Dive into Diagnostics to Discover Data Discrepancies

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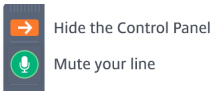
Making the most of this learning opportunity



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Agenda

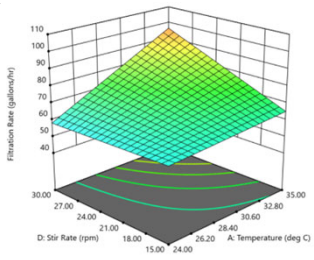
- **Analyzing DOE results – why check diagnostics?**
- Diagnostic basics
- Case Study – Well (bad diagnostics and a transformation)
- Wrap Up

Purpose of a Designed Experiment

Goal: Take DOE data (small sample) and → turn it into a predictive model (of a larger system).

Std	Run	Factor 1 A:Temperat... deg C	Factor 2 B:Pressure psig	Factor 3 C:Concentr... percent	Factor 4 D:Stir Rate rpm	Response 1 Filtration R... gallons/hr
11	1	24.00	15.00	2.00	30.00	45
9	2	24.00	10.00	2.00	30.00	43
12	3	35.00	15.00	2.00	30.00	104
13	4	24.00	10.00	4.00	30.00	75
15	5	24.00	15.00	4.00	30.00	70
14	6	35.00	10.00	4.00	30.00	86
2	7	35.00	10.00	2.00	15.00	71
3	8	24.00	15.00	2.00	15.00	48
7	9	24.00	15.00	4.00	15.00	80
10	10	35.00	10.00	2.00	30.00	100
8	11	35.00	15.00	4.00	15.00	65
1	12	24.00	10.00	2.00	15.00	45
4	13	35.00	15.00	2.00	15.00	65
6	14	35.00	10.00	4.00	15.00	60
16	15	35.00	15.00	4.00	30.00	96
5	16	24.00	10.00	4.00	15.00	68

Filtration Rate	=
+70.06	
+10.81	* A
+4.94	* C
+7.31	* D
-9.06	* AC
+8.31	* AD



The Statistical Tool - ANOVA

The statistical relationship between the factors and the responses is built using the statistical tool called analysis of variance (ANOVA).

ANOVA for selected factorial model

Response 1: Filtration Rate

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	5535.81	5	1107.16	56.74	< 0.0001	significant
A-Temperature	1870.56	1	1870.56	95.86	< 0.0001	
C-Concentration	390.06	1	390.06	19.99	0.0012	
D-Stir Rate	855.56	1	855.56	43.85	< 0.0001	
AC	1314.06	1	1314.06	67.34	< 0.0001	
AD	1105.56	1	1105.56	56.66	< 0.0001	
Residual	195.12	10	19.51			
Cor Total	5730.94	15				

Question: are the p-values, and related R^2 values, correct statistically?

ANOVA Assumptions

ANOVA validity assumes that the model is correct, and the residuals:

- Are (nearly) independent
- Have a mean = 0
- Have a constant variance
- Follow a "well-behaved" distribution (approx. normal)

➢ If the model is correct, then the residuals should look like a sample of random variables – no "signal" remaining.

➢ If the assumptions are violated, then the p-values, R-squared values, predictions, etc, are wrong.

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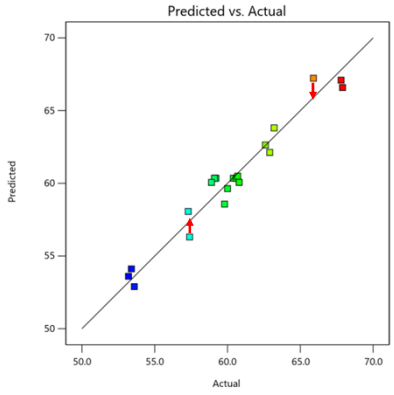
What is a residual?

Residual – difference between the actual data and the predicted value. $e_i = y_i - \hat{y}_i$



Reasons **not** to use the raw residuals to verify ANOVA:

- Sensitive to under-fitting or over-fitting of the model (too few or too many terms)
- Variance is not constant

Better residuals

Internally studentized residuals (standardized) – the raw residual divided by its estimated standard error. This helps with nonconstant variance but does not follow a t distribution.

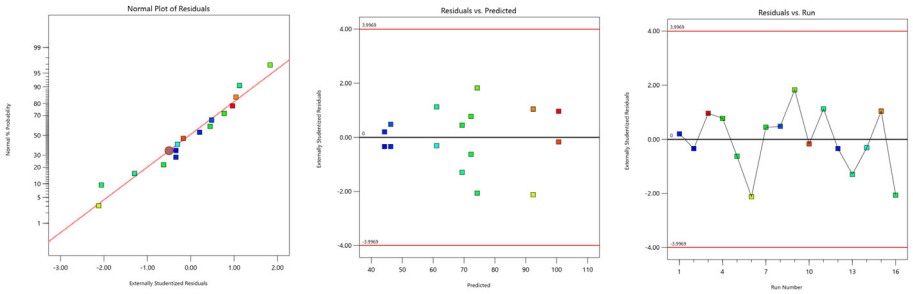
$$r_i = \frac{e_i}{\sqrt{MS_{res}(1 - h_{ii})}}$$

Externally studentized residuals (deleted) – adjusted to drop the *i*th data point. Corrects for nonconstant variance and follows a t distribution (which converges to the normal).

$$t_i = \frac{e_i}{\sqrt{MS_{res(-i)}(1 - h_{ii})}}$$

BEST for verifying assumptions

Diagnostic plots of Externally Std. Residuals



Normal plot of residuals – look for large violations of normality

Residuals vs Predicted – look for non-constant variance across range

Residuals vs Run – check for time-based trends or patterns

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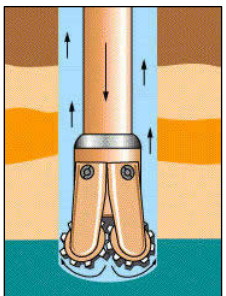
Well-Drilling Experiment
2^4 factorial – Background

This is a case study with a twist (pun-intended). The goal is to increase the advance rate of a drilling operation.

The drill is driven by a pipe, which carries a water-based mud down-hole to:

- Carry off the pulverized rock and
- Lubricate the drill-bit.


Mud circulation in the hole

The mud carries the bits of rock up the annulus of the borehole. It then runs through gratings to shed off the rock-cuttings before being re-circulated.

Well-Drilling Experiment

Input factors and ranges to study:

Factor	Units	Low Level (−)	High Level (+)
Load	tons	50	70
Flow	gal/min	180	220
Speed	1/sec	45000	55000
Mud	base gum	guar	xanthan

Open Well and analyze.

Well-Drilling Experiment

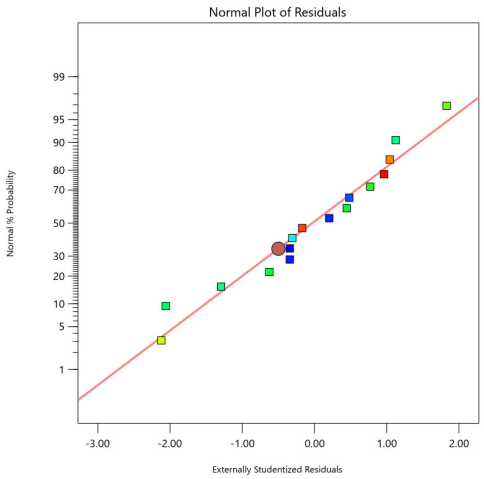
Fit a model and view ANOVA and Fit Statistics:

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	216.00	5	43.20	48.93	< 0.0001	significant
B-Flow	40.80	1	40.80	46.21	< 0.0001	
C-Speed	142.50	1	142.50	161.42	< 0.0001	
D-Mud	17.00	1	17.00	19.25	0.0014	
BC	8.48	1	8.48	9.61	0.0113	
CD	7.22	1	7.22	8.18	0.0169	
Residual	8.83	10	0.8828			
Cor Total	224.83	15				

Std. Dev.	0.9396		**R^2**	0.9607
Mean	5.92		**Adjusted R^2**	0.9411
C.V. %	15.86		**Predicted R^2**	0.8995
			Adeq Precision	19.5066

All looks good here!
Check diagnostics →

Normal plot of residuals – what it should be



The residuals should follow a well-behaved distribution.

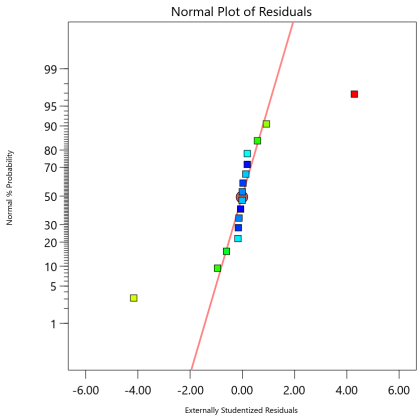
- Single peak
- Roughly symmetric
- Tails die rapidly

Roughly a normal distribution.

ANOVA is robust to moderate deviations from normality, so no need for a formal test (like Shapiro Wilks).

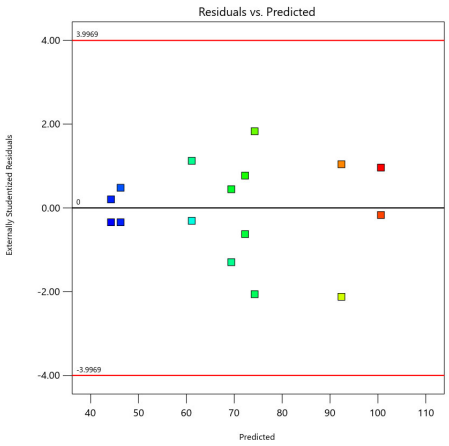
Well-Drilling Experiment
Diagnostic plots

Normal probability plot of residuals: want approximate normality



The residuals are not approximately normally distributed. This shows an S-shaped curve.

Residuals vs Predicted – what it should be

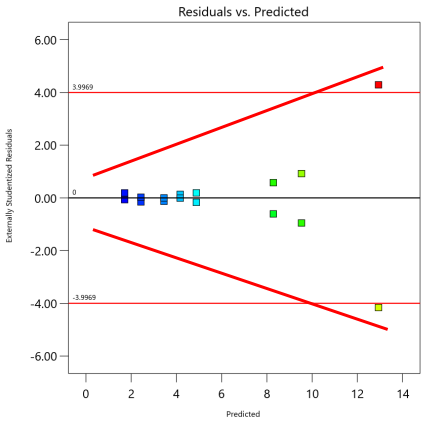


The plot should be a random scatter of points.

Look for systematic patterns or evidence of increasing variability as the predicted value increases.

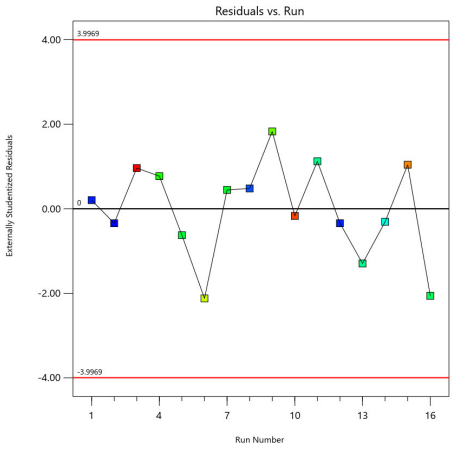
Well-Drilling Experiment
Diagnostic plots

Predicted vs Residuals: Look for constant variance left to right.



The residuals have small variation with small predictions and increasing variation with larger predictions.

Residuals vs Run Order – what it should be

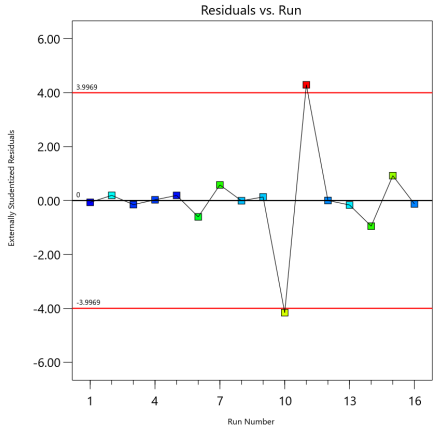


This time-ordered plot should show no patterns or trends.

- Watch for upward or downward trends, clumps of data.
- Watch for points not predicted well by the model, usually called "outliers".

Well-Drilling Experiment
Diagnostic plots

Residuals vs Run: want no time-based patterns/trends, no outliers

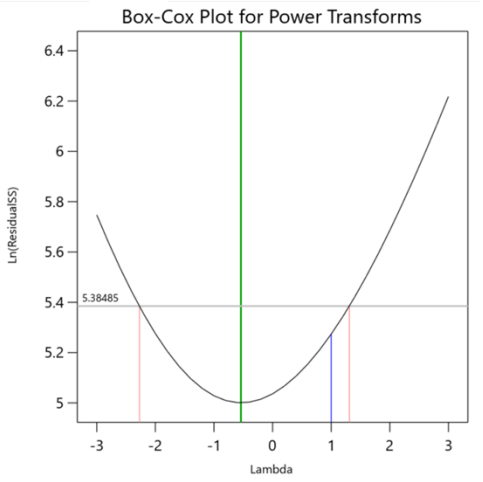


There are no particular trends, but there are 2 points that are not fit well by this model. "Outliers"??

Box Cox plot – what it should be

Current transform: None
Current Lambda = 1
Recommended transform: None

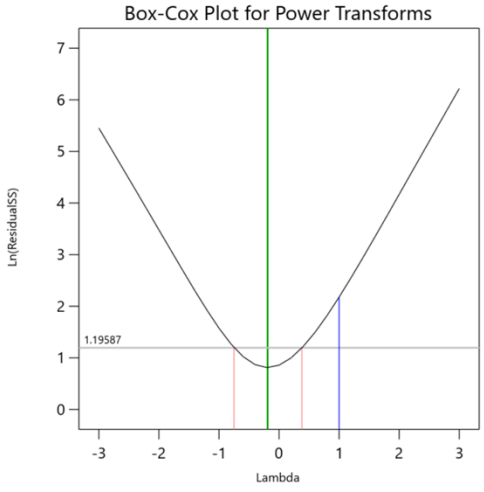
This plot will either recommend NO transformation or specify a particular legend.



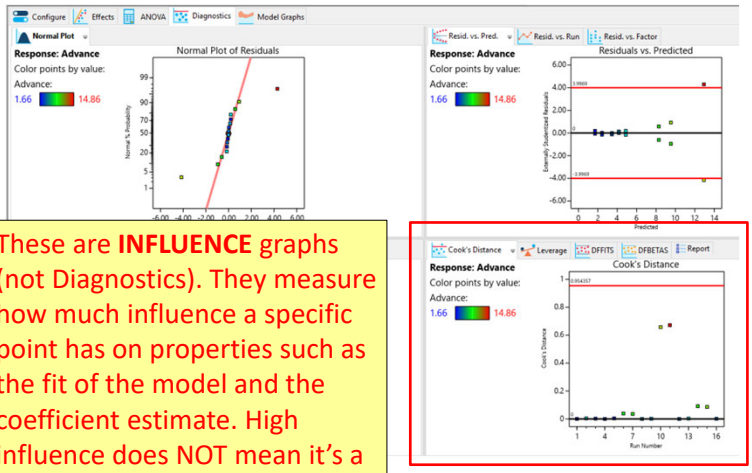
Well-Drilling Experiment
Box-Cox plot for transformations

Response: Advance
Current transform: None
Current Lambda = 1
Recommended transform: Log
(Lambda = 0)

The recommended transformation is a Log, so re-analyze the data using this scale.



Well-Drilling Experiment
What about the lower right graphs?



These are **INFLUENCE** graphs (not Diagnostics). They measure how much influence a specific point has on properties such as the fit of the model and the coefficient estimate. High influence does NOT mean it's a "bad" point!

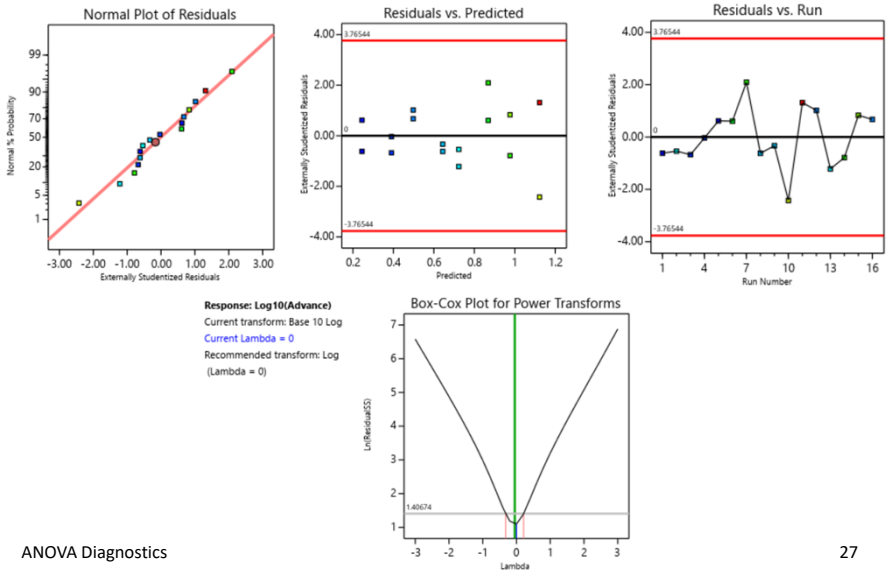
Well-Drilling Experiment
Re-analyze with log transform

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	1.26	3	0.4191	206.68	< 0.0001	significant
B-Flow	0.2568	1	0.2568	126.65	< 0.0001	
C-Speed	0.9155	1	0.9155	451.51	< 0.0001	
D-Mud	0.0849	1	0.0849	41.87	< 0.0001	
Residual	0.0243	12	0.0020			
Cor Total	1.28	15				

Std. Dev.	0.0450		**R^2**	0.9810
Mean	0.6835		**Adjusted R^2**	0.9763
C.V. %	6.59		**Predicted R^2**	0.9662
			Adeq Precision	38.9736

Fewer terms in the model, but it predicts better, explaining more variation.

Well-Drilling Experiment
Diagnostics after log transform



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Why check diagnostics?
Satisfy ANOVA Assumptions

ANOVA validity assumes that the model is correct,
and the residuals:

- Are (nearly) independent (Resid vs Run Order)
- Have a mean = 0 (given by math)
- Have a constant variance (Resid vs Predicted)
- Follow a "well-behaved" distribution (Normal probability plot)

➢ If the model is correct, then the residuals should look like a sample of random variables – no "signal" remaining.

What if the residuals remain messy?

- Check the science – could there be any additional variables to consider?
- This is a small sample – did you have some "bad luck" and it just happens to have some unknown random effects?
- Do confirmation runs – use the model as is (even if a bit messy), pick some plausible/desirable conditions, and run them. Compare results to the predicted values from Point Prediction.
- Do a replicate or collect more data to enhance the information.

The researcher must weigh the risks of using an imperfect model versus spending more money to get more data.

Self-study options for learning more

YouTube Channel: www.youtube.com/c/StatisticsMadeEasybyStatEase

Playlist: New to DOE?

A collection of webinars on basic to intermediate-level topics.

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