



Using Magruder Data More Than Just a Report Card!

- * Z Scores, What You Can Do?
- A Data Mining
 A
- * **Z Control Charts** (If there's time!)

Z Scores for the Magruder PT Program

Z is a Normalized measure of where you stand relative to the other participants in the scheme.

 Measured as the difference between your analysis (x_{LAB}) and the true analyte concentration (X_{AV}) described as:

o Assigned Value

- o Robust Mean
- o True Value
- o Etc., etc., ...
- And here's the twist; all divided by the robust SD (orob) of the participants.
- The robust SD is the fit-for-purpose SD in our PT scheme.
- So, Z is essentially "how many ffp SDs are you away from the truth, as we know it?".





Z Scoring for Analytical Chemistry

We all remember the Bell Curve!

check sample program

 The distribution of Analytical Chemistry results can be modeled with a Normal Bell Curve.

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- How many SDs (or Zs) away from the Robust Mean is acceptable?
- As long as you are within ± 3 SDs you pass or at least you "get away with it" – 99.7% capture!
- Beyond that you should try to start an investigation – some action is required – something is not quite right with the process!
- Green is GOOD!





Now, think about how much power σ has over your Z Score!



If σ is equal to the robust SD (σ_{Rob}) ~ 95% Pass. If σ is lower, Z is higher and many more fail! If σ is higher, Z is lower and many more pass! But, is the σ fit-for-<u>your</u>-purpose? magruder fertilizer check sample program



Fitness For Purpose (ffp) σ for Z Scores

- In the Magruder PT Program σ_{Rob} is the σ_{ffp} .
- However, you may have a client or a regulation or some other precision with which you must comply.
- In this case the Magruder σ_{ffp} may no longer be appropriate.
- Use an appropriate o_{ffp} and adjust the equation to fit your need.

$$Z = \frac{X_{LAB} - X_{AV}}{\sigma_{ffp}}$$

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Fitness For Purpose (ffp) σ for Z Scores

$$Z = \frac{X_{LAB} - X_{AV}}{\sigma_{ffp}}$$

The %RSD (relative standard deviation) is a popular measure of precision.



Example: For 3% RSD and X_{AV} = 15%

$$\sigma_{\rm ffp} = \frac{3}{100} \times 15 = 0.45$$

The Horwitz %RSD is another popular measure of precision.

Where C_{mf} is the mass fraction concentration.

Horwitz %RSD = $2 \times C_{mf}^{-0.1505}$

Example: For X_{AV} = 15%: Mass fraction = 15 parts / 100 parts = 0.15

$$\sigma_{\rm ffp} = \frac{2 \times 0.15_{\rm mf}^{-0.1505}}{100} \times 15 = 1.33$$

Fitness For Purpose (ffp)
$$\sigma$$
 for Z Scores





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Fitness For Purpose (ffp) σ for Z Scores

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$$Z = \frac{x_{\text{LAB}} - X_{\text{AV}}}{\sigma_{\text{ffp}}}$$

Or, just a hard limit like no more than ±100 ppm. A "designer" σ_{ffp} if you will! $\sigma_{ffp} = \frac{100}{3}$

Example: Sigma_{ffp} = 33.3: So within \pm 3 Z captures 99.7% of values.

And Barrison IA as a Fitness For Purpose Criteria

- Investigational Allowances (IA) can provide an industry standard ffp criteria.
- While this is not a Z Score, very simply:

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- ✓ Pass if: x_{LAB} is within $X_{AV} \pm IA_{AV}$ range.
- ✓ Fail if: x_{LAB} is outside $X_{AV} \pm IA_{AV}$ range.
- This is now shown in reports and report cards as IA Status.

$$IA Status = \begin{cases} Low & \text{if } x_{LAB} < X_{AV} - IA_{AV} \\ High & \text{if } x_{LAB} > X_{AV} + IA_{AV} \\ OK & Otherwise \end{cases}$$





In Summary:

- Z Scores are an "Alert!" tool and are NOT diagnostic.
- Be aware of "fitness-for-purpose" criteria.
- What Z-Score suits your needs?
- Z is **NOT** about the people, it's about the process!





We'll look at these 3 Method reports

Magruder Data Mining:

Where is the Mine?

Excel Data Downloads 2017

2017 Cumulative Analyte Data Report

2017 Cumulative Analyte Summary Report

2017 Cumulative Method Data Report

2017 Cumulative Method Summary Report

2017 Cumulative Method Precision Report

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Data Mining in the 2017 "Cumulative Method Summary Report"

Let's look at the New IA Ratio metric:

IA Ratio = $\frac{\text{Robust \%RSD}}{\text{IA \%RSD}}$

- Both %RSD's represent ~68% of data.
- This factor should be less than 1.
- Lower implies more precision relative to IA.
- Values <= 1 will appear in Green.</p>
- Values > 1 may appear in Green, Orange ,then Red if Significant (f).
- **Grey** is applied where the number of labs is < 6.

Data Mining in the "Cumulative Method Summary Report".

Two Potassium Methods.

Sample Number	Sample Name	# Labs	Assigned Value (%)	IA at Method Value	Robust sd	Robust % RSD	Method IA Ratio
Soluble	Potassium as K ₂ O,	STPB	Oxalate				
170611	Grade 2-15-15 w/PO3	10	17.79	1.003	0.571	3.21%	1.33
170811*	Grade 21-0-5	10	5.20	0.438	0.199	3.83%	1.06
170711	Grade 7-25-40	9	40.48	1.545	0.423	1.04%	0.64
171211	Grade 5-15-30	9	30.44	1.401	0.403	1.32%	0.67
Soluble	Potassium as K ₂ O,	AA (C	Dxalate)				
170611	Grade 2-15-15 w/PO3	8	17.53	0.994	1.98	11.29%	4.64
170411*	Grade 15-15-15 + Micros	7	2.47	0.410	0.372	15.02%	2.11
170711	Grade 7-25-40	7	40.22	1.542	1.70	4.22%	2.56
171211	Grade 5-15-30	6	30.79	1.410	1.68	5.45%	2.77

Data Mining in the "Cumulative Method Summary Report". Acid Soluble Boron (165) – All 2017 methods

Samples	# Labs	Assigned Value (%)	IA at Method Value	Robust SD	Robust % RSD	Method IA Ratio
Grade 5-15-30	19	0.255	0.041	0.032	12.5%	1.80
Grade 15-15-15 + Micros	18	0.292	0.047	0.039	13.2%	1.92
Grade 15-15-15 + Micros	13	0.274	0.044	0.038	13.9%	2.01
Grade 5-15-30	11	0.234	0.038	0.019	8.2%	1.18
Grade 5-15-30	11	0.248	0.040	0.026	10.4%	1.50
Grade 18-46-0 DAP	7	0.012	0.005	0.007	55.2%	3.30
Grade 15-15-15 + Micros	6	0.247	0.040	0.064	26.1%	3.75
MAP plus S, 12-40-0	6	0.008	0.004	0.007	94.6%	4.16
MAP plus S, 12-40-0	5	56.0	1.0	78.0	139.3%	181.74
Grade 16-1-0	\ 5	0.007	0.004	0.010	145.9%	5.93
Grade 21-0-5	5	0.003	0.003	0.003	105.9%	2.11

IA Ratio a little dodgy at the participation low end (< 6).

Acid Soluble Boron (165) – All 2017 methods

Sample Number	Sample Name	Method Code	# Labs	Assigned Value (%)	IA at Method Value	Robust sd	Robust % RSD	Method IA Ratio
171211	Grade 5-15-30	165.99	19	0.255	0.041	0.032	12.5%	1.80
170411	Grade 15-15-15 + Micros	165.99	18	0.292	0.047	0.039	13.2%	1.92
170411	Grade 15-15-15 + Micros	165.30	13	0.274	0.044	0.038	13.9%	2.01
171211	Grade 5-15-30	165.00	11	0.234	0.038	0.019	8.2%	1.18
171211	Grade 5-15-30	165.30	11	0.248	0.040	0.026	10.4%	1.50
170111	Grade 18-46-0 DAP	165.99	7	0.012	0.005	0.007	55.2%	3.30
170411	Grade 15-15-15 + Micros	165.00	6	0.247	0.040	0.064	26.1%	3.75
170911	MAP plus S, 12-40-0	165.99	6	0.008	0.004	0.007	94.6%	4.16

Does the IA for Boron adequately reflect the analytical dispersion?

Might need to reevaluate IA for Boron!

Data Mining the "Cumulative Method Precision" report.



Precision:

- Essentially estimating and separating out Intra Lab dispersion from Inter Lab dispersion. This is "Within" and "Between" lab precision respectively.
- Precision within (S_r) and between (S_R) labs is calculated according to ISO 5725-2 concepts. These are not robust procedures!
- Reproducibility (S_R) can form the basis for better estimates of IA values.
- o Repeatability (S_r) is highly indicative of method robustness.
- o Horwitz describes the S_R/S_r ratio as usually between 2 and 4 (skewed \rightarrow 2).

"Cumulative Method Precision Report"

		Th W i	is looks l hat you s n your lal	ike ee yo o. usu	s is what u don't ally see.	The Ratio: rom Horwitz ~ 2 to 4
Acid Soluble Boron,	2 Me	thods &	& Other*			
Sample Name Analyte Code: 165	# Labs	Mean	Between Labs %RSD	Repeatability %rsd	Reproducibility %RSD	sR/sr
Grade 5-15-30	9	0.24	6.4%	4.4%	7.8%	1.8
Grade 15-15-15 + Micros	11	0.28	11.6%	3.0%	12.0%	4.0
Grade 5-15-30	10	0.25	9.9%	2.2%	10.2%	4.6
Grade 15-15-15 + Micros*	16	0.28	15.4%	2.5%	15.6%	6.2
Grade 5-15-30*	17	0.25	9.5%	4.4%	10.5%	2.4
		Weight	ted Mean	3.41%	12.35%	3.6

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In general there is more variance between labs than within labs.

magruder fertil check sample pr	izer ogram		Thi wh in	s looks like at you see your lab.	This is what you don't usually see.							
"Cumulative Metho	od Pre	ecisio	n Repor	t" \	So	me Hig						
Total Nitrogen, Combustion (18%)												
Sample Name Method Code: 010.06	# Labs	Mean	Between Labs %RSD	Repeatability %rsd	Reproducibility %RSD	sR/sr						
Grade 18-46-0 DAP	49	18.3	1.5%	0.5%	1.6%	3.2						
Grade 27-0-0	50	26.6	3.5%	0.6%	3.6%	5.7						
Grade 28-0-0 Liquid SR	56	28.4	1.0%	0.5%	1.1%	2.3						
Grade 15-15-15 + Micros	56	20.1	1.4%	0.6%	1.5%	2.8						
Grade 16-1-0	54	16.9	0.9%	0.5%	1.0%	2.1						
Grade 2-15-15 w/PO ₃	53	2.1	9.0%	1.7%	9.2%	5.5						
Grade 7-25-40	52	6.6	12.5%	1.5%	12.6%	8.4						
Grade 21-0-5	54	21.1	1.4%	0.7%	1.5%	2.3						
MAP plus S, 12-40-0	54	12.5	1.4%	0.8%	1.6%	2.0						
Grade 12-0-0-26S	50	12.1	2.0%	0.7%	2.2%	3.0						
Grade 5-15-30	49	5.2	2.2%	1.2%	2.5%	2.1						
		Weigh	ited Mea	n 0.7%	2.85%	4.09						



"Cumulative Method Data Report" aka "All Tests" reports.

Data Mining in the New IA Cumulative Method Data Report.

Report"

A look at Total Sulfur Method 148.01 "Total Sulfur, Gravimetric - sulfate and elemental"

How the new IA metric "Method IA Status" (fixed dispersion) compares with Z Scores (variable dispersion).

$$IA Status = \begin{cases} Low & \text{if } x_{LAB} < X_{AV} - IA_{AV} \\ High & \text{if } x_{LAB} > X_{AV} + IA_{AV} \\ OK & Otherwise \end{cases}$$

$$Z = \frac{x_{LAB} - X_{AV}}{\sigma_{rob}}$$

Method	Analyte and	Lab	Lab	Data	Method Values				Magruder CS	Method IA	
Code	Method (Units)	Code	Value	Range	Rob Mean	Rob SD	R-bar	# Tests	Z Score	Status	Flag
171111	Grade 12-0-0-26S									ΙΔ = 1	
148.01	Total Sulfur, Gravimetric - sulfate and	0500	25.3	0.0000	26.4	0.56	0.1699	12	-1.95	Low	0
148.01	Total Sulfur Gravimetric - sulfate and	0534	25.6	0.2800	26.4	0.56	0 1699	12	-1.43	OK	0
148.01	Total Sulfur Gravimetric - sulfate and	0040	26.1	0 1000	26.4	0.56	0 1699	12	-0.60	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0231	26.1	0.0000	26.4	0.56	0.1699	12	-0.51	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0513	26.2	0.1300	26.4	0.56	0.1699	12	-0.37	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	26.5	0.1000	26.4	0.56	0.1699	12	0.12	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0029	26.5	0.1700	26.4	0.56	0.1699	12	0.29	ок	0
148.01	Total Sulfur, Gravimetric - sulfate and	0485	26.7	0.0628	26.4	0.56	0.1699	12	0.59	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0105	26.8	0.5200	26.4	0.56	0.1699	12	0.68	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0114	26.8	0.4000	26.4	0.56	0.1699	12	0.70	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0095	26.9	0.1200	26.4	0.56	0.1699	12	0.84	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0476	27.0	0.1556	26.4	0.56	0.1699	12	1.18	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0230	25.6	2.500	26.4	0.56	0.1699	12	-1.50	OK	1
148.0 1	Total Sulfur, Gravimetric - sulfate and	0530	2.6	0.0000	26.4	0.56	0.1699	12	- 42.83	Low	2
171211	Grade 5-15-30									IA = 0.46	
148.01	Total Sulfur, Gravimetric - sulfate and	0513	4.1	0.0900	5.2	1.07	0.1293	9	-0.93	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0476	4.1	0.0641	5.2	1.07	0.1293	9	-0.92	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0324	4.3	0.2900	5.2	1.07	0.1293	9	-0.78	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0444	4.5	0.1500	5.2	1.07	0.1293	9	-0.56	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0405	5.1	0.1400	5.2	1.07	0.1293	9	-0.07	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0055	6.0	0.0700	5.2	1.07	0.1293	9	0.71	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0534	6.1	0.1100	5.2	1.07	0.1293	9	0.77	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0040	6.1	0.2000	5.2	1.07	0.1293	9	0.80	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	6.3	0.0500	5.2	1.07	0.1293	9	0.97	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0114	4.7	0.7800	5.2	1.07	0.1293	9	-0.44	Low	4

Method	Analyte and	Lab	Lab	Data	Meth	od Val	ues		Magruder CS	Method IA	
Code	Method (Units)	Code	Value	Range	Rob Mean	Rob SD	R-bar	# Tests	Z Score	Status	Flag
170411	Grade 15-15-15 + Mid	cros								IA = 0.41	
148.01	Total Sulfur, Gravimetric - sulfate and	0513	2.4	0.0100	4.2	1.14	0.0852	14	-1.64	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0457	2.6	0.0700	4.2	1.14	0.0852	14	-1.42	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0073	3.4	0.1100	4.2	1.14	0.0852	14	-0.71	Low	0
148.01	Total Sulfur. Gravimetric - sulfate and	0177	3.5	0.0222	4.2	1.14	0.0852	14	-0.63	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0510	3.5	0.0004	4.2	1.14	0.0852	14	-0.61	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0029	3.7	0.0100	4.2	1.14	0.0852	14	-0.45	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0230	4.7	0.2300	4.2	1.14	0.0852	14	0.42	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0105	4.8	0.1100	4.2	1.14	0.0852	14	0.50	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	4.8	0.1500	4.2	1.14	0.0852	14	0.50	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0324	4.9	0.0500	4.2	1.14	0.0852	14	0.54	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0485	4.9	0.0700	4.2	1.14	0.0852	14	0.57	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0055	4.9	0.1200	4.2	1.14	0.0852	14	0.61	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0114	5.0	0.1000	4.2	1.14	0.0852	14	0.66	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0231	9.7	0.1400	4.2	1.14	0.0852	14	4.79	High	0
170811	Grade 21-0-5									IA = 0.47	
148.01	Total Sulfur, Gravimetric - sulfate and	0230	5.2	0.1800	5.4	0.19	0.0913	11	-1.11	ок	0
148.01	Total Sulfur, Gravimetric - sulfate and	0105	5.3	0.0200	5.4	0.19	0.0913	11	-0.75	ок	0
148.01	Total Sulfur, Gravimetric - sulfate and	0444	5.3	0.3000	5.4	0.19	0.0913	11	-0.75	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0040	5.3	0.0000	5.4	0.19	0.0913	11	-0.49	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0029	5.3	0.1000	5.4	0.19	0.0913	11	-0.44	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0500	5.3	0.0800	5.4	0.19	0.0913	11	-0.28	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0055	5.4	0.0100	5.4	0.19	0.0913	11	-0.05	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0102	5.4	0.1143	5.4	0.19	0.0913	11	0.28	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	5.5	0.0800	5.4	0.19	0.0913	11	0.59	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0073	8.1	0.0200	5.4	0.19	0.0913	11	13.90	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0534	8.6	0.1000	5.4	0.19	0.0913	11	16.41	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0324	5.2	0.5200	5.4	0.19	0.0913	11	-1.05	OK	1
148.01	Total Sulfur, Gravimetric - sulfate and	0485	0.0	0.0000	5.4	0.19	0.0913	11			4

Method	Analyte and	Lab	Lab	Data	Meth	od Val	ues		Magruder CS	Method IA	
Code	Method (Units)	Code	Value	Range	Rob Mean	Rob SD	R-bar	# Tests	Z Score	Status	Flag
170911	MAP plus S, 12-40-0									IA = 0.56	
148.01	Total Sulfur, Gravimetric - sulfate and	0534	6.5	0.0400	7.2	0.15	0.0771	17	-4.50	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0444	7.0	0.1200	7.2	0.15	0.0771	17	-1.39	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0230	7.1	0.0100	7.2	0.15	0.0771	17	-0.91	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0231	7.1	0.0500	7.2	0.15	0.0771	17	-0.84	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0481	7.1	0.0100	7.2	0.15	0.0771	17	-0.65	OK	О
148.01	Total Sulfur, Gravimetric - sulfate and	0105	7.2	0.0100	7.2	0.15	0.0771	17	-0.32	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0371	7.2	0.3200	7.2	0.15	0.0771	17	-0.29	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0073	7.2	0.0300	7.2	0.15	0.0771	17	-0.26	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0485	7.2	0.2107	7.2	0.15	0.0771	17	0.06	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0029	7.2	0.0700	7.2	0.15	0.0771	17	0.20	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0040	7.3	0.1000	7.2	0.15	0.0771	17	0.23	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0513	7.3	0.0500	7.2	0.15	0.0771	17	0.39	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0055	7.3	0.0700	7.2	0.15	0.0771	17	0.84	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0324	7.4	0.1900	7.2	0.15	0.0771	17	0.91	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0500	7.4	0.0200	7.2	0.15	0.0771	17	0.94	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	7.4	0.0000	7.2	0.15	0.0771	17	1.14	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0102	7.4	0.0100	7.2	0.15	0.0771	17	1.45	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0114	7.5	0.6300	7.2	0.15	0.0771	17	2.07	OK	1
161211	MAP plus S									IA = 0.63	
148.01	- Total Sulfur, Gravimetric - sulfate and	0444	4.8	0.0100	8.5	2.27	0.1904	12	-1.60	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0324	5.1	0.0000	8.5	2.27	0.1904	12	-1.49	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0230	5.5	0.5600	8.5	2.27	0.1904	12	-1.34	Low	0
148.01	Total Sulfur, Gravimetric - sulfate and	0055	8.7	0.0500	8.5	2.27	0.1904	12	0.10	OK	0
148.01	Total Sulfur, Gravimetric - sulfate and	0073	9.3	0.3700	8.5	2.27	0.1904	12	0.37	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0157	9.5	0.1600	8.5	2.27	0.1904	12	0.46	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0028	9.5	0.4000	8.5	2.27	0.1904	12	0.47	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0231	9.6	0.0100	8.5	2.27	0.1904	12	0.50	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0105	9.7	0.1000	8.5	2.27	0.1904	12	0.54	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0037	9.7	0.4950	8.5	2.27	0.1904	12	0.56	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0029	9.9	0.0400	8.5	2.27	0.1904	12	0.63	High	0
148.01	Total Sulfur, Gravimetric - sulfate and	0485	10.0	0.0900	8.5	2.27	0.1904	12	0.69	High	0





"Cumulative Method Data Report" aka "All Tests" reports.

We have just seen the lab results from 6 samples for one Method. "Total Sulfur, Gravimetric - sulfate and elemental"

Clearly, IA Status predicts a different outcome than Z Score, for only some Samples.

It is important to recognize:

- IA Status is derived from a fixed dispersion (IA) set by the fertilizer regulators.
- Z Scores are derived from variable dispersion (σ_{Rob}) set by participants in that round.



Data Mining in the Cumulative Reports

Much can be learned from just sorting the data:

- o Using the Excel Data Downloads available on the Magruder Website (easily sortable!).
- o Sort these 2017 reports by Method Code:
 - Cumulative Method Summary Report
 - Cumulative Method Precision Report
 - Cumulative Method Data Report
- o These files are the annual collection of information contained in sample reports you get every month on the DRW, which are:
 - Method All Tests Report
 - Individual Method Performance Summary
- o After sorting scroll down and look for methods of interest! (Hint: colors can really help!).
- o Cumulative Analyte Reports are also available (no precision!).



GET CREATIVE!

magruder fertilizer

check sample program

"There is a wealth of information out there just dying to spill it's guts!"

To Sum Up:

• We have talked about Z Scores – a simple calculation. $Z = \frac{X_{LAB} - X_{AV}}{\sigma_{HAB}}$

- Described fit-for-purpose sigmas.
- Discussed calculating your own ffp sigma.¹²
- All the hard work is provided by Magruder as X_{AV} (Assigned Value).

o We have talked about Magruder Data Mining.

- There are 5 Cumulative Excel data files produced for each year.
- The story here is "just sort to see"!

o We briefly touched upon the new IA metrics.

- IA Ratio: Robust %RSD / IA %RSD
- IA Status: Relative to $X_{AV} \pm IA_{AV}$





STRIVING FOR EXCELLENCE IN ANALYSIS



Control Charts

An Excel file you can download from the website.



STRIVING FOR EXCELLENCE IN ANALYSIS

Magruder Check Sample: Z Control Charts

Enter Lab # Below 0000 Get Current Data

First check the Sample list below to make sure you have downloaded the latest version from the website. The last Sample in the list should reflect the most current Sample for which reports have been released.

Now enter your Lab Number. When you hit the enter key your Lab Number will convert to the standard 4 character format (leading 0's).

Finally click the [Get Current Data] button and you will be switched to the Control Charts sheet. These control charts show Z-scores for the last 16 Magruder Check Samples by Analyte and Method submitted by you.

When in the Control Charts sheet you can scroll sequentially through your Methods by tapping the [Tap To Scroll Through Charts] button or select the method of interest directly in the scroll box. If you wish you can print this page using the Excel Print Preview and Print icons.

When you return to this sheet samples for which you submitted data will be marked with an astrix. To return just click on the "StartUp" tab below.

16 Samples in This Version Number Name *161011 MOP *161111 Grade 32-0-10 *161211 MAP plus S *170111 Grade 18-46-0 DAP *170211 Grade 27-0-0 *170311 Grade 28-0-0 Liquid SR *170411 Grade 15-15-15 + Micros *170511 Grade 16-1-0 *170611 Grade 2-15-15 w/PO3 *170711 Grade 7-25-40 *170811 Grade 21-0-5 *170911 MAP plus S, 12-40-0 *171011 Epsom Salts *171012 TSP. 0-45-0 *171111 Grade 12-0-0-26S *171211 Grade 5-15-30

THIS IS AN EXCEL FILE!

- On left the opening sheet.
- Check the list for latest sample.
- Enter your lab number.
- Click "Get Current Data" button
- On return to this sheet, stars will appear on sample numbers you submitted.



Analyte Chart (independent of method)



magruder fertilizer check sample program

	Analyte Code and Name										
	010 1	otal Nitro	gen (%)								
Number of	Samples	11		Analyte	Values	Your					
Sample Name &	Code	Z	# Labs	Rob Mean	Rob SD	Method					
Grade 32-0-10	161111	0.83	75	32.34	0.3510	010.60					
Grade 18-46-0 DAP	170111	0.37	67	18.29	0.2678	010.60					
Grade 27-0-0	170211	0.88	67	26.59	0.8404	010.60					
Grade 28-0-0 Liquid	170311	1.28	76	28.31	0.3561	010.60					
Grade 15-15-15 + Mi	170411	0.12	81	19.95	0.4052	010.60					
Grade 16-1-0	170511	0.37	78	16.88	0.2172	010.60					
Grade 2-15-15 w/PO	170611	-0.27	80	2.094	0.1521	010.60					
Grade 7-25-40	170711	0.54	67	6.770	0.5281	010.60					
MAP plus S, 12-40-0	170911	0.54	73	12.46	0.2121	010.60					
Grade 12-0-0-26S	171111	-0.82	69	12.12	0.2238	010.60					
Grade 5-15-30	171211	-0.28	67	5.140	0.1444	010.60					

Your Method Chart

magruder fertilizer check sample program



010.60 T	Method Code and Name 010.60 Total Nitrogen, Combustion (%)													
			Lab	Data	Threshold	Method	Values							
Code	Z	#Labs	Value	Range	<u> % _ P</u>	Rob Mean	Rob SD							
161111	0.70	55	32.64	0.0300		32.44	0.2845							
170111	0.34	54	18.39	0.0570	Sta	18.29	0.2722							
170211	0.82	55	27.33	0.0200	atu	26.52	0.9822							
170311	1.13	57	28.76	0.0600		28.39	0.3240							
170411	-0.40	58	19.99	0.0640	he	20.10	0.2578							
170511	0.13	56	16.96	0.0200	re	16.94	0.1643							
170611	-0.16	56	2.053	0.0680	in	2.082	0.1762							
170711	0.55	55	7.054	0.0474	T	6.749	0.5527							
170911	0.57	57	12.57	0.0760		12.46	0.2012							
<u>17111</u> 1	-0.73	53	11.94	0.1800	re	12.11	0.2301							
171211	-0.45	52	5.100	0.0600	A. (10)	5.160	0.1335							





Number of	Samples	12		Analyte	Values	Your				Lab I	Data	Threshold	Method	Values
Sample Name &	Code	Z	# Labs	Rob Mean	Rob SD	Method	Code	z	# Labs	Value	Range	% RSD	Rob Mean	Rob SD
Grade 32-0-10	161111	1.27	9	7.116	0.3816	148.07	161111	1.47	5	7.640	0.1000	4%	7.024	0.4191
MAP plus S	161211	-0.57	40	9.492	0.9896	148.07	161211	-0.37	11	8.930	1.300	2%	9.344	1.106
Grade 18-46-0 DAP	170111	2.92	10	2.192	0.0840	148.07	170111	2.63	6	2.455	0.1100	6%	2.195	0.0882
Grade 27-0-0	170211	0.36	7	0.2078	0.0552	148.07	170211	-0.18	4	0.2300	0.0040	2%	0.2406	0.0594
Grade 15-15-15 + Mi	170411	0.80	45	4.574	0.4957	148.07	170411	0.93	12	4.970	0.0400	3%	4.712	0.2768
Grade 16-1-0	170511	-1.36	41	19.12	0.7888	148.07	170511	-1.20	11	18.05*	3.500	3%	19.03	0.8235
Grade 21-0-5	170811	0.36	44	5.343	0.2401	148.07	170811	0.08	12	5.430	0.4200	0%	5.409	0.2556
MAP plus S, 12-40-0	170911	-0.05	47	7.023	0.3618	148.07	170911	0.90	12	7.005	0.1700	2%	6.774	0.2565
Epsom Salts	171011	2.15	51	13.19	0.5648	148.07	171011	1.81	13	14.40	0.6000	4%	13.22	0.6545
TSP, 0-45-0	171012	1.13	8	1.117	0.0916	148.07	171012	1.69	5	1.230	0.0000	5%	1.115	0.0676
Grade 12-0-0-26S	171111	-2.16	38	26.40	0.8319	148.07	171111	-1.44	12	24.60*	2.800	4%	26.62	1.406
Grade 5-15-30	171211	0.74	37	5,467	0.8675	148.07	171211	0.68	11	6.110	0.1800	8%	5.275	1.154

A slightly more erratic process, but still in control!



			Analyte Co	de and Name			Method Code and Name							
<i>4</i>	010 -	Total Nitro	gen (%)				010.60	Total Nitro	gen, Combu	stion (%)				
Number o	of Samples	13		Analyte	Values	Your				Lab [Data	Threshold	Method	Values
Sample Name 8	Code	z	# Labs	Rob Mean	Rob SD	Method	Code	Z	# Labs	Value	Range	% RSD	Rob Mean	Rob SD
Grade 32-0-10	161111	-0.91	75	32.34	0.3510	010.60	161111	-1.45	55	32.03	0.0300	1%	32.44	0.2845
MAP plus S	161211	1.00	72	12.06	0.2047	010.60	161211	1.05	57	12.27	0.0100	1%	12.07	0.1876
Grade 18-46-0 DAP	170111	1.56	67	18.29	0.2678	010.60	170111	1.50	54	18.70	0.1250	1%	18.29	0.2722
Grade 27-0-0	170211	-4.01	67	26.59	0.8404	010.60	170211	-3.36	55	23.23*	0.0700	6%	26.52	0.9822
Grade 28-0-0 Liquid	170311	-0.49	76	28.31	0.3561	010.60	170311	-0.82	57	28.13	0.0600	0%	28.39	0.3240
Grade 15-15-15 + Mi	170411	1.23	81	19.95	0.4052	010.60	170411	1.35	58	20.45	0.0300	1%	20.10	0.2578
Grade 16-1-0	170511	1.53	78	16.88	0.2172	010.60	170511	1.65	56	17.21	0.0200	1%	16.94	0.1643
Grade 2-15-15 w/PO	170611	-0.13	80	2.094	0.1521	010.60	170611	-0.04	56	2.075	0.0300	0%	2.082	0.1762
Grade 7-25-40	170711	-5.63	67	6.770	0.5281	010.60	170711	-5.34	55	3.795*	0.0100	22%	6.749	0.5527
Grade 21-0-5	170811	0.05	82	21.05	0.3075	010.60	170811	-0.13	56	21.06	0.0400	0%	21.10	0.2994
MAP plus S, 12-40-0	170911	19.53	73	12.46	0.2121	010.60	170911	20.58	57	16.60	0.4000	17%	12.46	0.2012
Grade 12-0-0-26S	171111	-1.24	69	12.12	0.2238	010.60	171111	-1.15	53	11.85	0.0500	1%	12.11	0.2301
Grade 5-15-30	171211	-0.31	67	5.140	0.1444	010.60	171211	-0.48	52	5.095	0.0300	1%	5.160	0.1335

This visual certainly indicates sporadic problems!



Γ	Analyte Code and Name							Method Code and Name								
~ ~ ~	101 Acid Soluble Calcium (%)							101.30 Acid Soluble Calcium, ICP, test portion inorg (%)								
Number o	11		Analyte Values		Your				Lab Data		Threshold Method Val		Values			
Sample Name & Code		Z	# Labs	Rob Mean	Rob SD	Method	Code	z	# Labs	Value	Range	% RSD	Rob Mean	Rob SD		
Grade 32-0-10	161111	43.66	12	0.0944	0.0080	101.30	161111	1.56	5	0.4445	0.0190	84%	0.1654	0.1562		
MAP plus S	161211	7.85	14	0.2201	0.0532	101.30	161211	5.48	6	0.6375	0.0910	93%	0.2236	0.0673		
Grade 18-46-0 DAP	170111	4.95	14	0.2803	0.0538	101.30	170111	5.62	8	0.5465	0.0230	49%	0.2749	0.0442		
Grade 27-0-0	170211	3.03	56	4.502	0.2419	101.30	170211	3.48	21	5.235	0.1100	8%	4.496	0.2124		
Grade 15-15-15 + Mi	170411	3.93	23	0.3360	0.0534	101.30	170411	7.84	8	0.5460	0.0420	27%	0.3553	0.0222		
Grade 16-1-0	170511	6.21	17	0.4945	0.0407	101.30	170511	2.62	6	0.7470	0.0880	22%	0.5162	0.0784		
Grade 21-0-5	170811	1.37	17	6.730	0.4868	101.30	170811	0.98	7	7.395	0.0300	5%	6.783	0.5655		
MAP plus S, 12-40-0	170911	5.28	16	0.4252	0.0358	101.30	170911	1.67	8	0.6140	0.0360	17%	0.4607	0.0840		
TSP, 0-45-0	171012	1.55	62	13.48	0.7251	101.30	171012	1.19	25	14.60	0.2000	4%	13.48	0.9366		
Grade 12-0-0-26S	171111	1.10	3	0.0738	0.0764	101.30	171111		2	0.1580	0.0340					
Grade 5-15-30	171211	3.29	44	0.3850	0.0656	101.30	171211	3.97	15	0.6010	0.0020	31%	0.3700	0.0582		

Time to start thinking about a possible Method Bias!



ſ	Analyte Code and Name							Method Code and Name								
	010 1	Total Nitro	gen (%)				010.60	Total Nitro	gen, Combu	stion (%)						
Number of Samples 13				Analyte Values		Your				Lab Data		Threshold	Threshold Method Val			
Sample Name & Code		Z	# Labs	Rob Mean	Rob SD	Method	Code	Z	# Labs	Value	Range	% RSD	Rob Mean	Rob SD		
Grade 32-0-10	161111	0.66	75	32.34	0.3510	010.60	161111	0.49	55	32.58	0.1100	0%	32.44	0.2845		
MAP plus S	161211	0.73	72	12.06	0.2047	010.60	161211	0.76	57	12.21	0.0200	1%	12.07	0.1876		
Grade 18-46-0 DAP	170111	1.10	67	18.29	0.2678	010.60	170111	1.05	54	18.58	0.0200	1%	18.29	0.2722		
Grade 27-0-0	170211	0.56	67	26.59	0.8404	010.60	170211	0.55	55	27.06	0.1480	1%	26.52	0.9822		
Grade 28-0-0 Liquid	170311	0.62	76	28.31	0.3561	010.60	170311	0.40	57	28.53	0.3700	0%	28.39	0.3240		
Grade 15-15-15 + Mi	170411	0.93	81	19.95	0.4052	010.60	170411	0.89	58	20.33	0.1100	1%	20.10	0.2578		
Grade 16-1-0	170511	-0.96	78	16.88	0.2172	010.60	170511	-1.64	56	16.67	0.0400	1%	16.94	0.1643		
Grade 2-15-15 w/PO	170611	-1.38	80	2.094	0.1521	010.60	170611	-1.12	56	1.885	0.0700	5%	2.082	0.1762		
Grade 7-25-40	170711	0.11	67	6.770	0.5281	010.60	170711	0.15	55	6.830	0.1000	1%	6.749	0.5527		
Grade 21-0-5	170811	0.18	82	21.05	0.3075	010.60	170811	0.01	56	21.10	0.3600	0%	21.10	0.2994		
MAP plus S, 12-40-0	170911	-0.40	73	12.46	0.2121	010.60	170911	-0.41	57	12.38	0.0300	0%	12.46	0.2012		
Grade 12-0-0-26S	171111	4.68	69	12.12	0.2238	010.60	171111	4.61	53	13.17	0.0000	4%	12.11	0.2301		
Grade 5-15-30	171211	-1.35	67	5.140	0.1444	010.60	171211	-1.61	52	4.945	0.1100	2%	5.160	0.1335		

So, when this happens, don't get too worried!



Summary:

- o These "Control" charts provide a quick process visual over time.
- o They are not strictly control charts but more like Z tracking charts.
 - Each sample is different (somewhat handled by Z normalization!).
 - But remember, each Z is derived from a different dispersion σ_{Rob} .
- o But useful nonetheless!
- o The Control charts are easily accessible from the Website.
- o Each Lab can and should visually track Z Scores over time.
- o All the critical data is provided for both Analyte and Method Z Scores.