defined by E = ABCD

Notation 4. *Product of upright letters (e.g.* ABCD*) is a shorthand for taking Hadamard (element-wise) product of the corresponding column vector in the design table.*

A	B	C	D	E	A	B	C	D	E
-	-	-	-	+	-	-	-	+	-
+	-	-	-	-	+	-	-	+	+
-	+	-	-	-	-	+	-	+	+
+	+	-	-	+	+	+	-	+	-
-	-	+	-	-	-	-	+	+	+
+	-	+	-	+	+	-	+	+	-
-	+	+	-	+	-	+	+	+	-
+	+	+	-	-	+	+	+	+	+

Table 19. E=ABCD design

The equation

$$\mathrm{E} = \mathrm{ABCD}$$

is called the generator of the design. Multiplying both sides of the generator by E gives:

$$\mathrm{I} = \mathrm{ABCDE}, \tag{6}$$

where I is a column of positive signs and (6) is called the **defining relation** of the design. We can easily obtain its confounding pattern by multiplying (6) on both sides by any main or interaction effect, e.g., A = BCDE, B = ACDE, AB = CDE, which means the effects on both sides of the equality is confounded with each other. The expected values of the estimations are:

$$\begin{aligned}
\mathbb{E}(\bar{y}_1) &= \eta + A\,B\,C\,D\,E/2 \\
\mathbb{E}(\hat{A}_1) &= A + B\,C\,D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B}_1) &= A\,B + C\,D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B\,C}_1) &= A\,B\,C + D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B\,C\,D}_1) &= A\,B\,C\,D + E
\end{aligned}$$

Combining two half-fractions. Suppose we are allowed to run another 2^{5-1} experiment with defining relation E = −ABCD. Let δ be the block effect of the second run, $\hat{A}_2, \ldots, \widehat{ABCD}_2$ be the estimations for the corresponding effects in the second run, then we have

$$\begin{aligned}
\mathbb{E}(\bar{y}_2) &= \eta + \delta - A\,B\,C\,D\,E/2 \\
\mathbb{E}(\hat{A}_2) &= A - B\,C\,D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B}_2) &= A\,B - C\,D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B\,C}_2) &= A\,B\,C - D\,E \\
&\vdots \\
\mathbb{E}(\widehat{A\,B\,C\,D}_2) &= A\,B\,C\,D - E.
\end{aligned}$$

Thus, we can obtain unbiased estimation of each effect by combining two estimations. e.g.

$$\begin{aligned}
\mathbb{E}[(\hat{A}_1 + \hat{A}_2)/2] &= A \\
\mathbb{E}[(\widehat{A\,B}_1 + \widehat{A\,B}_2)/2] &= A\,B,
\end{aligned}$$

while the grand mean is still confounded by the block effect δ.

4.3 Resolution

Definition 3. *The **resolution** of a two-level fractional design is length of the shortest non-identity word in the defining relation.*

Interpretation: A design with **Resolution R** means that **Any p-factor effect** (an effect that involves p factors, such as a main effect where $p=1$ or an interaction where $p>1$) is **not** confounded with any other effect that involves fewer than $\boldsymbol{R-p}$ **factors**.

- A design with **Resolution III** means that while the mean effect are not aliased with one another, they may be aliased with two-factor interactions.
- A design with **Resolution IV** ensures that main effects are unconfounded with two-factor interactions while two-factor interactions might be aliased with each other.
- In a **Resolution V** design, main effects and two-factor interactions are not aliased with each other. In other words, any confounding (aliasing) involves interactions of order three or higher.

4.3.1 Half-fractional design for the highest resolution

To construct a half-fraction of the highest resolution (i.e., a 2^{k-1} design) with maximal clarity for estimating lower-order effects:

1. Start with a Full Factorial: Construct a full 2^{k-1} factorial design for the first $k-1$ factors.
2. Generate the k th Factor: Define the k th factor as the product of the first $k-1$ factors (i.e., $x_k = x_1 \times x_2 \times \cdots \times x_{k-1}$). This leads to the defining relation:

$$\mathrm{I} = \mathrm{F}_1\mathrm{F}_2 \ldots \mathrm{F}_k$$

   where F_i denotes the ith factor, and the defining relation has length k.

This approach produces the highest possible resolution for a 2^{k-1} design because a longer defining word (length k) ensures that any aliasing only involves high-order interactions (order k or more). As a consequence, main effects and low-order interactions (which are usually of primary interest) remain unconfounded, maximizing the interpretability of the experimental results.

Remark 7. If we remove any one column in a 2^{k-1} design, the remaining four columns form a complete 2^k factorial. A fractional factorial design of resolution R is constructed in such a way that every $R-1$ factors appears as a complete factorial.

4.3.2 Sequential use of fractional designs

It is generally advisable for an experimenter planning a 2^5 design in 32 runs to first conduct a half-fraction (16 runs), review the results, and then decide how to proceed. Here are the key points:

1. **Within-Fraction Randomization:**
   Randomize the order of runs within each half-fraction.
2. **Orthogonal Blocking When Combining Fractions:**
   If you choose to run another fraction later, structure them as randomized orthogonal blocks of the complete factorial design.
3. **Retention of Information:**
   No information is lost except for the interaction effect that becomes confounded with the block effect.
4. **Enhanced Precision:**
   Running the design as two randomized fractions can provide greater precision than a full random order because the block effect is removed.

4.3.3 Construction of Resolution III designs

Resolution III designs involving $2^k - 1$ variables can be constructed by "saturating" a 2^k factorial design with additional variables. For instance, let $k = 4$, a 2^{15-11}_{III} design (a design with 2^{15-11} runs and resolution III) may be obtained by the following procedure:

1. **Full Factorial Formation:**
   Start by constructing a full factorial design on variables 1, 2, 3, and 4.

2. **Association with Interaction Columns:**
   Assign the additional variables, numbered 5 through 15, to the 11 interaction columns corresponding to the interactions:

$$\pm F_1F_2,\ \pm F_1F_3,\ \pm F_1F_4,\ \pm F_2F_3,\ \pm F_2F_4,\ \pm F_3F_4,$$
$$\pm F_1F_2F_3,\ \pm F_1F_2F_4,\ \pm F_1F_3F_4,\ \pm F_2F_3F_4,\ \pm F_1F_2F_3F_4.$$

   In this context, each distinct assignment of the $\pm$ signs to these interaction terms defines one fraction of the design.

Example 8. (2^{7-4}_{III} design) Use generators F_4=F_1F_2, F_5=F_1F_3, F_6=F_2F_3 and F_7=$F_1F_2F_3$

1	2	3	4	5	6	7
-	-	-	+	+	+	-
+	-	-	-	-	+	+
-	+	-	-	+	-	+
+	+	-	+	-	-	-
-	-	+	+	-	-	+
+	-	+	-	+	-	-
-	+	+	-	-	+	-
+	+	+	+	+	+	+

Table 20. 2^{7-4}_{III} design

If we run another half-fractional design by switching the sign for 4, 5, 6, 7, then F_4=-F_1F_2, F_5=-F_1F_3, F_6=-F_2F_3 and F_7=-$F_1F_2F_3$ then the shortest defining relation becomes

$$I = (F_1F_2 \cdot F_4)(F_1F_3 \cdot F_5) = F_2F_4F_3F_5.$$

The resolution is 4 and we therefore have a 2^{7-3}_{IV} design.

4.3.4 Plackett-Burman Designs

Saturated fractional factorial designs are valued for their **orthogonality**: in any two columns of the design matrix, exactly half the runs in column A are "+," and among those, half are "+" and half "–" in column B; the same balance holds for the runs where column A is "–." Under the assumption that all interactions are negligible, this balance guarantees unbiased, minimum-variance estimates of all main effects for $k = N - 1$ factors in just N runs.

- **Classical limitation:** Regular 2^{k-p} designs exist only when N is a power of 2.

- **Plackett & Burman (1946):** Extended this orthogonality to any N that is a multiple of 4, allowing efficient main-effects screening with non–power-of-2 runs.

- **Example ($k = 11$, $N = 12$):**

    1. Write the first row of 11 signs (e.g. "+ − + + − ..."). If you have a Hadamard matrix of order N, remove the **1** column. Any one of the remaining rows of length $N - 1$ can be the first row. Standard choices of first rows are summarized in table 22.

    2. Generate each subsequent row by cyclically shifting the previous row one column to the right.

    3. Add a final 12th row of all "–" signs.

This simple "shifted-row" construction produces a 12×11 Plackett–Burman design that retains the key orthogonality property for unbiased estimation of main effects.

Run	1	2	3	4	5	6	7	8	9	10	11
1	+	-	+	-	-	-	+	+	+	-	+
2	+	+	-	+	-	-	-	+	+	+	-
3	-	+	+	-	+	-	-	-	+	+	+
4	+	-	+	+	-	+	-	-	-	+	+
5	+	+	-	+	+	-	+	-	-	-	+
6	+	+	+	-	+	+	-	+	-	-	-
7	-	+	+	+	-	+	+	-	+	-	-
8	-	-	+	+	+	-	+	+	-	+	-
9	-	-	-	+	+	+	-	+	+	-	+
10	+	-	-	-	+	+	+	-	+	+	-
11	-	+	-	-	-	+	+	+	-	+	+
12	-	-	-	-	-	-	-	-	-	-	-

Table 21. Plackett-Burman design for $k = 11$ and $N = 12$

4.3.5 Construction of Resolution IV Designs

You can obtain a 2_{IV}^{k-p} design from any resolution III fraction in three steps:

1. **Base Fraction (Resolution III):**
   Construct a $2_{\text{III}}^{(k-1)-p}$ design on the first $k - 1$ factors.

2. **Add a "Pure" Column:**
   Append a kth factor column consisting entirely of "+" signs to that design.

3. **Foldover:**
   Create a second block of runs by flipping every sign in the first block. Together, the original block and its foldover form a resolutionrIV design on k factors.

Example 9. Constructing a 2_{IV}^{7-3} design from 2_{III}^{6-3} Design

1. **Base 2_{III}^{6-3} Design.** Define the generators:

$$\text{F}_4 = \text{F}_1\text{F}_2, \quad \text{F}_5 = \text{F}_1\text{F}_3, \quad \text{F}_6 = \text{F}_2\text{F}_3.$$

   The defining relation for the first $2^{6-3} = 8$ runs is:

$$\text{I} = \text{F}_1\text{F}_2\text{F}_4 = \text{F}_1\text{F}_3\text{F}_5 = \text{F}_2\text{F}_3\text{F}_6.$$

2. **Add the seventh factor $\mathbf{F_7}$.** Assign $\mathrm{F}_7 = +1$ in the first half, introducing the word

$$\mathrm{I} = \mathrm{F}_7.$$

3. **Fold-over to Resolution IV.** Create a second set of 8 runs by flipping every sign in the first half. Its defining relation becomes:

$$I = -\mathrm{F}_1\mathrm{F}_2\mathrm{F}_4 = -\mathrm{F}_1\mathrm{F}_3\mathrm{F}_5 = -\mathrm{F}_2\mathrm{F}_3\mathrm{F}_6 = -\mathrm{F}_7.$$

4. **Combine Both Halves.** When the two halves are pooled, each length-3 word appears once with "+" and once with "–," so they cancel. The shortest remaining aliasing words involve four factors, yielding a *resolution IV* design.

Example 10. Constructing a 2^{7-3}_{IV} design from 2^{7-4}_{III} Design.

1. **Base 2^{7-4}_{III} design**: Use generators

$$\mathrm{F}_4 = \mathrm{F}_1\mathrm{F}_2, \quad \mathrm{F}_5 = \mathrm{F}_1\mathrm{F}_3, \quad \mathrm{F}_6 = \mathrm{F}_2\mathrm{F}_3, \quad \mathrm{F}_7 = \mathrm{F}_1\mathrm{F}_2\mathrm{F}_3.$$

Its defining relation is

$$\begin{aligned}\mathrm{I}_1 =& \mathrm{F}_1\mathrm{F}_2\mathrm{F}_4 = \mathrm{F}_1\mathrm{F}_3\mathrm{F}_5 = \mathrm{F}_2\mathrm{F}_3\mathrm{F}_6 = \mathrm{F}_1\mathrm{F}_2\mathrm{F}_3\mathrm{F}_7 \\ &= \mathrm{F}_2\mathrm{F}_3\mathrm{F}_4\mathrm{F}_5 = \mathrm{F}_1\mathrm{F}_3\mathrm{F}_4\mathrm{F}_6 = \mathrm{F}_3\mathrm{F}_4\mathrm{F}_6\mathrm{F}_7 \\ &= \mathrm{F}_1\mathrm{F}_2\mathrm{F}_5\mathrm{F}_6 = \mathrm{F}_2\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7 = \mathrm{F}_1\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7 \\ &= \mathrm{F}_1\mathrm{F}_2\mathrm{F}_3\mathrm{F}_4\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7.\end{aligned}$$

2. **Second Fraction by Sign-Switching**: Flip every sign in all columns of the first fraction. Its defining relation becomes

$$\begin{aligned}\mathrm{I}_2 =& -\mathrm{F}_1\mathrm{F}_2\mathrm{F}_4 = -\mathrm{F}_1\mathrm{F}_3\mathrm{F}_5 = -\mathrm{F}_2\mathrm{F}_3\mathrm{F}_6 = \mathrm{F}_1\mathrm{F}_2\mathrm{F}_3\mathrm{F}_7 \\ &= \mathrm{F}_2\mathrm{F}_3\mathrm{F}_4\mathrm{F}_5 = \mathrm{F}_1\mathrm{F}_3\mathrm{F}_4\mathrm{F}_6 = -\mathrm{F}_3\mathrm{F}_4\mathrm{F}_6\mathrm{F}_7 \\ &= \mathrm{F}_1\mathrm{F}_2\mathrm{F}_5\mathrm{F}_6 = -\mathrm{F}_2\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7 = -\mathrm{F}_1\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7 \\ &= -\mathrm{F}_1\mathrm{F}_2\mathrm{F}_3\mathrm{F}_4\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7.\end{aligned}$$

3. **Combine to Resolution IV**: Pooling both fractions cancels all length-3 and length-7 words, leaving only length-4 words as the shortest aliases. The final defining relation is

$$\mathrm{I} = \mathrm{F}_1\mathrm{F}_2\mathrm{F}_3\mathrm{F}_7 = \mathrm{F}_2\mathrm{F}_3\mathrm{F}_4\mathrm{F}_5 = \mathrm{F}_1\mathrm{F}_3\mathrm{F}_4\mathrm{F}_6 = \mathrm{F}_1\mathrm{F}_2\mathrm{F}_5\mathrm{F}_6 = \mathrm{F}_3\mathrm{F}_5\mathrm{F}_6\mathrm{F}_7 = \mathrm{F}_2\mathrm{F}_4\mathrm{F}_6\mathrm{F}_7 = \mathrm{F}_1\mathrm{F}_4\mathrm{F}_5\mathrm{F}_7.$$

Remark 8. (Selection of Resolution IV and V Designs)

- A *main effect* or *two-factor interaction* (2-fi) is said to be ***clear*** if none of its aliases is a main effect or two-factor interaction.
- A main effect or two-factor interaction is said to be ***strongly clear*** if none of its aliases is a main effect, two-factor interaction, or three-factor interaction (3-fi).

1. In any Resolution IV design, all main effects are clear.
2. In any Resolution V design, all main effects are strongly clear and all two-factor interactions are clear.

3. Among Resolution IV designs with fixed k and p, those maximizing the number of clear two-factor interactions are preferred.

A Plackett–Burman Table

Variable	12	16	20	24	32
1	+	+	+	+	-
2	+	-	+	+	-
3	-	-	-	+	-
4	+	-	-	+	-
5	+	+	+	+	+
6	+	-	+	-	-
7	-	-	+	+	+
8	-	+	+	-	-
9	-	+	-	+	+
10	+	-	+	+	+
11	-	+	-	-	+
12	·	-	+	-	-
13	·	+	-	+	+
14	·	+	-	+	+
15	·	+	-	-	-
16	·	·	-	-	-
17	·	·	+	+	-
18	·	·	+	-	+
19	·	·	-	+	+
20	·	·	·	-	+
21	·	·	·	-	+
22	·	·	·	-	+
23	·	·	·	-	-
24	·	·	·	·	-
25	·	·	·	·	+
26	·	·	·	·	+
27	·	·	·	·	-
28	·	·	·	·	+
29	·	·	·	·	-
30	·	·	·	·	-
31	·	·	·	·	+

Table 22. Plackett–Burman Table