DOE, cont'd.

BONING

MANOVA & MODEL FIT

- ANOVA builds a model for the data, and reports on the significance of terms (or dependencies) in the model:

$$y_{ti} = \mu + \tau_t + \beta_i + \varepsilon_{ti}$$ ← assumed real response

$$\hat{y}_{ti} = \hat{\mu} + \hat{\tau}_t + \hat{\beta}_i$$ ← predicted response, prediction model

\# Model Coefficients = 1 ($\hat{\mu}$), k ($\hat{\tau}_t$), n ($\hat{\beta}_i$)

BUT recall that our $\hat{\tau}_t$, $t = 1, 2, \ldots k$ are NOT all independent model coefficients, because $\sum \tau_t = 0$
$\Rightarrow$ really only have k-1 indep. model coeffs $\Rightarrow \nu_T = k-1$

\# Model Coeffs (Independent) = 1, $\nu_T = k-1$, $\nu_B = n-1$

- ANOVA uses F test to check significance of $\hat{\tau}_t$, $\hat{\beta}_i$ sets
$\Rightarrow$ Retain a model with only the significant factors,
e.g. we might find β_i not significant, then $\hat{y}_{ti} = \hat{\mu} + \hat{\tau}_t$.

- "Goodness of fit" – R^2
Question answered: How much better does the model do than just using the grand average?

$$R^2 = \frac{S_T' + S_B'}{S' - S_A} = \frac{S_T + S_B}{S_D} \quad ; \quad 0 \le R^2 \le 1$$

τ, β Explain ALL deviation around the grand ave.

- Adjusted R^2
For "fair" comparison between models with different #'s of coefficients:

$$R^2_{adj} = 1 - \underbrace{\frac{S_R/\nu_R}{S_D/\nu_D}}_{\text{Variation remaining in residual}} = 1 - \frac{s^2_R}{s^2_D} = 1 - \frac{\text{Mean Sq. Resid}}{\text{Mean Sq. Total}}$$

Recall $\nu_R = \nu_D - \nu_T - \nu_B$

TWO - WAY FACTORIAL DESIGN

- With the blocked treatment design, we make a couple of assumptions:
  (1) additivity of effects - impact of block can just be added to impact of treatment
  (2) the goal of the design is to isolate & guard against "unwanted" variation in the block factor while retaining or improving precision (randomization guards against first but at cost of increased error variance and precision loss).

- The next step is to ease up on these assumptions
  (1) explicitly check for interactions (or other additivity problems)
  (2) treat both variables as legitimate factors

MODEL

$$y_{tij} = \mu_{ti} + e_{tij}$$

IID, $N(0,\sigma^2)$

t = treatment factor
i = "block" or second factor
j = replicant

an effect that depends on both t & i factors simultaneously

or

$$y_{tij} = \mu + \tau_t + \beta_i + \omega_{ti}$$
$$= \bar{y} + (\bar{y}_t - \bar{y}) + (\bar{y}_i - \bar{y}) + (\bar{y}_{ti} - \bar{y}_t - \bar{y}_i + \bar{y})$$

$$\omega_{ti} \triangleq \text{INTERACTION TERM} = \bar{y}_{ti} - \bar{y}_t - \bar{y}_i + \bar{y}$$

τ_t, β_i $\triangleq$ MAIN EFFECTS

$t = 1, 2, \ldots k \Rightarrow k = \#$ levels of 1st factor
$i = 1, 2, \ldots n \Rightarrow n = \#$ levels of 2nd factor
$j = 1, 2, \ldots m \Rightarrow m = \#$ replicants at i,j th combination of factor levels

ANOVA for TWO-WAY DESIGN with INTERACTIONS

Source of Variation	Sum of Square	D.O.F.	Mean Square	E(mean square)	Ratio of Mean Sq
Between levels of Factor 1 (T)	S_T'	$k-1$	s^2_T	$\sigma^2 + mn \sum' \tau_t^2/(k-1)$	s^2_T / s^2_E
Between levels of Factor 2 (B)	S_B'	$n-1$	s^2_B	$\sigma^2 + mk \sum' \beta_i^2/(n-1)$	s^2_B / s^2_E
Interaction	S_I'	$(k-1)(n-1)$	s^2_I	$\sigma^2 + m \sum \sum \omega_{ti}^2/(n-1)(k-1)$	s^2_I / s^2_E
Within Groups (Error)	S_E'	$nk(m-1)$	s^2_E		
Total (corrected)	S_D'	$nkm-1$			

where significance of variation source is judged by F test w/ appropriate d.o.f.

Effect Test

Source	Nparm	DF	Sum of Squares	F Ratio	Prob > F
Block	1	1	150.0000	•	•
Treatment	2	2	1200.0000	•	•
Block *Treatmen	2	2	28.0000	•	•

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	5	1378.0000	275.600	•
Error	0	0.0000	•	Prob > F
C Total	5	1378.0000		•

Problem:
- No error degrees of freedom! ⇒ No replication
- In blocked design, assumed additivity & used interaction terms to help estimate variance!

Example - TWO-WAY (2 FACTOR) FACTORIAL DESIGN

FACTOR 1: Etch Recipe
- 3 levels

FACTOR 2: Bake Recipe
- 2 levels

Response: Effective Linewidth

Two way factorial experiment for DLeff.

Etch Rec	Bake	DLeff	Etch Rec	Bake	DLeff
1	1	0.31	1	2	0.40
2	1	0.82	2	2	0.49
3	1	0.43	3	2	0.31
4	1	0.45	4	2	0.71
1	1	0.45	1	2	0.23
2	1	1.10	2	2	1.24
3	1	0.45	3	2	0.40
4	1	0.71	4	2	0.38
1	1	0.46	1	3	0.22
2	1	0.88	2	3	0.30
3	1	0.63	3	3	0.23
4	1	0.66	4	3	0.30
1	1	0.43	1	3	0.21
2	1	0.72	2	3	0.37
3	1	0.76	3	3	0.25
4	1	0.62	4	3	0.36
1	2	0.36	1	3	0.18
2	2	0.92	2	3	0.38
3	2	0.44	3	3	0.24
4	2	0.56	4	3	0.31
1	2	0.29	1	3	0.23
2	2	0.61	2	3	0.29
3	2	0.35	3	3	0.22
4	2	1.02	4	3	0.33

Anova Table for 2-way DLeff Factorial

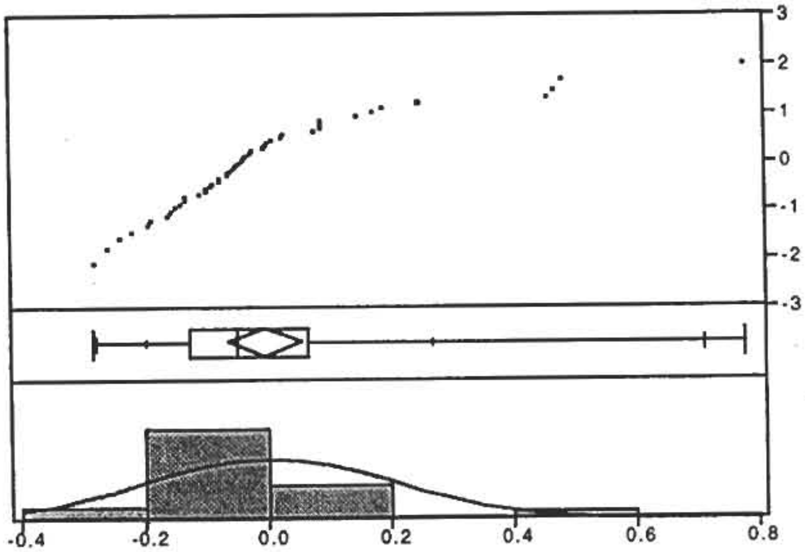
Effect Test

Source	Nparm	DF	Sum of Squares	F Ratio	Prob>F
Etch Recipe	3	3	0.9212063	13.8056	0.0000
Bake Proc	2	2	1.0330125	23.2217	0.0000
Etch Rec*Bake Pro	6	6	0.2501375	1.8743	0.1123

Analysis of Variance

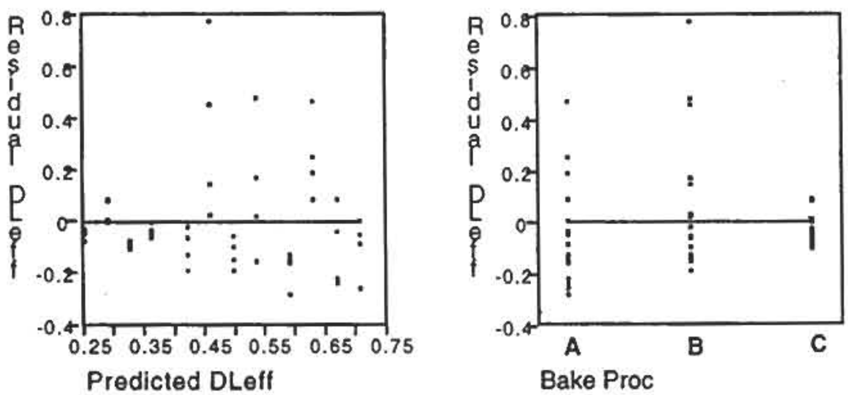
Source	DF	Sum of Squares	Mean Square	F Ratio
Model	11	2.2043563	0.200396	9.0097
Error	36	0.8007250	0.022242	Prob>F
C Total	47	3.0050813		0.0000

Residual Statistics for DLeff



• Longer tail than Normal

Diagnostics for DLeff



Bake choice affects residual!

Anova Table for 2-way ln(DLeff) Factorial

Effect Test

Source	Nparm	DF	Sum of Squares	F Ratio	Prob>F
Etch Recipe	3	3	3.5571735	21.9295	0.0000
Bake Proc	2	2	5.2374726	48.4324	0.0000
Etch Rec*Bake Pro	6	6	0.3957467	1.2199	0.3189

← Improvement with the transform

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	11	9.190393	0.835490	15.4520
Error	36	1.946516	0.054070	Prob>F
C Total	47	11.136909		0.0000

APPROACHES FOR DEPENDENT RESIDUALS

- In diagnostic examination of residuals, often see variance that depends on μ:

Variance dependency:

$$\sigma_y = c\,\mu^{\alpha}$$

$$\log \sigma_y = \log c + \alpha \log \mu$$

$$\log s_R = c' + \alpha \log \bar{y}$$

Data Transform:

$$Y = y^{\lambda}$$
$$\lambda = 1 - \alpha$$

$\Rightarrow$ A plot of log s.d. vs. log $\bar{y}$ can suggest power dependencies, and data transformations to remove

- Curvilinear Relationships in residuals are often an indication of nonadditivity. Suppose, for example, that

$$y_{ti} = \mu + \tau_t \beta_i + \epsilon_{ti}$$ is actual dependency.

Then a fit to $\hat{\mu} + \hat{\tau}_t + \hat{\beta}_i$ can't be expected to do well. An alternative is

$$\log (y_{ti} - \mu) = \log \tau_t + \log \beta_i$$ assuming $e_t \sim N(0, \sigma^2)$

will be a much better approximation

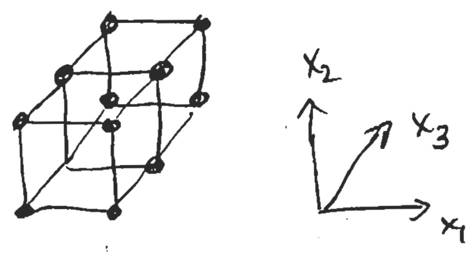
- Tests for nonadditivity exist, Box-Cox transformations improve result and increase precision substantially (and can remove apparent interaction effects)

General Factorial Designs

- Multiple Factors & Levels

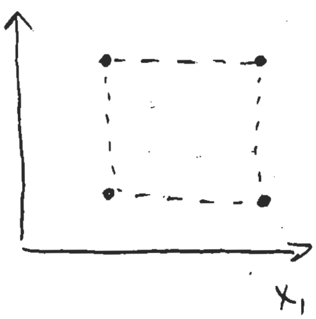
  $l_1 \times l_2 \times l_3$ points

  $2 \times 2 \times 3$

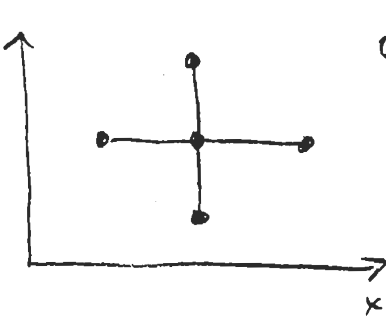


- Focus: Two-Level Factorial

2^k pts
(k = # factors)



vs.



One factor at a time

⟹ Can detect interactions between factors x_1, x_2
(need replication to distinguish interactions from errors)

That is to say, we know the relevance of factor x_1 across a larger space in factorial design, while we only know x_1's effect at a specific value of x_2 in the single factor at a time experiment.

Q: what if the process really is additive (no interaction)?

⟹ Still a win! The factorial results in more precision. In case of additivity, we get additional effective replication (via projection onto each factor), thus increasing our ability to discern/distinguish real effects.

(In general, require k-fold, or $\frac{k+1}{2}$-fold number of runs in one-at-a time approach for same precision)

FULL FACTORIAL DESIGNS – ANALYSIS

- In addition to the ANOVA approaches which help identify and test significance of factors, we also desire ways to explore the model components:

  - MAIN EFFECTS eg. τ_t, β_i
  - INTERACTIONS e.g. ω_{ti}
    - .. 2 way for two factor
    - .. 3 way for three factor design
    - up to .. k-way for k-factor design

- CONVENTIONS for defining and analyzing factorial designs (applicable to both nominal and continuous factors)

Data from a 2^3 factorial design, pilot plant example

test condition number	temperature (°C) T	concentration (%) C	catalyst (*A* or *B*) K	yield (grams) y
		a. Original units of variables		
1	160	20	*A*	60
2	180	20	*A*	72
3	160	40	*A*	54
4	180	40	*A*	68
5	160	20	*B*	52
6	180	20	*B*	83
7	160	40	*B*	45
8	180	40	*B*	80
		b. Coded units of variables		
1	–	–	–	60
2	+	–	–	72
3	–	+	–	54
4	+	+	–	68
5	–	–	+	52
6	+	–	+	83
7	–	+	+	45
8	+	+	+	80

temperature (°C)		*concentration (%)*		*catalyst*	
–	+	–	+	–	+
160	180	20	40	*A*	*B*

(1) CALCULATION OF MAIN EFFECTS

– Typically interested in the effect of each factor:

EFFECT $\triangleq$ change in response from – to + level of factor

e.g. 4 measures of temperature effect in experiment.

individual measure of the effect of changing temperature from 160 to 180°C	condition at which comparison is made: concentration C	catalyst K
$y_2 - y_1 = 72 - 60 = 12$	20	*A*
$y_4 - y_3 = 68 - 54 = 14$	40	*A*
$y_6 - y_5 = 83 - 52 = 31$	20	*B*
$y_8 - y_7 = 80 - 45 = 35$	40	*B*
main effect of temperature $T = 23$		

⇒ average effect of T across all other parameters

MAIN EFFECT $= \bar{y}_+ - \bar{y}_-$ where $\bar{y}_+$ & $\bar{y}_-$ are average responses for one specific factor

temperature effect $$T = \frac{72 + 68 + 83 + 80}{4} - \frac{60 + 54 + 52 + 45}{4} = 75.75 - 52.75 = 23$$

concentration effect $$C = \frac{54 + 68 + 45 + 80}{4} - \frac{60 + 72 + 52 + 83}{4} = 61.75 - 66.75 = -5$$

catalyst effect $$K = \frac{52 + 83 + 45 + 80}{4} - \frac{60 + 72 + 54 + 68}{4} = 65.0 - 63.5 = 1.5$$

NOTE:

- ALL observations used to supply info on each main effect
- Each effect determined with precision of a fourfold replicated difference.

(2) TWO - FACTOR INTERACTIONS

- See that the effect of one factor on the response also depends on the level of another factor (e.g. T effect larger for catalyst B) ⇒ interaction!

catalyst	average temperature effect
(+)B	33
(−)A	13
difference	20

$T \times K$ interaction $= \frac{20}{2} = 10$

temperature (°C)	average catalyst effect
(+)180	11.5
(−)160	−8.5
difference	20.0

$T \times K$ interaction $= \frac{20}{2} = 10$

By convention, interaction term is ½ difference in levels across interactiv factor...

- Alternative Picture: CONTRASTS

$T \times K = 10$
$T \times C = 1.5$
$C \times K = 0$

catalyst	average temperature effect
(+)B	$33 = \frac{31+35}{2} = \frac{1}{2}(y_6 - y_5 + y_8 - y_7)$
(−)A	$13 = \frac{12+14}{2} = \frac{1}{2}(y_2 - y_1 + y_4 - y_3)$

$$T \times K \text{ interaction} = \tfrac{1}{2}\text{ difference} = \frac{33-13}{2} = 10$$

$$= \tfrac{1}{4}(y_1 - y_2 + y_3 - y_4 - y_5 + y_6 - y_7 + y_8)$$

$$= \frac{y_1 + y_3 + y_6 + y_8}{4} - \frac{y_2 + y_4 + y_5 + y_7}{4}$$

Interaction as differences between averages

⇒ diagonal faces

(3) THREE - FACTOR INTERACTIONS

$T \times C$ interaction with catalyst B (+):

$$\frac{(y_8 - y_7) - (y_6 - y_5)}{2} = \frac{(80-45)-(83-52)}{2} = \frac{35-31}{2} = 2$$

$T \times C$ interaction with catalyst A (−):

$$\frac{(y_4 - y_3) - (y_2 - y_1)}{2} = \frac{(68-54)-(72-60)}{2} = \frac{14-12}{2} = 1$$

- How does catalyst affect the T×C interaction?

Geometric Picture of Contrasts – Main Effects & Interactions

Summary of Results – Example

Calculated effects and standard errors for the 2^3 factorial design, pilot plant example

effect	estimate ± standard error
average	64.25 ± 0.7
main effects	
temperature T	23.0 ± 1.4
concentration C	−5.0 ± 1.4
catalyst K	1.5 ± 1.4
two-factor interactions	
$T \times C$	1.5 ± 1.4
$T \times K$	10.0 ± 1.4
$C \times K$	0.0 ± 1.4
three-factor interaction	
$T \times C \times K$	0.5 ± 1.4

⇒ significant effects & interactions circled

KEY: how calculate the std error?
⇝ ANOVA approaches

TABLE OF CONTRASTS – Quick Effects

Signs for calculating effects from the 2^3 factorial design, pilot plant example

	mean	T	C	K	TC	TK	CK	TCK	yield averages
	+	−	−	−	+	+	+	−	60
	+	+	−	−	−	−	+	+	72
	+	−	+	−	−	+	−	+	54
	+	+	+	−	+	−	−	−	68
	+	−	−	+	+	−	−	+	52
	+	+	−	+	−	+	−	−	83
	+	−	+	+	−	−	+	−	45
	+	+	+	+	+	+	+	+	80
divisor	8	4	4	4	4	4	4	4	

E.g. T main effect by avg. of +' − avg of −' rows
& similarly for interactions

$$TC = \frac{60+68+52+80}{4} - \frac{72+54+83+45}{4}$$

$$= 65 - 63.5 = 1.5$$

(A) Estimating std errors from REPLICATED RUNS

- As we saw previously, if we have no replicates and use all interactions, NO way to estimate underlying process/measurement variance ⇒ Replication Helps!

E.g. m_i replicants at i_{th} set of conditions
$\Rightarrow s_i^2$ with $\nu_i = m_i - 1$

Can POOL the replicants across all runs

$$\Rightarrow s^2 = \frac{\nu_1 s_1^2 + \nu_2 s_2^2 + \dots \nu_g s_g^2}{\nu_1 + \nu_2 + \dots \nu_g}$$

(g total condition combinations)

- Minimal case: 2 replicants

Estimation of the variance, pilot plant example

average response value (previously used in the analysis)	T	C	K	results from individual runs*		difference of duplicate	estimated variance at each set of conditions s_i^2 = (difference)^2/2
60	−	−	−	59$^{(6)}$	61$^{(13)}$	−2	2
72	+	−	−	74$^{(2)}$	70$^{(4)}$	4	8
54	−	+	−	50$^{(1)}$	58$^{(16)}$	−8	32
68	+	+	−	69$^{(5)}$	67$^{(10)}$	2	2
52	−	−	+	50$^{(8)}$	54$^{(12)}$	−4	8
83	+	−	+	81$^{(9)}$	85$^{(14)}$	−4	8
45	−	+	+	46$^{(3)}$	44$^{(11)}$	2	2
80	+	+	+	79$^{(7)}$	81$^{(15)}$	−2	2
						total	64

s^2 = pooled estimate of σ^2 = average of estimated variances
= $\frac{64}{8}$ = 8 with ν = 8 degrees of freedom

* Superscripts give the order in which the runs were made.

$s^2 = 8$, $\nu = 8$
$s = 2.8$

- Once we have estimated variance, can determine SAMPLING variances used in calculating effects

$$V(\text{effect}) = V(\underbrace{\bar{y}_+ - \bar{y}_-}_{8 \text{ runs in each}}) = \frac{s^2}{8} + \frac{s^2}{8} = \frac{s^2}{4} \Rightarrow \text{s.e. } 1.41$$

Note: the average is calculated with all 16 runs, so s.e. $= \frac{s}{\sqrt{N=16}} = 0.7$

- Identifying Significant Effects / Interaction (Large Designs)

  - Once we know the std. error for each effect/interaction, we can do a t-test to evaluate significance of effect

  - A graphical approach:

    Suppose really is nothing but random variation in the data ⇒ then effects will be normally distributed (related to sampling from process w/. underlying variation).

- Related approach to increase precision in error estimates
  - Count insignificant effects/interactions as replicants ⇒ pool across these when calculating s^2

ADDITIONAL ISSUES in <u>FACTORIAL DESIGNS</u>

① BLOCKING

- May still have additional conditions that <u>may</u> affect our experiment. Again possible (sometimes) to arrange experiment to guard against this ... <u>to a degree</u>

- Can block, for example, against extra variable affecting the main effects only; but if we don't make this a full factor, we will <u>CONFOUND</u> possible interactions with the blocking parameter with other model interaction terms.

② FRACTIONAL FACTORIAL

- Sometimes we do not need the full <u>resolution</u> of a design, i.e. we do not need (or believe the likelihood is very low) to study j-way interactions

  ⇒ can trade off # runs with ability to distinguish between different combinations of factors

- Good references (e.g. BHH) that describe methods to carefully control what gets confounded with what in different fractional designs... e.g. "generators"

MODELING: GOAL of EXPERIMENTAL DESIGN: "MAP" A SPACE

- We desire quantitative models of the relationship between one or more responses and some number of factors.

- Visualization / Understanding
- Optimization

FACTORS may be

- Nominal (choices) as done so far

or

- Continuous

KEY ISSUE: How choose experimental points to get the most value / information from the data?

... especially important for continuous parameters!