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:

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

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:

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

Source	SS	df	$\mathbb{E}(\mathrm{MS}=\mathrm{SS}/\mathrm{df})$
	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	$\sum_{ij} (y_{ij}-y_{..})^2$	$b\,t-1$	
	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	$\sum_{ij} (y_{ij}-y_{..})^2$	$b\,t-1$	

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:

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

Example 1. (4 × 4 Design)

	μ_{jk}				$\mu_{j.}$	p_j	$(pq)_{jk}$			
	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
$\mu_{\cdot k}$	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 2. *A contrast for the main effects of factor P is defined as*

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

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

Example 3. (Simple Pairwise Comparison)

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

Definition 4. *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 5. Test whether the difference between levels of P depends on trhe 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 $q=3$

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

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

Table 4.

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

The columns of $\mathbf{X}$ w.r.t. different parameter groups are orthognal. 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

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

Note that the number of parameter equals to the number of observations, $\mathbf{X}$ is invertable, $\hat{\beta}$ is the solutoin 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:

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

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:

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

The sum of squares are defined as:

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

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 $\tilde{\mu}_{jk} = y_{j..} + y_{\cdot k\cdot} - y_{...}$ denote the estimated value of μ_{jk} assuming no inetractions.

2. To assess the homogeneity of variance in interactions, create a plot of the residuals $y_{jkl} - \hat{\mu}_{\mathrm{jk}}$ against the fitted values $\hat{\mu}_{\mathrm{jk}}$. A consistent spread of residuals across different values of $\hat{\mu}_{\mathrm{jk}}$ 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.

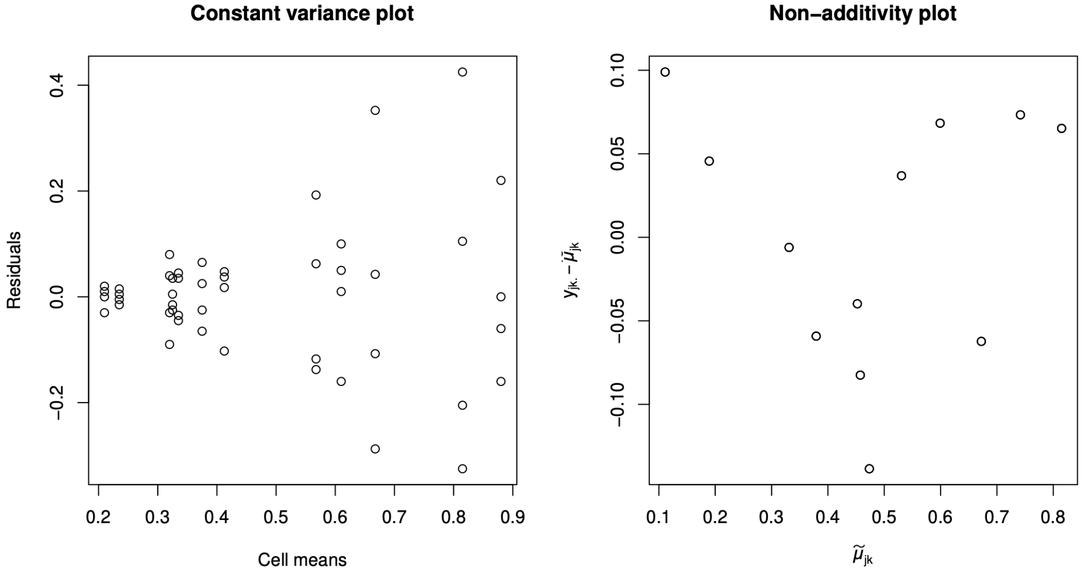

Figure 1. Model checking plots suggesting heteroscedasticity and non-additivity

2.6 Transformations