

# ST 5203: Experimental Design

(Semester 1, AY 2017/2018)

**Text book:** *Experiments: Planning, Analysis, and Optimization*  
(2nd. edition)

by Jeff Wu and Mike Hamada

## Topic 2: Experiments with a Single Factor; One way ANOVA

- One-way layout with fixed effects.
- Analysis of Variance (ANOVA).
- Multiple Comparison.
- Contrast Test.
- Quantitative treatment factors and Orthogonal Polynomials.
- Model diagnosis.
- One-way layout with random effects.

## An Example to One-way Layout Data

- **Objective:** Study whether some form of controlled gas atmosphere would provide a more effective packaging environment for meat storage.
- **Response:** Psychrotrophic bacteria [ $\log(\text{count}/\text{cm}^2)$ ] after 9 days.
- **Factor:** Packaging conditions.
- **Factor levels:** “Commercial plastic wrap”; “Vacuum package”; “1% CO, 40% O<sub>2</sub>, 59% N”; “100% CO<sub>2</sub>”.
- **Randomization:** use some randomization mechanism to randomly assign 12 beef steaks (units) to four treatment groups, three beef steaks each.

# Data Collection

- Table for the experiment outputs:

Data Table for Meat Storage Experiment

Packaging Condition	Psychrotrophic Bacteria Log(count/cm <sup>2</sup> )		
Commercial plastic wrap	7.66	6.98	7.80
Vacuum packaged	5.26	5.44	5.80
1% CO, 40% O <sub>2</sub> , 59% N	7.41	7.33	7.04
100% CO <sub>2</sub>	3.51	2.91	3.66

# One-way Layout Model

- Cell means model:  $y_{ij} = \mu_i + e_{ij}$ ,  $i = 1, \dots, k$ ,  $j = 1, \dots, n_i$ , where,

$y_{ij}$  = the  $j$ th observation from the  $i$ th treatment group.

$\mu_i$  = the mean of the  $i$ th treatment population;

$e_{ij}$  = error, independent  $N(0, \sigma^2)$ .

- Treatment effects model:  $y_{ij} = \eta + \tau_i + e_{ij}$ ,  $i = 1, \dots, k$ ,  $j = 1, \dots, n_i$ , where,

$\eta = \sum_{i=1}^k \mu_i / k$ , the average of the population mean.

$\tau_i = \mu_i - \eta$ , the treatment effects.

**Note:**  $\sum_{i=1}^k \tau_i = 0$ . (Explain)

# Model Fitting

- Least Squares (on board)

- Decomposition:

$$\begin{aligned} \text{(cell means model)} \quad y_{ij} &= \bar{y}_{i\cdot} + (y_{ij} - \bar{y}_{i\cdot}) \\ &= \hat{\mu}_i + \hat{e}_{ij} \end{aligned}$$

$$\begin{aligned} \text{(treatment effects model)} \quad y_{ij} &= \bar{y}_{\cdot\cdot} + (\bar{y}_{i\cdot} - \bar{y}_{\cdot\cdot}) + (y_{ij} - \bar{y}_{i\cdot}) \\ &= \hat{\eta} + \hat{\tau}_i + \hat{e}_{ij} \end{aligned}$$

$$\text{where } \bar{y}_{i\cdot} = \sum_{j=1}^{n_i} y_{ij} / n_{i\cdot}$$

## Analysis of Variance (ANOVA)

- Following the treatment effects model decomposition (explain).

$$\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{..})^2 = \sum_{i=1}^k n_i (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i.})^2$$
$$\text{SST} = \text{SSTr} + \text{SSE}$$

- ANOVA table:  $N = \sum_{i=1}^k n_i$ , the total number of trials in the experiment.

ANOVA Table

Source	D.F.	Sum of Squares	Mean Squares
Treatments	$k - 1$	SSTr	$\text{MSTr} = \text{SSTr} / (k - 1)$
Error	$N - k$	SSE	$\text{MSE} = \text{SSE} / (N - k)$
Total	$N - 1$	SST	

## F-test and Its Properties

- The  $F$  statistic for testing the significance among the treatments, i.e.,

$$H_0 : \mu_1 = \mu_2 = \dots = \mu_k \quad [(or) \tau_1 = \tau_2 \dots = \tau_k = 0,]$$

is

$$F = \text{MSTr}/\text{MSE} \sim F_{k-1, N-k}.$$

- Properties of  $F$ -test in ANOVA table
  - Its rejection region is one-sided, say, for any given significant level  $\alpha$ ,  $p\text{-value} = P(F \geq f_{\text{obs}})$  with  $F \sim F_{k-1, N-k}$ .
  - If all the assumptions for the model (normal, equal variance and independent) are all satisfied, given any value of  $\alpha$  (type I error), the  $F$ -test has the smallest probability of a type II error.
  - The  $F$ -test is robust against the violations of the normality and constant variance, but not robust against the lack of independence.



## ANOVA for Meat Storage Experiment

	D.F.	Sum of Squares	Mean Squares	F
Treatments	3	32.873	10.958	94.584
Error	8	0.927	0.116	
Total	11	33.800		

- $p\text{-value} = P(F_{3,8} > 94.584) = 0.000$ , thus declaring a significant packaging condition difference in meat storage.
- Further question: among  $6 = \binom{4}{2}$  pairs of packaging conditions, what pairs show significant difference? We may need multiple comparisons to answer this question.

# Statistical Properties

(Derivations on board)

- $E(\text{MSE}) = \sigma^2$ .
- $E(\text{MSTr}) = \frac{\sum_{i=1}^k n_i(\tau_i - \bar{\tau})^2}{k-1} + \sigma^2$ , where  $\bar{\tau} = \sum_{i=1}^k n_i\tau_i/N$ .
- $\text{SSE}/\sigma^2 \sim \chi_{N-k}^2$ .
- $\text{SSTr}/\sigma^2 \sim \chi_{k-1}^2$  under  $H_0 : \tau_1 = \dots = \tau_k = 0$ .
- SSE and SSTr are independent.
- $F = \text{MSTr}/\text{MSE} \sim F_{k-1, N-k}$  under  $H_0 : \tau_1 = \dots = \tau_k = 0$ .

## Multiple Comparison

- If we would like to compare only one pair of treatments ( $H_{0,ij} : \mu_i = \mu_j$  versus  $H_{a,ij} : \mu_i \neq \mu_j$ ), it is common to use the  $t$ -test,

$$T_{ij} = \frac{\bar{y}_{i\cdot} - \bar{y}_{j\cdot}}{\hat{\sigma} \sqrt{1/n_i + 1/n_j}} \sim t_{N-k},$$

where  $n_j$  = number of observations for treatment  $j$ ,  
 $\hat{\sigma}^2 = MSE$  in ANOVA table (explain); thus, reject " $H_{0,ij} : \mu_i = \mu_j$  at level  $\alpha$ " if  $|T_{ij}| > t_{N-k, \alpha/2}$ .

- Suppose we are simultaneously performing  $k'$  tests.  
*Experiment-wise error rate* (EER) = probability of making at least one type I error.
- In multiple comparison literature, EER is also called *Family-wise error rate* (FWER).

## Example

- In our “meat storage experiment”, suppose  $k'$  tests are performed to test  $\{H_{0,ij} : \mu_i = \mu_j, 1 \leq i < j \leq k\}$ . There are  $k' = 6 = \binom{4}{2}$  pairs to compare.

$\mu_1$ & $\mu_2$	$\mu_1$ & $\mu_3$	$\mu_1$ & $\mu_4$	$\mu_2$ & $\mu_3$	$\mu_2$ & $\mu_4$	$\mu_3$ & $\mu_4$
7.12	0.80	14.82	-6.33	7.70	14.03

Need to use multiple comparisons to control EER.

- Note: Here  $k' = 6$  is just an example, actually,  $k'$  can be any integer value. For example, in the above example, if we are only interest in testing  $\mu_1 = \mu_2$  and  $\mu_3 = \mu_4$  are simultaneously true, then,  $k' = 2$ .  **$k'$  is the number of simultaneous tests you want to perform.**

## Bonferroni Method: Theory

- Suppose we want to control EER by  $\alpha$ , i.e. we want  $P(EER) \leq \alpha$ .
- On the other hand

$$\begin{aligned} P(EER) &= P(\text{make AT LEAST 1 type I error out of } k' \text{ tests}) \\ &= P(\cup_{i=1}^{k'} \{\text{make type I error for } i\text{th test}\}) \\ &\leq \sum_{i=1}^{k'} P(\text{make type I error for } i\text{th test}) \end{aligned}$$

- How can we make  $P(EER) \leq \alpha$  true?
- Bonferroni's idea: get each  $P(\text{make type I error for } i\text{th test})$  controlled by  $\alpha/k'$ .
- In other words: set each test's type I error (significant level) as  $\alpha/k'$ .

## Bonferroni Method

- Declare “ $\mu_i$  different from  $\mu_j$  at level  $\alpha$ ” if  $|t_{i,j}| > t_{N-k, \frac{\alpha}{2k'}}$ , where  $k' =$  the number of tests.
- For one-way layout with  $k$  treatments, if we would like to make multiple comparison on all combinations of  $\mu_i$ 's, then  $k' = \binom{k}{2} = k(k-1)/2$ . As  $k$  increases,  $k'$  increases, and the critical value  $t_{N-k, \frac{\alpha}{2k'}}$  gets bigger.
- Drawbacks: since  $k'$  can be very large, it tends to be conservative in rejecting hypothesis. Actually, Bonferroni method is a very conservative multiple testing approach.
- Advantages: (1). No assumption on the independence; (2). Work for any number  $k'$ .
- For our example, choose  $\alpha = 0.05$ , then,  $k' = 6$ ,  $t_{8, 0.05/12} = 3.479$ . Among the 6  $t_{i,j}$  values,  $\mu_1$  &  $\mu_2$ ,  $\mu_1$  &  $\mu_4$ ,  $\mu_2$  &  $\mu_3$ ,  $\mu_2$  &  $\mu_4$ ,  $\mu_3$  &  $\mu_4$  are bigger than 3.479, thus, these pairs are declared as different at level 0.05.

## Tukey Method: Theory

- **Note:** Tukey method is only applicable in comparing difference of treatment effects.
- Tukey method is owing to the following fact:

$$\sqrt{2} \max_{i,j} \frac{|\bar{y}_{i\cdot} - \bar{y}_{j\cdot}|}{\hat{\sigma} \sqrt{1/n_i + 1/n_j}} \sim Q_{k,N-k}$$

i.e.  $\sqrt{2} \max_{i,j} |T_{ij}| \sim Q_{k,N-k},$

where  $Q_{k,N-k}$  is the Studentized Range statistic,  $k$  and  $N - k$  are degrees of freedom.

## Tukey Method

- Another way to test  $\{H_{0,ij} : \mu_i = \mu_j, 1 \leq i < j \leq k\}$ : reject if

$$\max_{i,j} |T_{ij}| \geq q_{k,N-k,\alpha}/\sqrt{2},$$

where  $q_{k,N-k,\alpha}$  is the upper  $\alpha$  quantile of the **studentized range distribution** with degrees of freedom  $k$  and  $N - k$ .

- Tukey method for multiple comparison: declare “ $\mu_i$  different from  $\mu_j$  at level  $\alpha$ ” if

$$|T_{ij}| > \frac{1}{\sqrt{2}} q_{k,N-k,\alpha}.$$

- For meat storage experiment

$\frac{1}{\sqrt{2}} q_{k,N-k,\alpha} = \frac{1}{\sqrt{2}} q_{4,8,0.05} = \frac{4.53}{\sqrt{2}} = 3.20$ . Again, only  $\mu_1$  &  $\mu_2$  with  $t_{1,2} = 0.8$  does not exceed 3.20.

- Tukey method is more powerful than Bonferroni method since 3.20 is smaller than 3.479. (why?)



# Tukey Method

v	$k$														
	2	3	4	5	6	7	8	9	10	11	12	13	14	15	
1	17.97	26.98	32.82	37.08	40.41	43.12	45.40	47.36	49.07	50.59	51.96	53.20	54.33	55.36	
2	6.08	8.33	9.80	10.88	11.74	12.44	13.03	13.54	13.99	14.39	14.75	15.08	15.38	15.65	
3	4.50	5.91	6.82	7.50	8.04	8.48	8.85	9.18	9.46	9.72	9.95	10.15	10.35	10.52	
4	3.93	5.04	5.76	6.29	6.71	7.05	7.35	7.60	7.83	8.03	8.21	8.37	8.52	8.66	
5	3.64	4.60	5.22	5.67	6.03	6.33	6.58	6.80	6.99	7.17	7.32	7.47	7.60	7.72	
6	3.46	4.34	4.90	5.30	5.63	5.90	6.12	6.32	6.49	6.65	6.79	6.92	7.03	7.14	
7	3.34	4.16	4.68	5.06	5.36	5.61	5.82	6.00	6.16	6.30	6.43	6.55	6.66	6.76	
8	3.26	4.04	4.53	4.89	5.17	5.40	5.60	5.77	5.92	6.05	6.18	6.29	6.39	6.48	
9	3.20	3.95	4.41	4.76	5.02	5.24	5.43	5.59	5.74	5.87	5.98	6.09	6.19	6.28	
10	3.15	3.88	4.33	4.65	4.91	5.12	5.30	5.46	5.60	5.72	5.83	5.93	6.03	6.11	
11	3.11	3.82	4.26	4.57	4.82	5.03	5.20	5.35	5.49	5.61	5.71	5.81	5.90	5.98	
12	3.08	3.77	4.20	4.51	4.75	4.95	5.12	5.27	5.39	5.51	5.61	5.71	5.80	5.88	
13	3.06	3.73	4.15	4.45	4.69	4.88	5.05	5.19	5.32	5.43	5.53	5.63	5.71	5.79	
14	3.03	3.70	4.11	4.41	4.64	4.83	4.99	5.13	5.25	5.36	5.46	5.55	5.64	5.71	
15	3.01	3.67	4.08	4.37	4.59	4.78	4.94	5.08	5.20	5.31	5.40	5.49	5.57	5.65	
16	3.00	3.65	4.05	4.33	4.56	4.74	4.90	5.03	5.15	5.26	5.35	5.44	5.52	5.59	

$\alpha$ =upper tail probability,  $v$ =degrees of freedom,  $k$ =number of treatments

For complete tables corresponding to various values of  $\alpha$  refer to Appendix E.

## Residual Analysis: Theory

- Define the residual for the  $i$ th observation  $\mathbf{x}_i$  as

$$r_i = y_i - \hat{y}_i, \quad \hat{y}_i = \mathbf{x}_i' \hat{\boldsymbol{\beta}},$$

$\hat{y}_i$  contains information given by the model;  $r_i$  is the “difference” between  $y_i$  (observed) and  $\hat{y}_i$  (fitted) and contains information on possible model inadequacy.

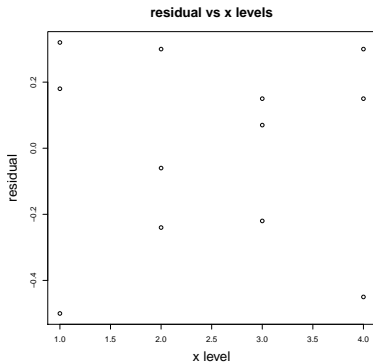
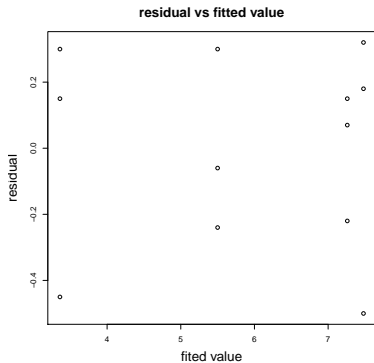
Vector of residuals  $\mathbf{r} = (r_1, r_2, \dots, r_N)' = \mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ .

- Question: what are the forms of  $\mathbf{x}_i$ ,  $\mathbf{X}$ ,  $\mathbf{y}$  and  $\hat{\boldsymbol{\beta}}$  for our one-way layout model?
- If all model assumptions are correct, it can be shown that
  - $E(\mathbf{r}) = 0$ ,
  - $\mathbf{r}$  and  $\hat{\mathbf{y}}$  are independent,
  - variances of  $r_i$  are nearly constant for “nearly balanced” designs, namely, all treatments have roughly the same number of runs.

## Residual Plots

1. Plot  $r_i$  vs.  $\hat{y}_i$ : It should appear as a parallel band around 0. Otherwise, it would suggest some violation of model assumption. For example, if the spread of  $r_i$  increases as  $\hat{y}_i$  increases, then the error variance of  $y$  increases with mean of  $y$ , and we need a transformation of  $y$ . (Will be explained in Topic 3.)
2. Plot  $r_i$  vs.  $x_i$ : If not a parallel band around 0, relationships between  $y_i$  and  $x_i$  are not fully captured. Revise the  $\mathbf{X}\beta$  part of the model.
3. Plot  $r_i$  vs. time sequence: to see if there is a time trend or autocorrelation over time.
4. Plot  $r_i$  from replicates per treatment: to see if error variance depends on treatment.

## Plot $r_i$ vs. $\hat{y}_i$ and $r_i$ vs. $x_i$



## Normal Probability Plot (Q-Q plot)

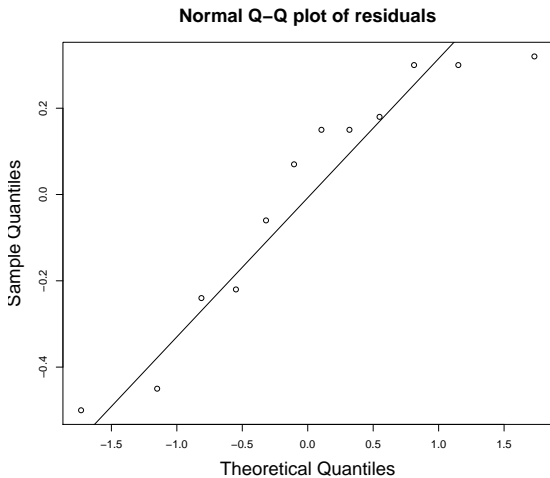
- Purpose: To visually check if a set of numbers are from a normal distribution. e.g., if the residuals follow a normal distribution, the points should be close to a straight line.
- How to draw: for residuals  $r_i, i = 1, 2, \dots, N$ .
  - Order  $r_1, r_2, \dots, r_N$  to have:  $r_{(1)} \leq r_{(2)} \leq \dots \leq r_{(N)}$ .
  - Find all  $(i - 0.5)/N$ th standard normal percentiles, say,  $z_{\frac{1-0.5}{N}}, z_{\frac{2-0.5}{N}}, \dots, z_{\frac{N-0.5}{N}}$ , where  $z_{\frac{i-0.5}{N}}, i = 1, 2, \dots, N$  are corresponding solutions for

$$P(Z < z_{\frac{i-0.5}{N}}) = (i - 0.5)/N, \quad i = 1, 2, \dots, N,$$

where  $Z \sim N(0, 1)$ .

- Plot  $r_{(i)}$  versus  $z_{\frac{i-0.5}{N}}, i = 1, 2, \dots, N$ .

## QQ plot of $r_i$



## More on the Constraint Condition

- Without posing constraint condition on  $y_{ij} = \eta + \tau_i + e_{ij}$ , it is not identifiable. (Explain)
- Mathematically, there exist infinite many possible constraint conditions on the model parameters  $\eta$  and  $\tau_i$ , such that the model is identifiable. So, which one should we use?
- Constraint conditions should take into account two aspects: mathematical validity (i.e. model identifiability) and meaningful interpretation in real application.
- One good constraint condition we have used so far is the "zero sum constraint condition"  $\sum_{i=1}^k \tau_i = 0$ .
- Another type of widely adopted constraint condition is the "baseline constraint condition".

## Baseline Constraint Condition (cont.)

- Recall that we have  $k$  treatment groups for one-way lay out design. The basic idea of baseline constraint condition is to **treat one group as baseline (controlled group)**, and the others as **treatment groups**.
- Example: in a clinical trial, to test which medicine out of 3 is the best,
  - 100 patients are recruited to join the study;
  - One group of 25 randomly selected patients is assigned to take placebo;
  - For the other 3 groups, each group with 25 patients is assigned to one kind of medicine.
- Here, the group taking placebo is usually labeled as the controlled group, whereas the other groups taking medicines are treatment groups.



## Baseline Constraint Condition (cont.)

- Instead of modeling  $\tau_i$  as the difference between levels of the factor and the grand mean, we can model it as the difference between treatment groups and the controlled group.
- Without loss of generality, if we assume group 1 ( $i = 1$ ) as the controlled group, then  $\tau_i$  has a clear meaning: the difference between treatment group  $i$  and the controlled group. Clearly, now  $\tau_1 = 0$ , i.e. the difference between the controlled group and itself is 0;  $\eta$  now stands for the population mean of the controlled group.
- In summary, one-way layout model with baseline constraint condition is given by:

$$y_{ij} = \eta + \tau_i + e_{ij},$$

with the baseline constraint condition  $\tau_1 = 0$ .

- Question: Estimators of parameters? Statistical inference? How is the model above comparable/different to the model with “sum up to zero” constraint?

## Contrast Test

- A **contrast** among means is defined as

$$C = \sum_{i=1}^k c_i \mu_i = c_1 \mu_1 + c_2 \mu_2 + \dots + c_k \mu_k,$$

where  $\sum_{i=1}^k c_i = 0$ .  $\mathbf{c} = (c_1, \dots, c_k)'$  is the **contrast vector**.

- Examples:

$$C_1 = \mu_1 - \frac{1}{3}(\mu_2 + \mu_3 + \mu_4)$$

$$C_2 = \mu_2 - \frac{1}{2}(\mu_3 + \mu_4)$$

- To test  $H_0 : C = 0$  versus  $H_a : C \neq 0$ , we use the test statistic

$$T_C = \frac{\sum_{i=1}^k c_i \hat{\mu}_i}{s.e.(\sum_{i=1}^k c_i \hat{\mu}_i)} \sim t_{N-k}.$$

## Contrast Test (cont.)

- In one-way layout model,  $\hat{\mu}_i = \bar{y}_i$ . We have

$$\hat{C} = \sum_{i=1}^k c_i \hat{\mu}_i = \sum_{i=1}^k c_i \bar{y}_i.$$
$$\text{Var}(\hat{C}) = \sum_{i=1}^k c_i^2 \frac{\sigma^2}{n_i}$$

- Therefore, the  $t$ -statistic is given by

$$T_C = \frac{\sum_{i=1}^k c_i \bar{y}_i}{\sqrt{\sum_{i=1}^k c_i^2 \frac{\hat{\sigma}^2}{n_i}}}$$

where  $\hat{\sigma}^2$  is the estimated error variance (MSE).

- More about contrast can be found in Chapter 3 of *Design and Analysis of Experiments* by Douglas C. Montgomery.

# A Quantitative Factor Experiment Example

- Data

$y$  = gain yields of crop,

$x$  = plant density at 10, 20, 30, 40 and 50.

Plant Density ( $x$ )				
10	20	30	40	50
12.2	16.0	18.6	17.6	18.0
11.4	15.5	20.2	19.3	16.4
12.4	16.5	18.2	17.1	16.6

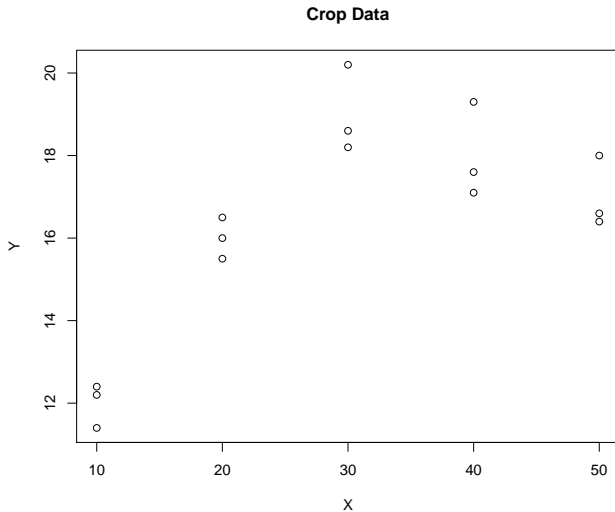
# One-way ANOVA

- ANOVA table

Source	D.F.	Sum of Squares	Mean Squares	F
x	4	87.600	21.900	29.278
Residuals	10	7.480	0.748	
Total	14	95.08		

- Conclusion: the plant density has significant effect on the yield.
- However, multiple comparison cannot provide desirable explanation for the effect. (why?)
- The effects of a quantitative factor like the plant density can be decomposed into linear, quadratic, etc.

# Scatter Plot



## Why Orthogonal Polynomial

- For one-way quantitative factor experiments, the response trend can be better explained by polynomial models.
- If the factor has  $k$  levels, the polynomial can be fitted up to the order  $k - 1$ .
- For meaningful explanation of the observed data trend, we can check the orthogonal contrasts among the treatment factor levels that measure the linear, quadratic or higher level polynomial effects.
- If  $y_1, y_2, y_3$  are observed at levels  $x = 10, 20, 30$ , then
  - $(y_3 - y_2) + (y_2 - y_1) = y_3 - y_1$  is called the *linear contrast*;
  - $(y_3 - y_2) - (y_2 - y_1) = y_3 - 2y_2 + y_1$  is called the *quadratic contrast*;
  - Note that their contrast vectors  $\mathbf{c}_1 = (-1, 0, 1)'$  and  $\mathbf{c}_2 = (1, -2, 1)'$  are orthogonal to each other.

# Orthogonal Polynomial

- Polynomial regression model:

$$y = \alpha_0 + \alpha_1 P_1(x) + \dots + \alpha_{k-1} P_{k-1}(x) + e$$

- The  $P_i(x)$  are  $i$ th-order orthogonal polynomial.

- Mean:  $P_0(x) = 1$ .
- Linear:  $P_1(x) = \lambda_1 \left[ \frac{x - m}{\Delta} \right]$
- Quadratic:  $P_2(x) = \lambda_2 \left[ \left( \frac{x - m}{\Delta} \right)^2 - \left( \frac{k^2 - 1}{12} \right) \right]$
- ...

where  $\Delta$  = distance between factor levels.  $\lambda_i$  makes  $P_i(x)$  integer values for all designed  $x$ .  $m$  is the mean of levels of designed  $x$ .

Values of  $\lambda_i$  and more orthogonal polynomials are given in Appendix G of the textbook.



# Advantages of Orthogonal Polynomial

- For factors with numerical nature, it offers predictions not only for designed factor levels but also for other factor values.
- The polynomial functions are well designed, such that the design matrix for regression model:

$$y = \beta_0 P_0(x) + \beta_1 P_1(x) + \beta_2 P_2(x) + \dots + \beta_{k-1} P_{k-1}(x) + \epsilon$$

is orthogonal. Then..., why good?

1. Low computational complexity.
2. High accuracy in the estimation of  $\beta_i$ , since no multicollinearity.
  - High order polynomials are usually not preferred: why?  
Parsimonious models are preferred.

## Results for the Crop Example

- The estimated equation is

$$\hat{y}_i = 16.4 + 1.2P_1(x_i) - 1.0P_2(x_i) + 0.1P_3(x_i) + 0.1P_4(x_i)$$

- Check the supplementary R codes for how to fit such orthogonal polynomial regression.
- The significance of the effects can be tested by ANOVA table.
- For each  $x$  value (not necessarily in the treatment assignment),  $\hat{y}$  can be estimated by plugging in  $x$  to the above fitted equation.

## Example: A Special Case, $k = 3$

- Data:
  - $y$  = bonding strength of composite material.
  - $x$  = laser power at 40, 50 and 60.

Strength Data, Composite Experiment

Laser Power (watts)		
40	50	60
25.66	29.15	35.73
28.00	35.09	39.56
20.65	29.79	35.66

- For three evenly spaced levels,  $m - \Delta$ ,  $m$  and  $m + \Delta$ , the first and second degree polynomials are given by
  - $P_1(x) = \frac{x - m}{\Delta}$  has 3 possible values: -1, 0 and 1, respectively corresponding to  $x = m - \Delta$ ,  $x = m$  and  $x = m + \Delta$ .
  - $P_2(x) = 3\left\{\left(\frac{x - m}{\Delta}\right)^2 - \frac{2}{3}\right\}$  has 3 possible values: 1, -2 and 1, respectively corresponding to  $x = m - \Delta$ ,  $x = m$  and  $x = m + \Delta$ .

## Example: A Special Case, $k = 3$

- Polynomial regression mode:

$$y = \beta_0 + \beta_1 P_1(x)/\sqrt{2} + \beta_2 P_2(x)/\sqrt{6} + e.$$

The fitted values are  $\hat{\beta}_0 = 31.0322$ ,  $\hat{\beta}_1 = 8.636$  and  $\hat{\beta}_2 = -0.381$ .

- Fitted model:

$$\hat{y} = 31.0322 + 8.636 P_1(x)/\sqrt{2} - 0.381 P_2(x)/\sqrt{6}.$$

- To compute  $\hat{y}$  at any  $x$ , plug in the  $x$  to the above fitted model. For example  $x = 55$ ,  $m = 50$ ,  $\Delta = 10$ ,

$$\begin{aligned} P_1(55) &= \frac{55 - 50}{10} = \frac{1}{2} \\ P_2(55) &= 3 \left\{ \left( \frac{55 - 50}{10} \right)^2 - \frac{2}{3} \right\} = -\frac{5}{4}, \end{aligned}$$

therefore,

$$\begin{aligned} \hat{y} &= 31.0322 + 8.636(0.3536) - 0.381(-0.5103) \\ &= 34.3803. \end{aligned}$$

## Revisiting Meat Storage Example; One-way Random Effects Model

- In the meat storage example,  $\tau_i$  are so called **fixed** effects because the study interest is to compare the four **specific** packaging conditions.
- What if these four packaging conditions were randomly chosen from a population of packaging conditions? The interest would usually be the variation among all packaging conditions in the population.
- If four packaging conditions are randomly selected from the population, the variation among the packaging conditions for the population is referred to as **random** effects.

# One-way Random Effects Model

- One-way random effects model:

$$y_{ij} = \eta + a_i + e_{ij},$$

- $e_{ij} \overset{i.i.d.}{\sim} N(0, \sigma_e^2)$ .
  - $a_i$  are independent  $N(0, \sigma_a^2)$ .
  - $e_{ij}$  and  $a_i$  are assumed to be independent of one another.
  - $\sigma_e^2$  and  $\sigma_a^2$  are the two variance components of the model.
  - The variance among packaging conditions is measured as  $\sigma_a^2$ .
- Question: What is the distribution of  $y_{ij}$  now?

## ANOVA and Variance Components

- The null hypothesis for fixed effects model:  
 $\tau_1 = \tau_2 = \dots = \tau_k = 0$  should now be replaced by

$$H_0 : \sigma_a^2 = 0.$$

**The  $F$  test and the ANOVA table for fixed effects model still hold, i.e.**

$$F = \frac{\text{MSTr}}{\text{MSE}} = \frac{\text{SSTr}/(k-1)}{\text{SSE}/(N-k)} \sim F_{k-1, N-k},$$

and we reject  $H_0 : \sigma_a^2 = 0$  if the p-value  $P(F > f_{\text{obs}})$  is very small.

- We can still apply the same ANOVA and  $F$  test in the fixed effects case for analyzing data. However, we need to compute the expected mean squares under the alternative of  $\sigma_a^2 > 0$  to estimate the variance components.

## Expected Mean Squares

- For balanced designs ( $n_1 = n_2 = \dots = n_k = n$ ),

$$E(\text{MSE}) = \sigma_e^2 \quad (1)$$

$$E(\text{MSTr}) = \sigma_e^2 + n\sigma_a^2 \quad (2)$$

- For unbalanced designs,  $n$  in (2) is replaced by

$$\frac{1}{k} \left[ \sum_{i=1}^k n_i - \frac{\sum_{i=1}^k n_i^2}{\sum_{i=1}^k n_i} \right].$$



## ANOVA Tables (Balanced Designs)

If  $n_1 = n_2 = \dots = n_k = n$ ,

ANOVA Table

Source	D.F.	S.S	M.S.	E(M.S.)
Treatments	$k - 1$	SSTrt	$MSTr = SSTrt / (k - 1)$	$\sigma_e^2 + n\sigma_a^2$
Error	$N - k$	SSE	$MSE = SSE / (N - k)$	$\sigma_e^2$
total	$N - 1$	SST		

Meat Storage Experiment

	D.F.	S.S.	M.S.	E(M.S.)
Treatments	3	32.873	10.958	$\sigma_e^2 + 3\sigma_a^2$
Error	8	0.927	0.116	$\sigma_e^2$
Total	11	33.800		

## Estimation of $\sigma_e^2$ and $\sigma_a^2$

- From (1) and (2), we have the following unbiased estimates of the variance components:

$$\hat{\sigma}_e^2 = \text{MSE} \quad \text{and} \quad \hat{\sigma}_a^2 = \frac{\text{MSTr} - \text{MSE}}{n}.$$

- In the case that  $\text{MSTr} \leq \text{MSE}$ ,  $\hat{\sigma}_a^2 \leq 0$ . On the other hand,  $\text{MSTr} \leq \text{MSE}$  is equivalent to  $F \leq 1$ . Obviously the null hypothesis  $H_0 : \sigma_a^2 = 0$  is not rejected when  $F \leq 1$ .
- Since the variance cannot be negative, a negative estimate (when  $\text{MSTr} < \text{MSE}$ ) can be replaced by 0. This does not indicate that the  $\sigma_a^2$  is zero! It only indicates that there is not enough information in the data to get a good estimate of  $\sigma_a^2$ .
- For the meat storage experiment,  $\hat{\sigma}_e^2 = 0.116$ ,  
 $\hat{\sigma}_a^2 = (10.958 - 0.116)/3 = 3.614$ .

## Inference for Overall Mean $\eta$

- In a random effects model,  $\eta$ , the population mean, is often of interest. From  $E(y_{ij}) = \eta$ , we use the estimate

$$\hat{\eta} = \bar{y}_{..}$$

- $\text{Var}(\hat{\eta}) = \text{Var}(\bar{a}_{..} + \bar{e}_{..}) = \frac{\sigma_a^2}{k} + \frac{\sigma_e^2}{N}$ .
- For balanced designs,

$$\text{Var}(\hat{\eta}) = \frac{\sigma_a^2}{k} + \frac{\sigma_e^2}{nk} = \frac{1}{nk} (\sigma_e^2 + n\sigma_a^2).$$

Using Equation (2), an unbiased estimate of  $\text{Var}(\hat{\eta})$  is  $\frac{\text{MSTr}}{nk}$ .

- Confidence interval for  $\eta$  is then:

$$\hat{\eta} \pm t_{k-1, \alpha/2} \sqrt{\frac{\text{MSTr}}{nk}}.$$