

Data Analysis: Total S

- definition of variances
- results from analyte report compared to IA and Horwitz
- comparing methods

Informed use of statistical methods
requires an understanding of the
underlying reasoning

Introduction to the Practice of Statistics,
D.S. Moore and G.P. McCabe, 1996

**DEFINITIONS ARE CRITICAL FOR
EFFECTIVE COMMUNICATION**

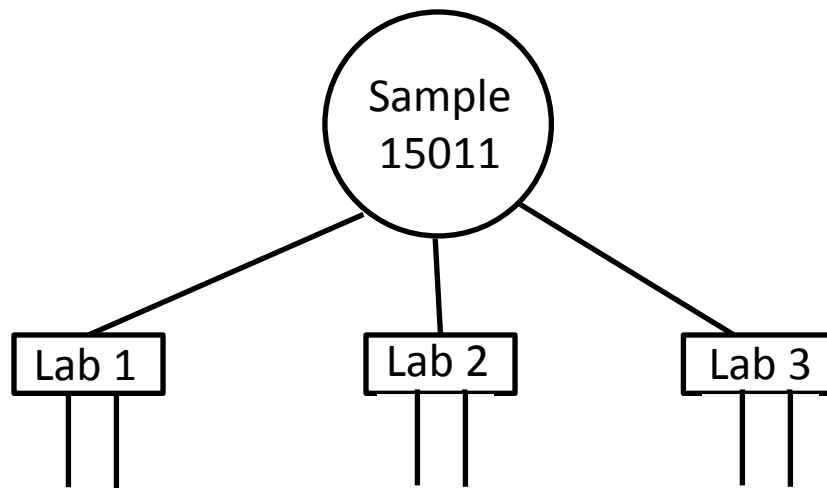
$$S_{\text{total}}^2 = S_{\text{part 1}}^2 + S_{\text{part b}}^2 + S_{\text{part c}}^2 + S_{\text{part d}}^2 + \dots$$

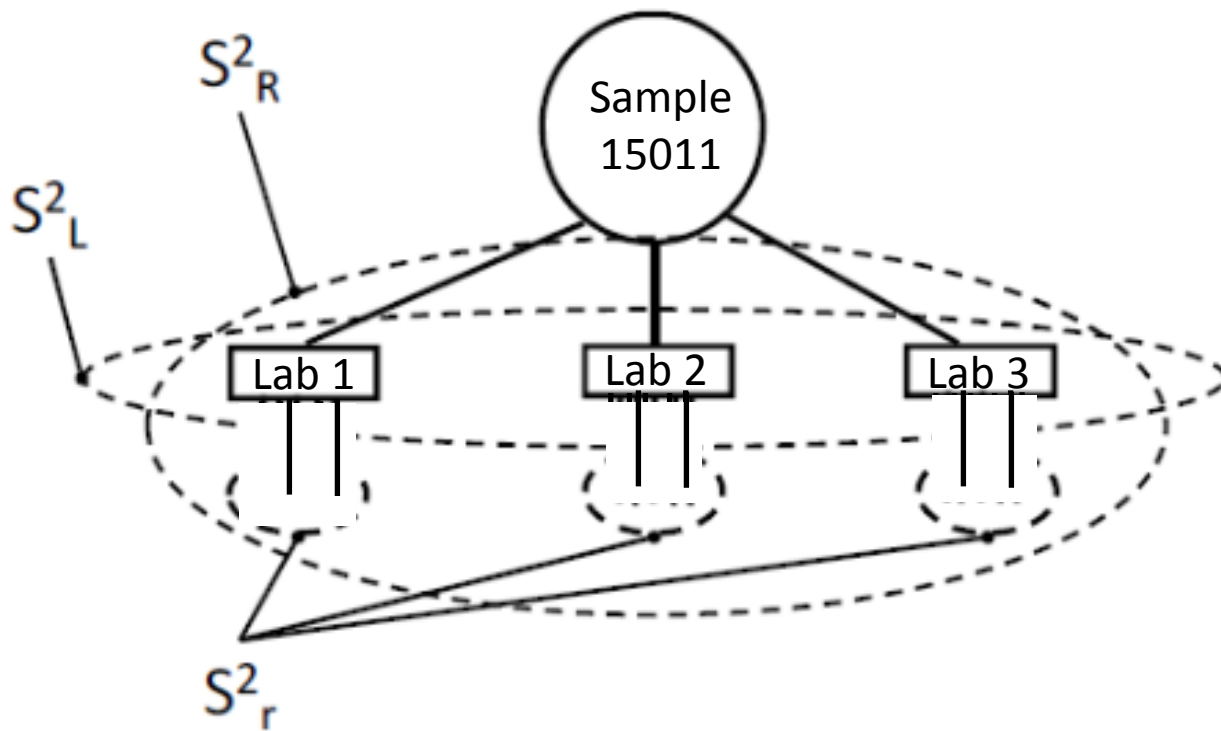
$$\text{Reproducibility } S_R^2 = S_L^2 + S_r^2$$

Between lab

Within lab

repeatability

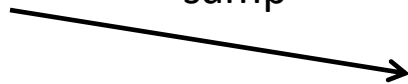




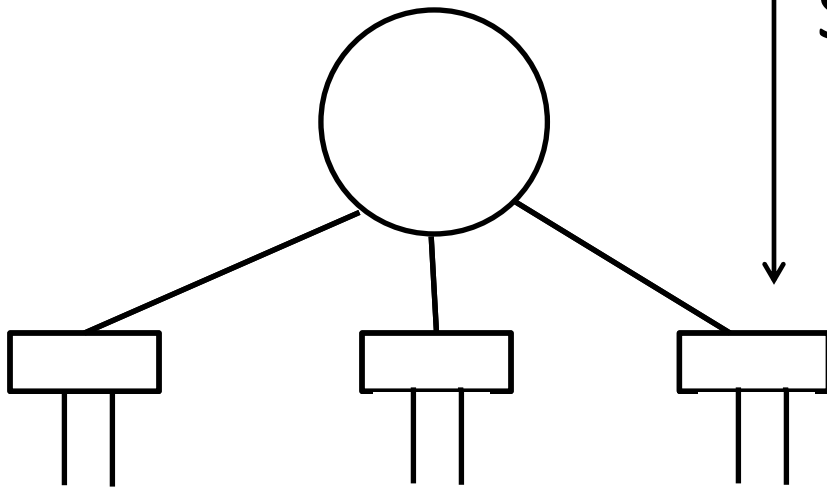


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S_{samp}^2



S_{prep}^2



$$S_R = \sqrt{S_L^2 + S_r^2}$$

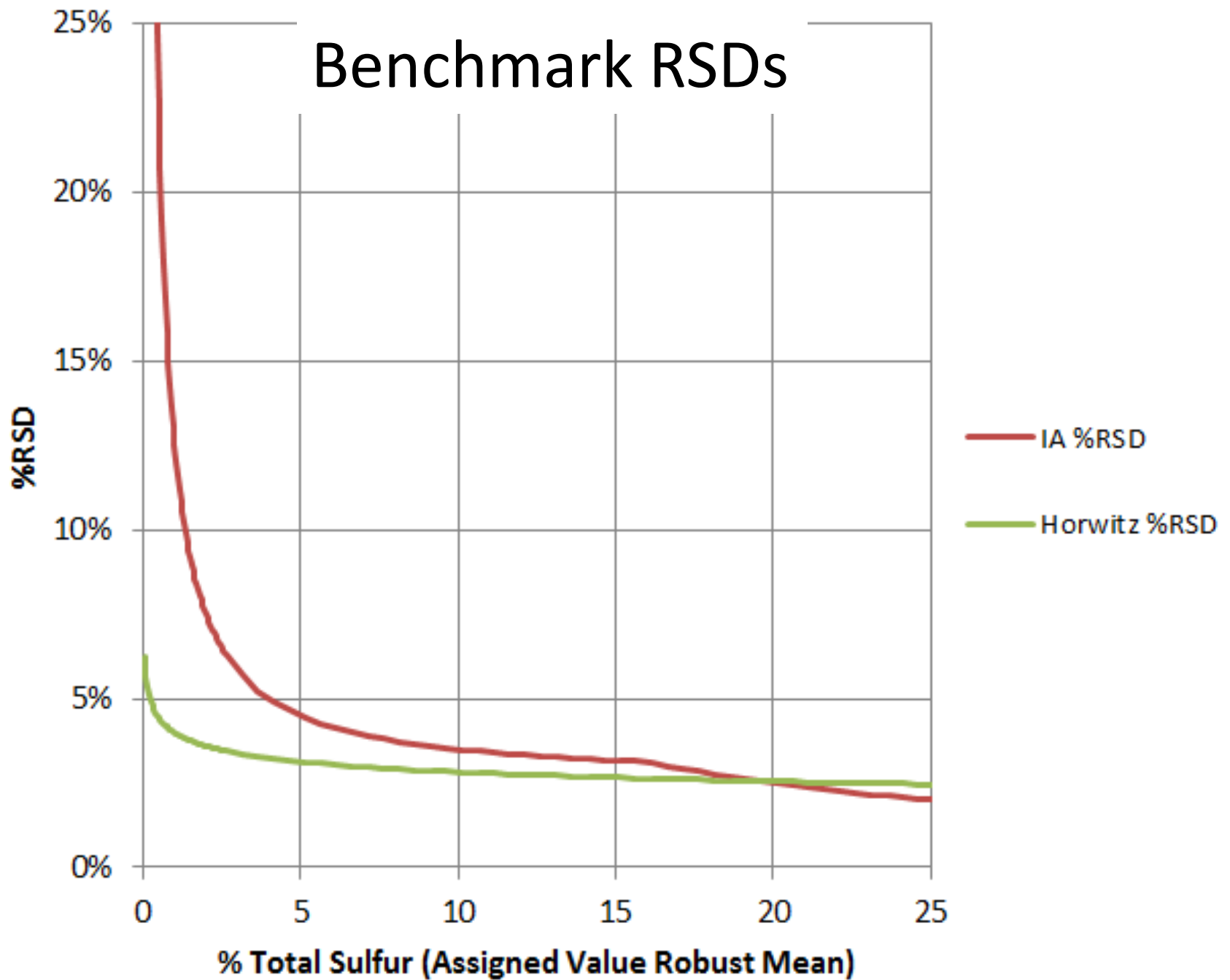
$$S_{IA} = \sqrt{S_L^2 + S_r^2 + S_{\text{prep}}^2 + S_{\text{samp}}^2}$$

$$\text{RSD}_R = \sqrt{\text{RSD}_L^2 + \text{RSD}_r^2}$$

$$\text{RSD}_{IA} = \sqrt{\text{RSD}_L^2 + \text{RSD}_r^2 + \text{RSD}_{\text{prep}}^2 + \text{RSD}_{\text{samp}}^2}$$

RSD_R compared to $\text{RSD}_{\text{Horowitz}} = 2 \times C^{-0.15}$

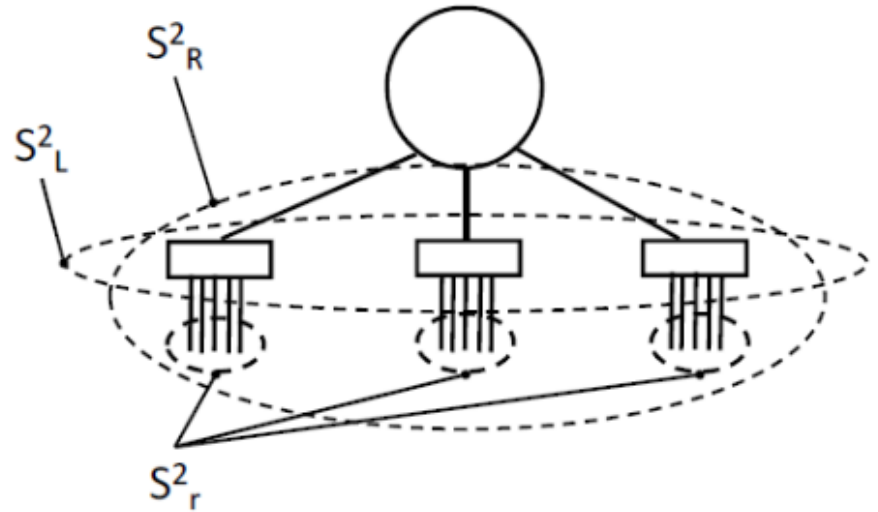
Benchmark RSDs

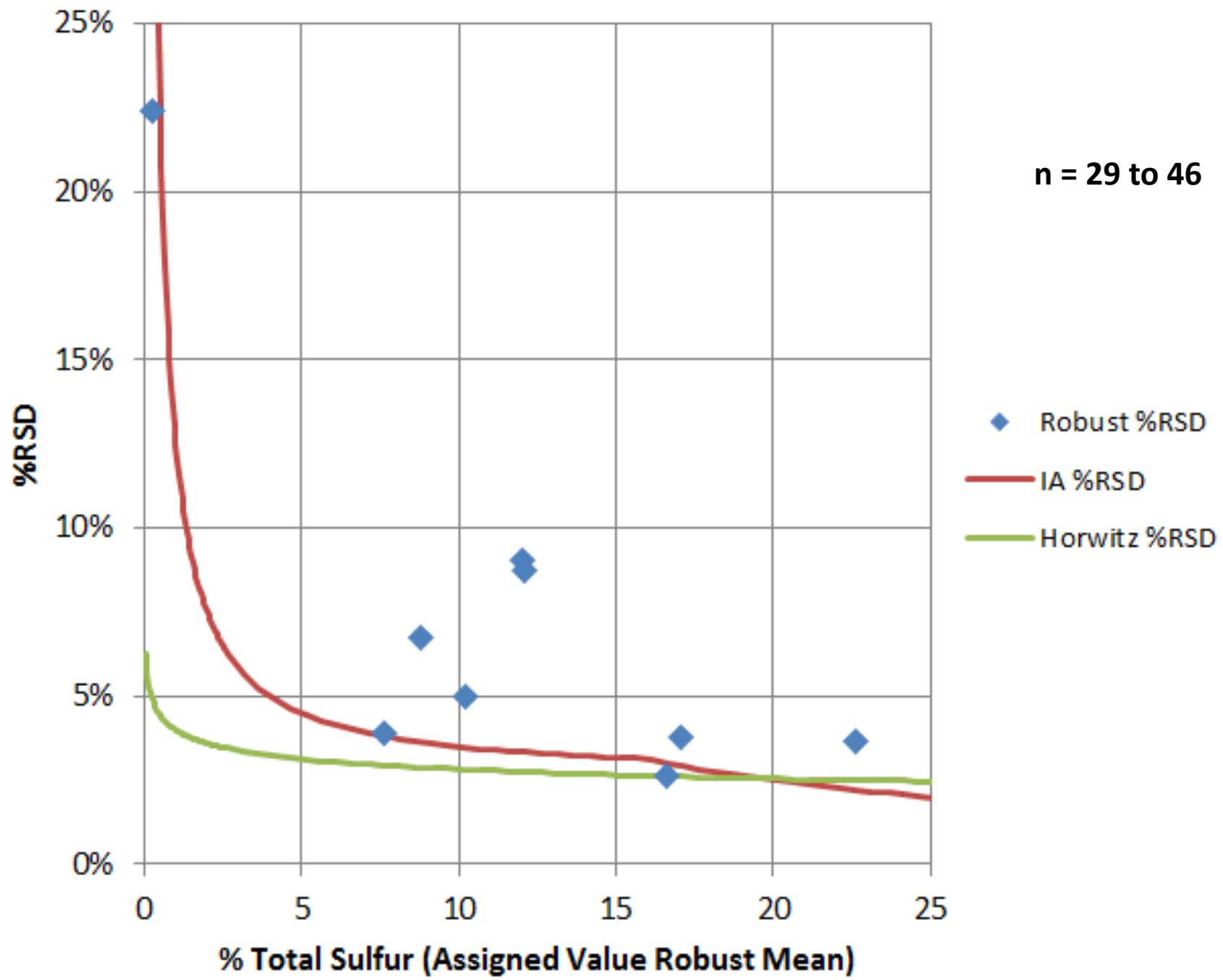


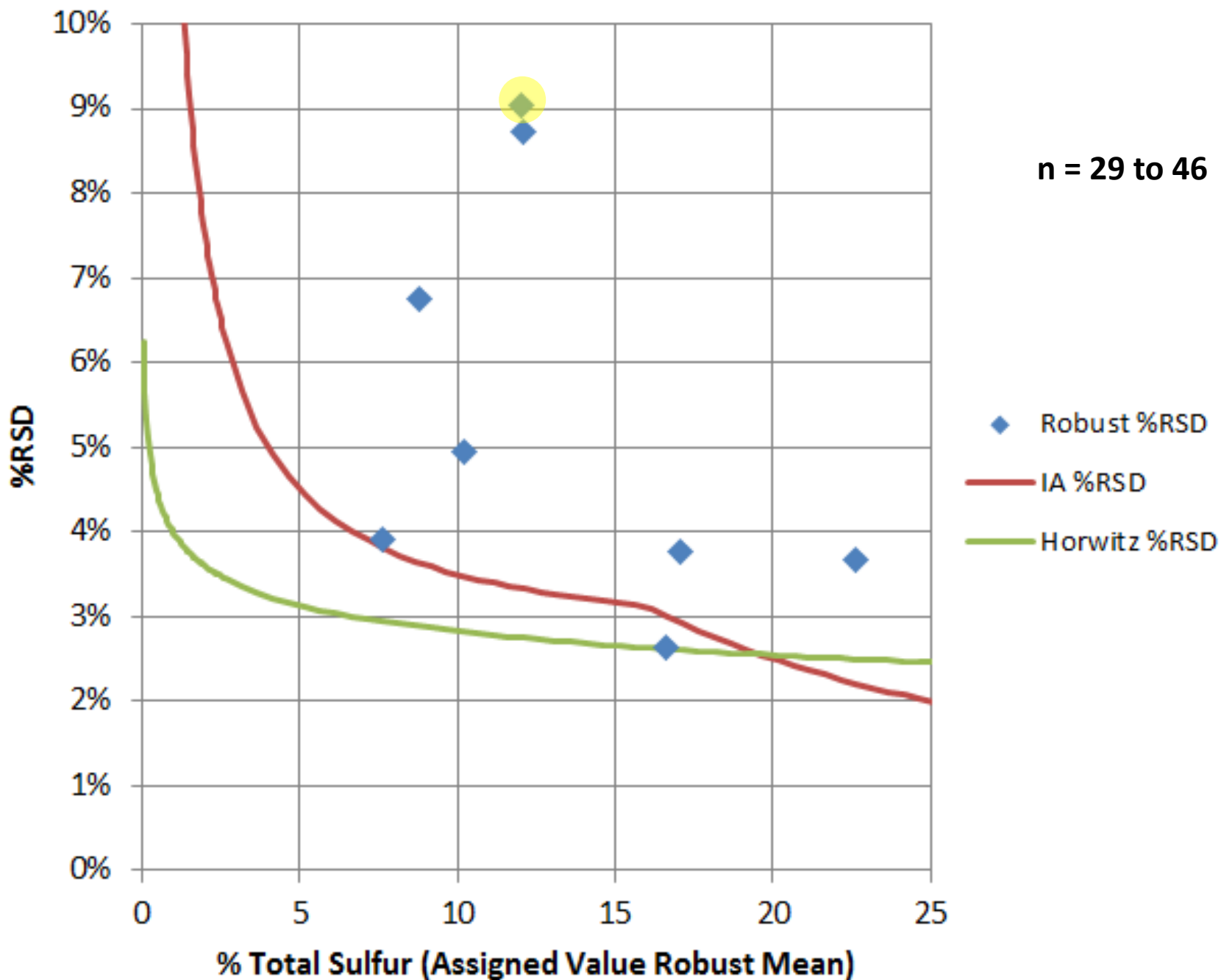
$$\text{RSD}_{\text{Horowitz}} = 2 \times C^{-0.15}$$

$$\text{RSD}_{\text{IA}} = \sqrt{\text{RSD}_{\text{L}}^2 + \text{RSD}_{\text{r}}^2 + \text{RSD}_{\text{prep}}^2 + \text{RSD}_{\text{samp}}^2}$$

$$\text{RSD}_{\text{Robust}} \approx \sqrt{\text{RSD}_{\text{L}}^2}$$







Magruder 160512 Micro Mix

Sulfur (S)* 9.0 %

Combined Sulfur (S)*9.0 %

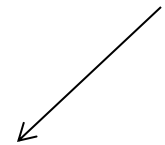
Analyte Group	Analyte (Units)	Lab Code	Lab Data		Method Values			# Tests	Magruder CS Z Score	Your Method	Flag
			Value	Range	Rob Mean	Rob SD	R-bar				
148	Total Sulfur (9%)	0519	9.130*	0.0600	12.10	1.055	0.2261	45	-2.81	148.07	0
148	Total Sulfur (9%)	0117	9.237*	0.0720	12.10	1.055	0.2261	45	-2.71	148.07	0
148	Total Sulfur (9%)	0354	9.721*	0.1640	12.10	1.055	0.2261	45	-2.25	148.99	0
148	Total Sulfur (9%)	0406	10.30*	0.5100	12.10	1.055	0.2261	45	-1.71	148.07	0
148	Total Sulfur (9%)	0486	10.31*	0.2900	12.10	1.055	0.2261	45	-1.70	148.07	0
148	Total Sulfur (9%)	0520	10.82*	0.3400	12.10	1.055	0.2261	45	-1.21	148.01	0
148	Total Sulfur (9%)	0444	10.97*	0.2300	12.10	1.055	0.2261	45	-1.07	148.01	0
148	Total Sulfur (9%)	0231	11.16*	0.0200	12.10	1.055	0.2261	45	-0.89	148.01	0
148	Total Sulfur (9%)	0482	11.20*	0.0000	12.10	1.055	0.2261	45	-0.85	148.99	0
148	Total Sulfur (9%)	0444	11.34	0.1800	12.10	1.055	0.2261	45	-0.72	148.07	0
148	Total Sulfur (9%)	0040	11.40	0.0000	12.10	1.055	0.2261	45	-0.66	148.01	0
148	Total Sulfur (9%)	0102	11.41	0.1230	12.10	1.055	0.2261	45	-0.65	148.01	0
148	Total Sulfur (9%)	0481	11.58	0.0300	12.10	1.055	0.2261	45	-0.49	148.01	0
148	Total Sulfur (9%)	0325	11.65	0.7000	12.10	1.055	0.2261	45	-0.42	148.07	0
148	Total Sulfur (9%)	0506	11.70	0.4000	12.10	1.055	0.2261	45	-0.37	148.99	0
148	Total Sulfur (9%)	0096	11.74	0.1800	12.10	1.055	0.2261	45	-0.34	148.99	0
148	Total Sulfur (9%)	0043	11.77	0.1000	12.10	1.055	0.2261	45	-0.31	148.01	0
148	Total Sulfur (9%)	0485	11.80	0.1700	12.10	1.055	0.2261	45	-0.28	148.01	0
148	Total Sulfur (9%)	0422	11.92	0.3700	12.10	1.055	0.2261	45	-0.17	148.07	0
148	Total Sulfur (9%)	0105	12.04	0.3000	12.10	1.055	0.2261	45	-0.05	148.01	0
148	Total Sulfur (9%)	0095	12.09	0.0400	12.10	1.055	0.2261	45	-0.01	148.01	0
148	Total Sulfur (9%)	0291	12.11	0.0800	12.10	1.055	0.2261	45	0.01	148.99	0
148	Total Sulfur (9%)	0157	12.25	0.1000	12.10	1.055	0.2261	45	0.15	148.01	0
148	Total Sulfur (9%)	0029	12.29	0.0300	12.10	1.055	0.2261	45	0.18	148.01	0
148	Total Sulfur (9%)	0292	12.30	0.0300	12.10	1.055	0.2261	45	0.19	148.07	0
148	Total Sulfur (9%)	0360	12.31	0.6400	12.10	1.055	0.2261	45	0.20	148.00	0
148	Total Sulfur (9%)	0073	12.33	0.5700	12.10	1.055	0.2261	45	0.22	148.01	0
148	Total Sulfur (9%)	0157	12.35	0.3000	12.10	1.055	0.2261	45	0.24	148.00	0
148	Total Sulfur (9%)	0023	12.38	0.6180	12.10	1.055	0.2261	45	0.27	148.07	0
148	Total Sulfur (9%)	0114	12.45	0.2000	12.10	1.055	0.2261	45	0.34	148.01	0
148	Total Sulfur (9%)	0102	12.48	0.0060	12.10	1.055	0.2261	45	0.37	148.07	0
148	Total Sulfur (9%)	0230	12.50	0.2000	12.10	1.055	0.2261	45	0.38	148.01	0
148	Total Sulfur (9%)	0025	12.57	0.1000	12.10	1.055	0.2261	45	0.45	148.00	0

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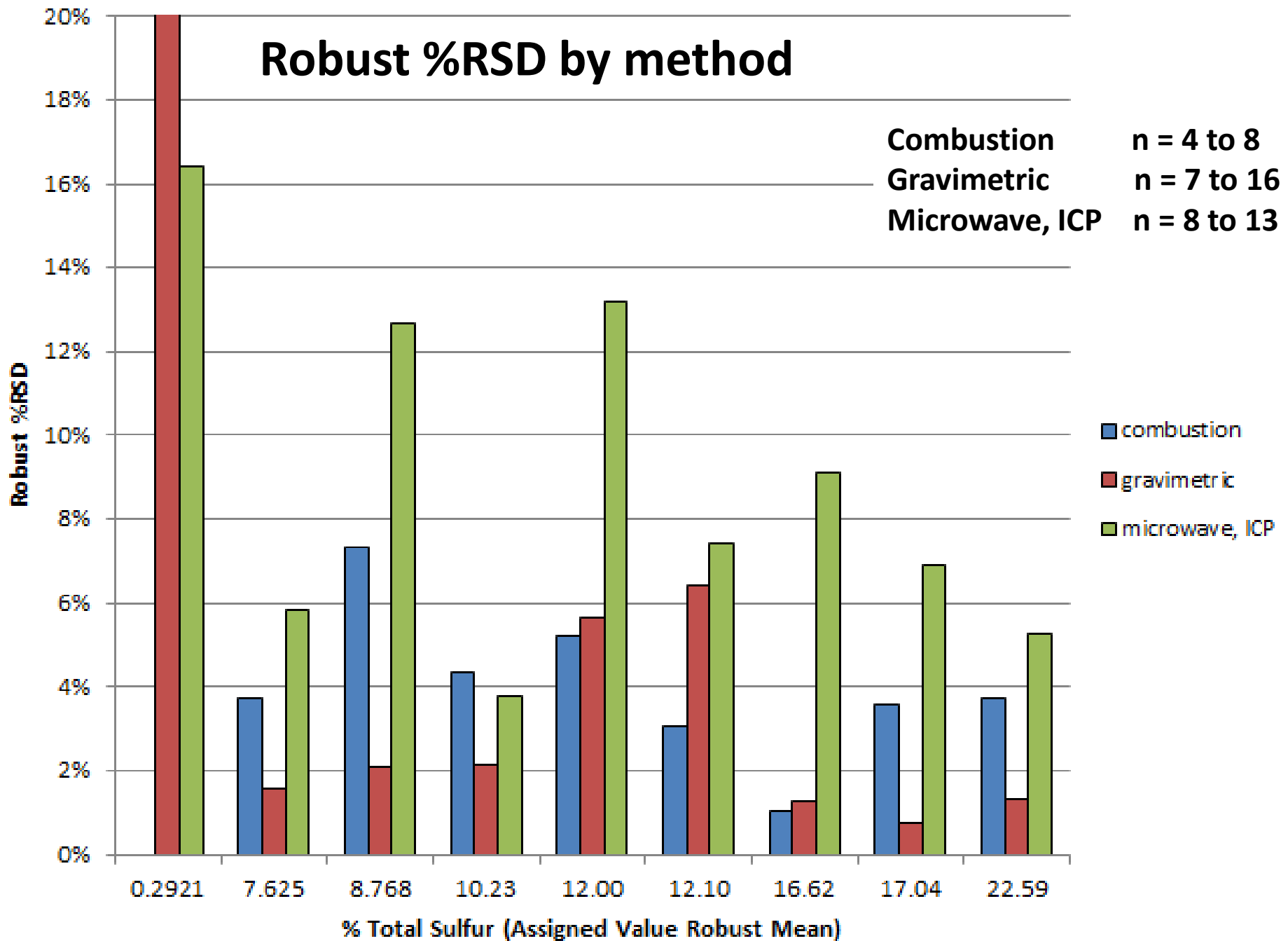
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148	Total Sulfur (9%)	0482	11.20*	0.0000	12.10	1.055	0.2261	45	-0.85	148.99	0



148.01 gravimetric
 148.07 microwave – ICP
 148.99 other

Robust %RSD by method

Combustion n = 4 to 8
Gravimetric n = 7 to 16
Microwave, ICP n = 8 to 13



Within Labs %rsd by method

