Eliminate or accommodate outliers? A comparison between standard and robust approaches for the analysis of collaborative study data

Michael J. Morton

Michael.J.Morton@altria.com
Altria Client Services LLC, Richmond, VA 23219
Center for Research and Technology

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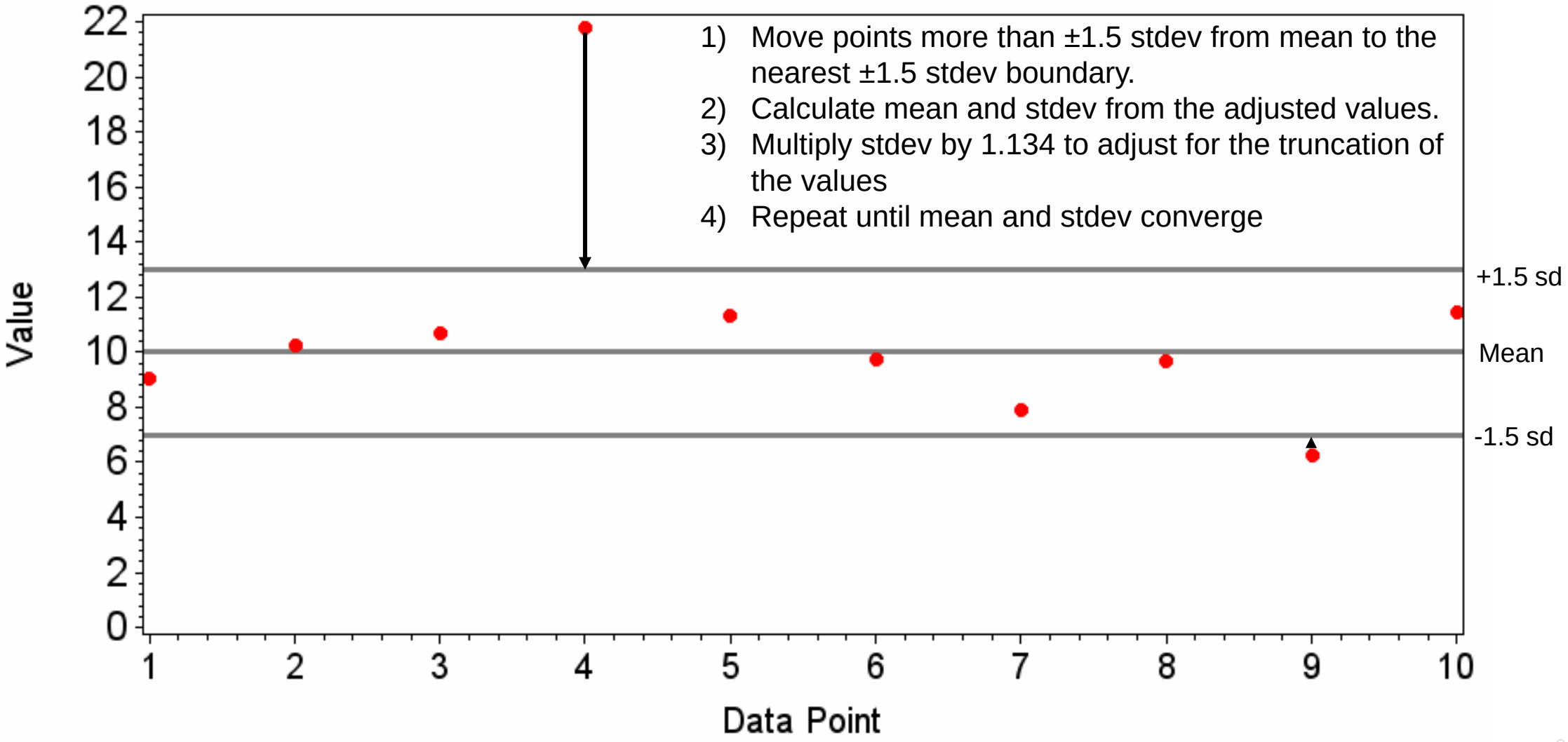
Collaborative Studies

- Collaborative studies are carried out to characterize the consistency of analytical methods both within and between laboratories.
- It is commonplace for there to be occasional outliers – points that are quite different than the remainder of the results and can strongly affect conventional measures of variability.
- The most common approach is to identify those outliers and eliminate them.
  - This is the approach described in ISO 5725-2, though with much latitude in its application.
- An alternative approach is to use robust calculation procedures that are *resistant* to small numbers of outliers.
  - This approach is recommended in ISO 5725-5, and there is less need for latitude in application of the approach.

Robust Estimator (Algorithm A, based on lab means)



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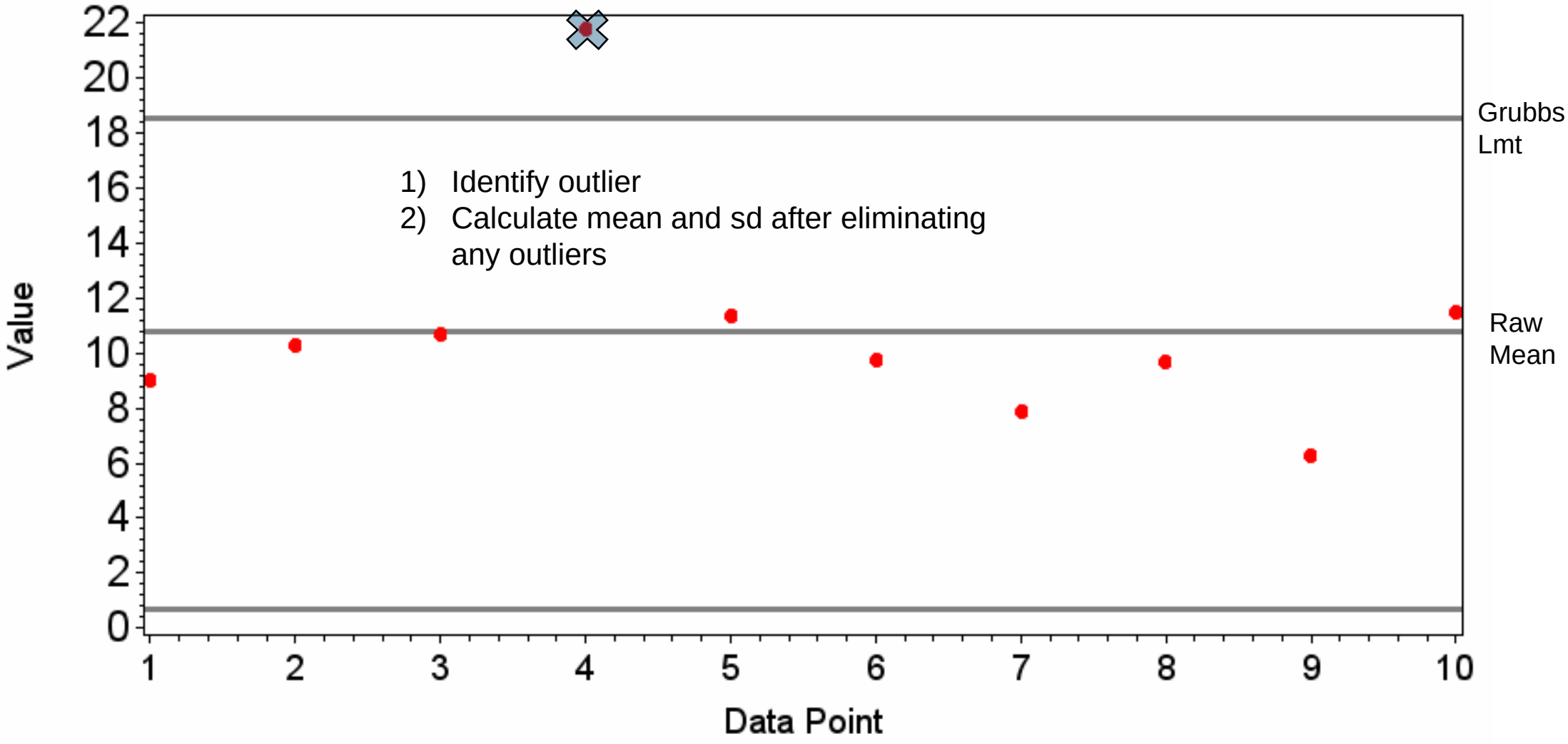
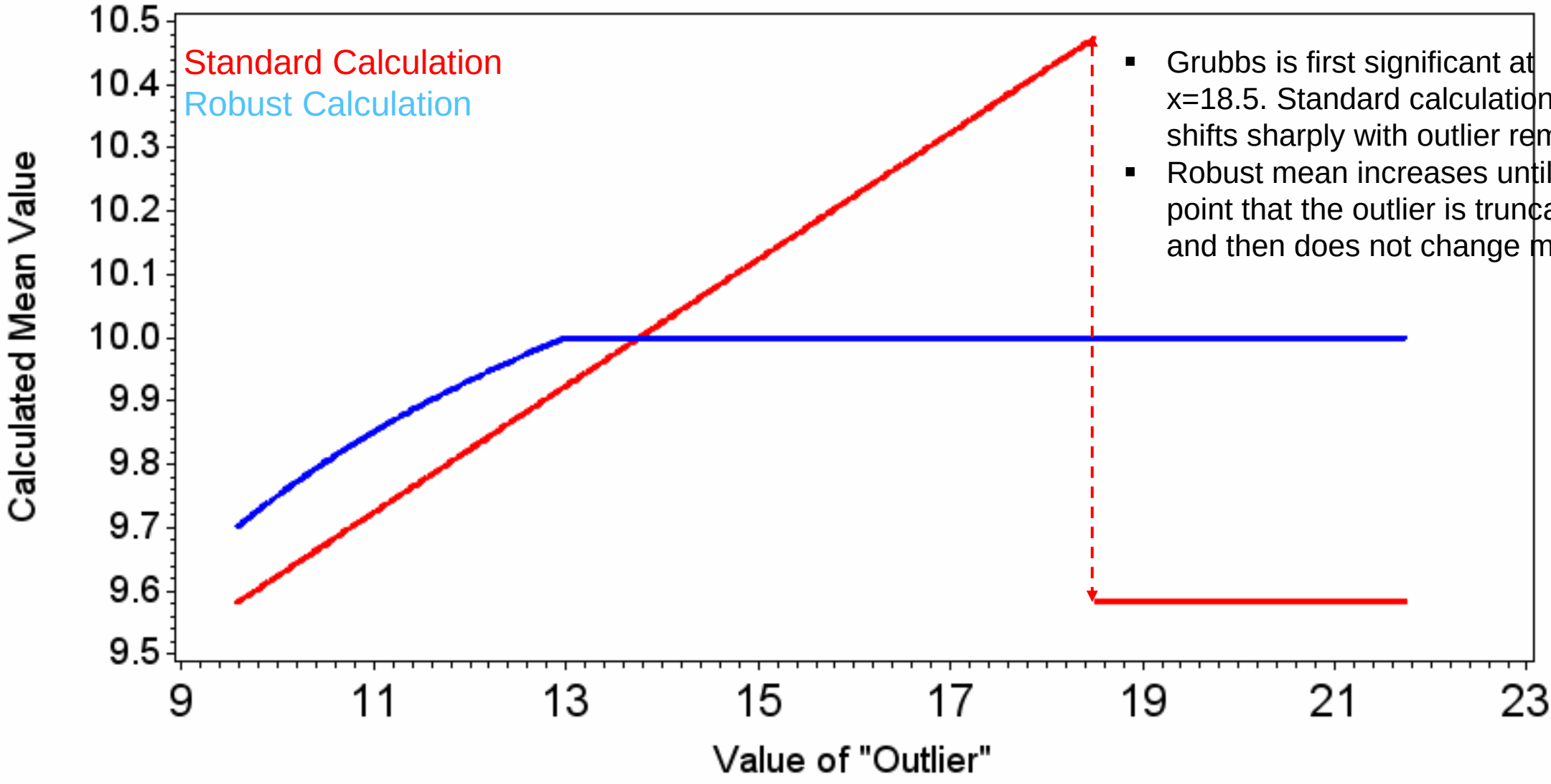
Standard calculation with lab mean outlier removal

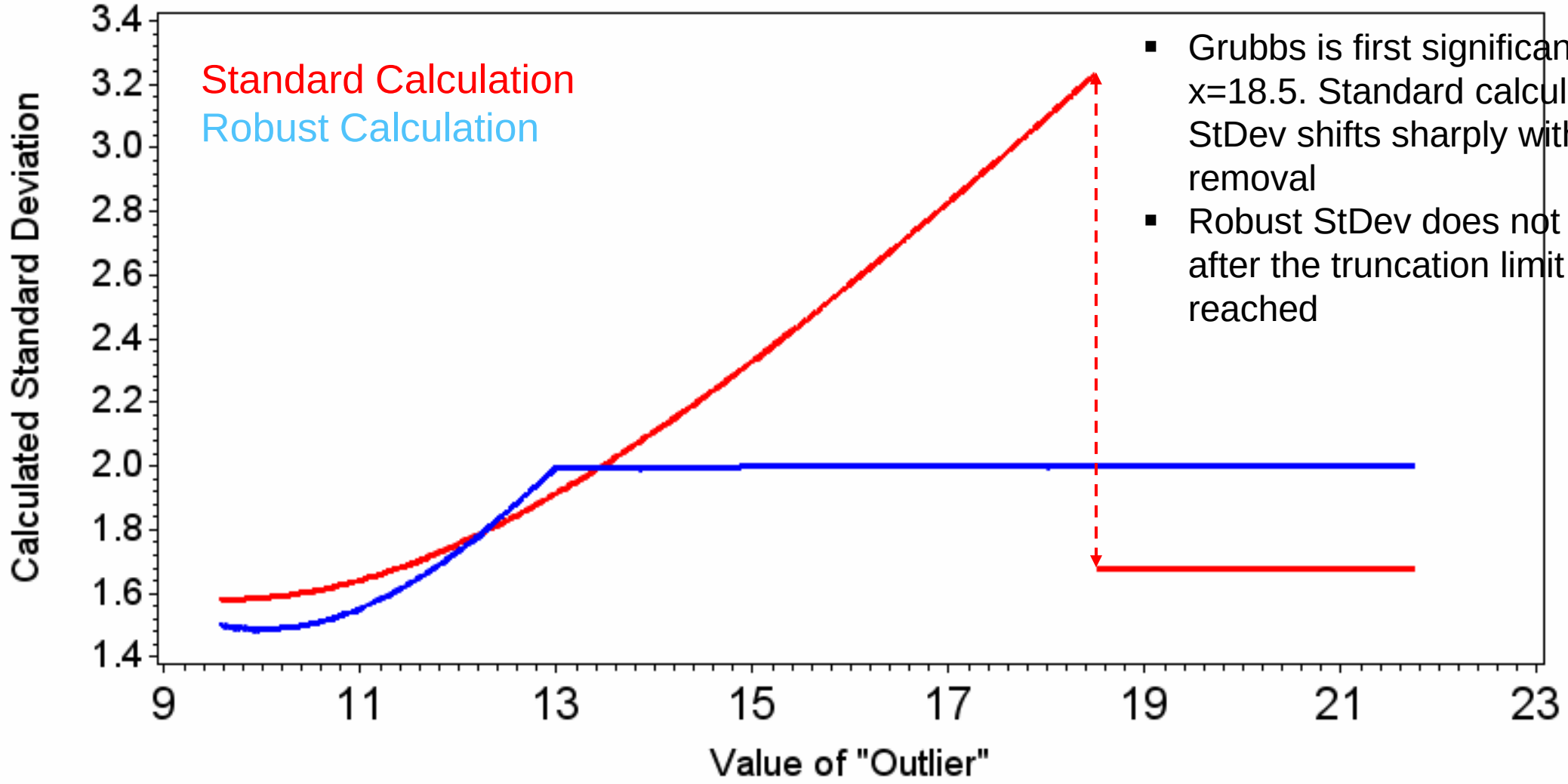


Mean Value Sensitivity



- Grubbs is first significant at x=18.5. Standard calculation mean shifts sharply with outlier removal
- Robust mean increases until the point that the outlier is truncated and then does not change more

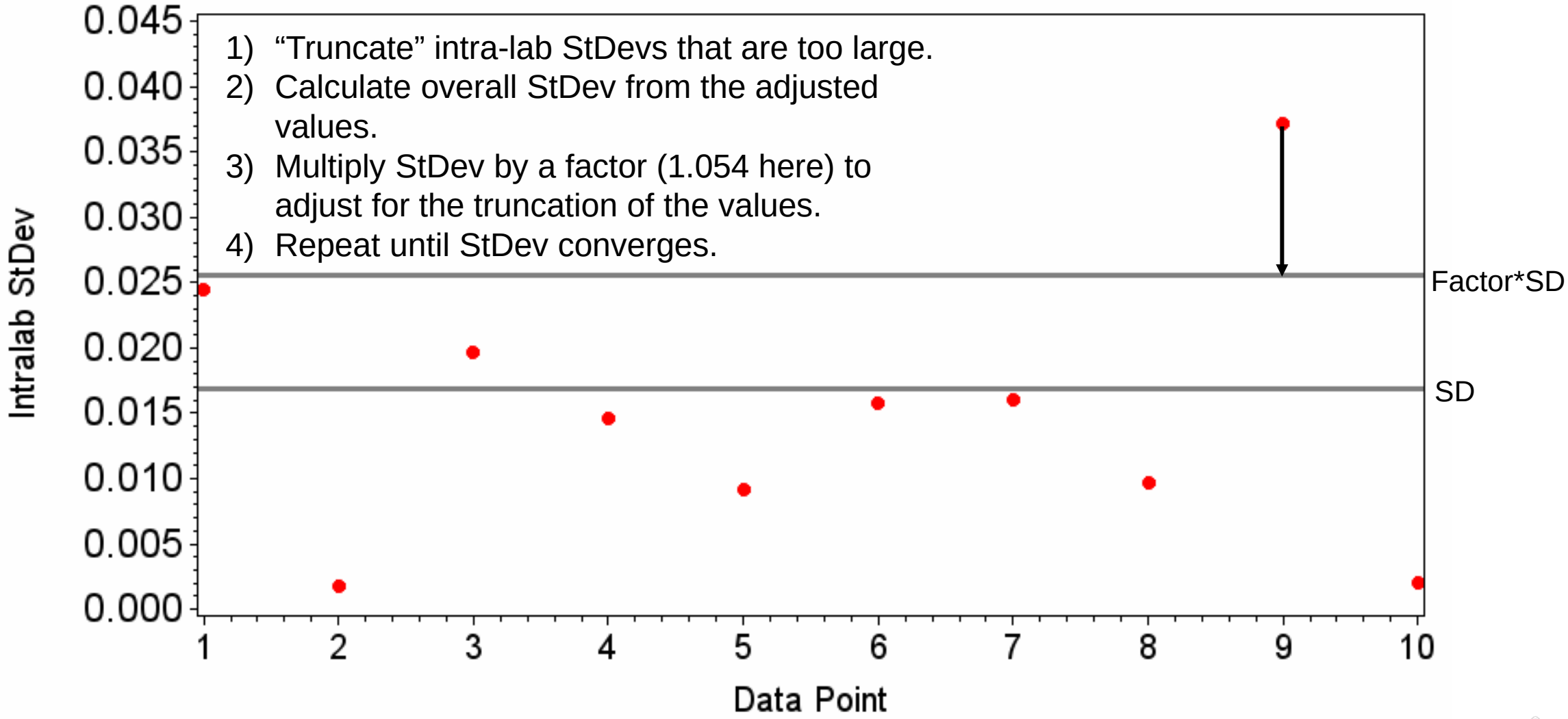
Standard deviation sensitivity



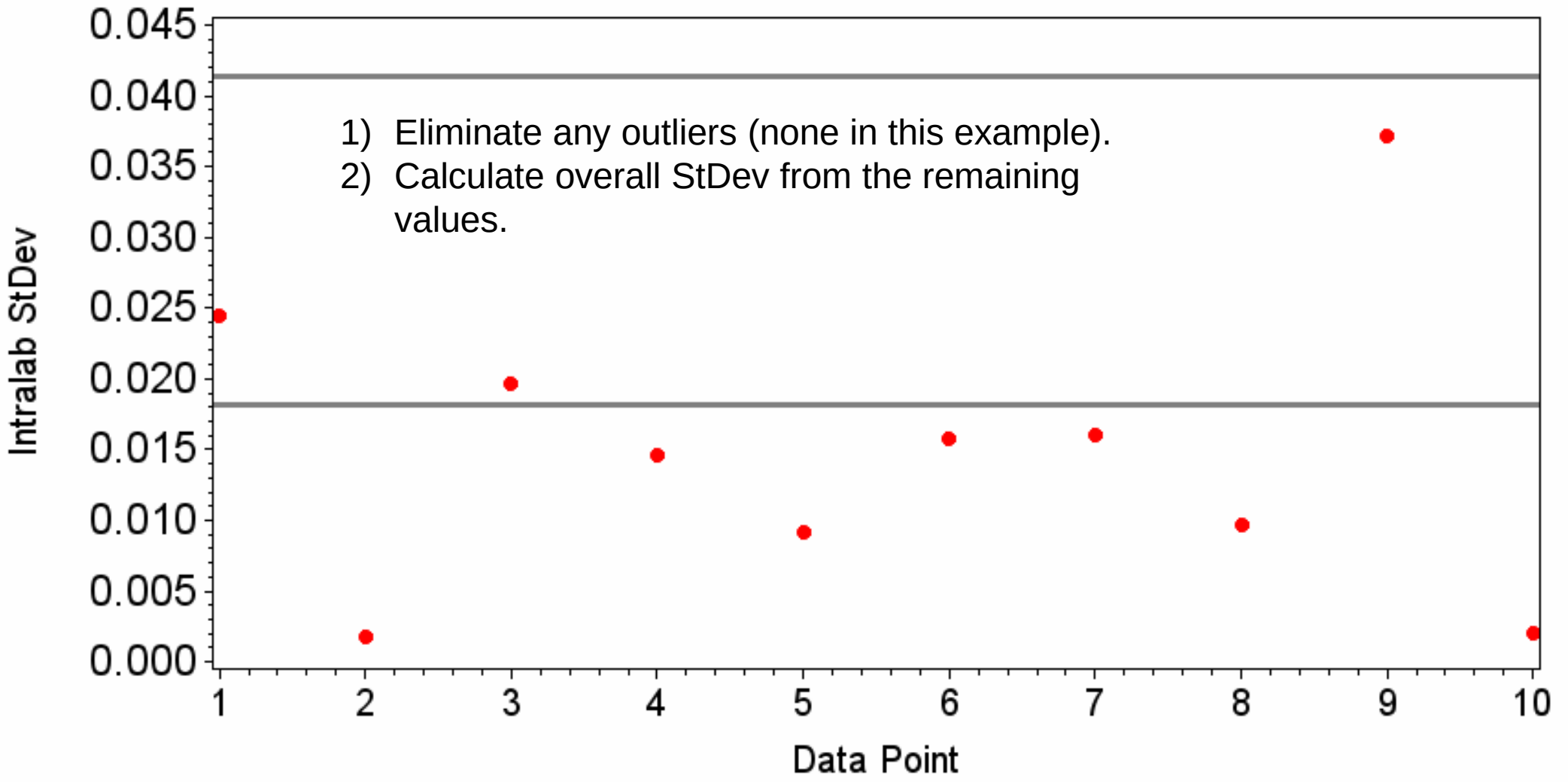
- Grubbs is first significant at x=18.5. Standard calculation StDev shifts sharply with outlier removal
- Robust StDev does not change after the truncation limit is reached

Robust Estimator Intra-lab StDev (Algorithm S)

1) "Truncate" intra-lab StDevs that are too large.
2) Calculate overall StDev from the adjusted values.
3) Multiply StDev by a factor (1.054 here) to adjust for the truncation of the values.
4) Repeat until StDev converges.

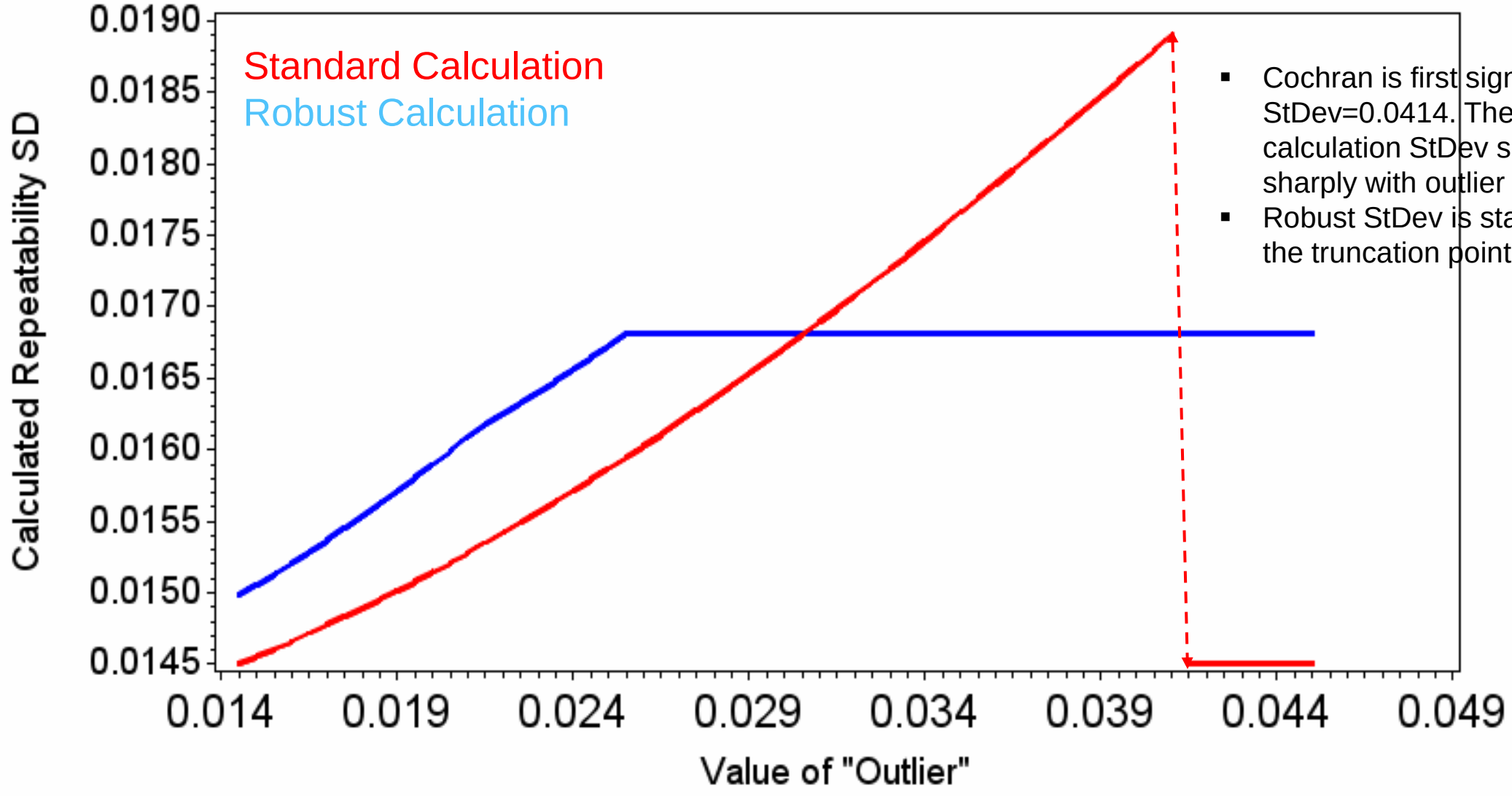


Standard Procedure for Intra-lab StDev



1) Eliminate any outliers (none in this example).
2) Calculate overall StDev from the remaining values.

Repeatability StDev calculation sensitivity

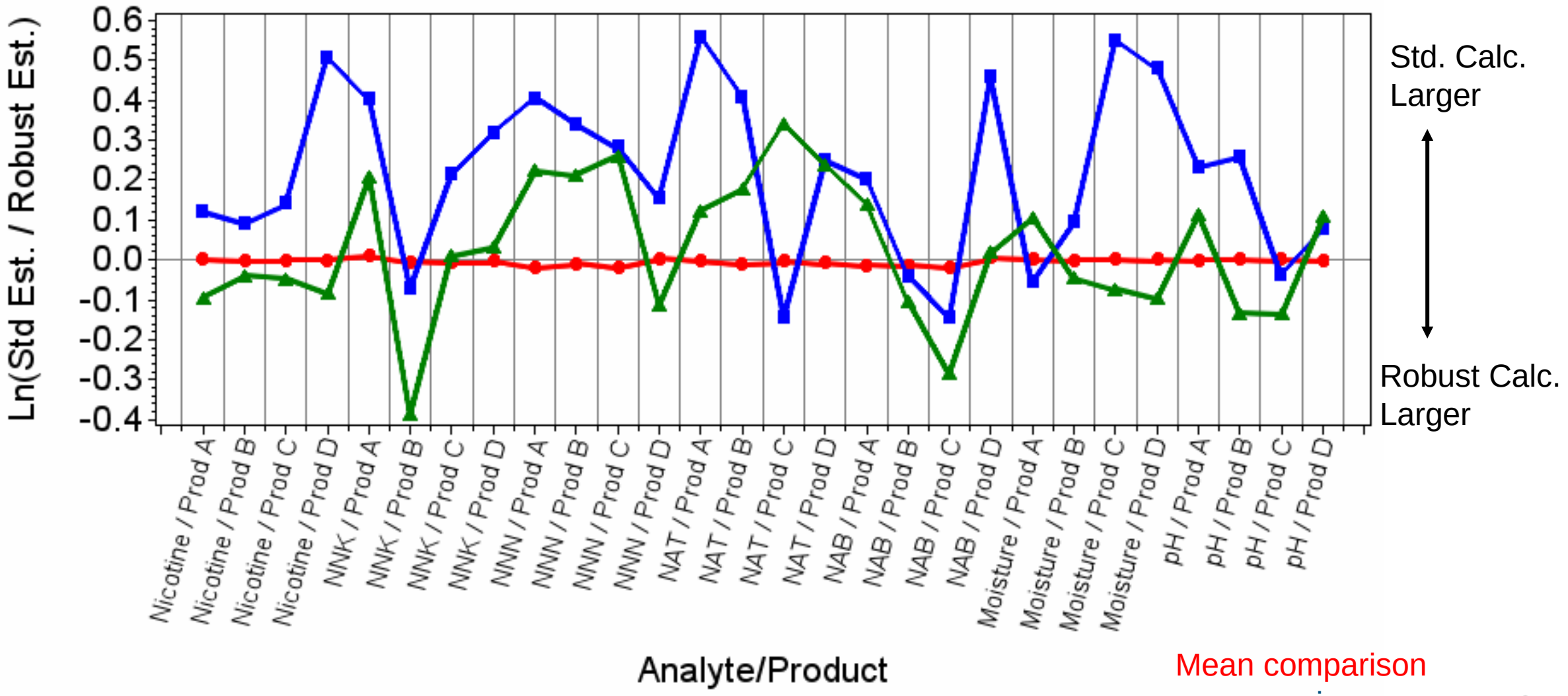


- Cochran is first significant at StDev=0.0414. The standard calculation StDev shifts sharply with outlier removal
- Robust StDev is stable after the truncation point is reached

Comparison of r & R for several data sets

- A collaborative study with 4 products and 7 analytes
- 16 participating labs (not all labs provided data for every analyte)
- r & R using ISO 5725-2 was calculated using Cochran's Test and Grubbs' Test applied iteratively for outlier identification
- r & R using ISO 5725-5 was calculated with no outlier identification using the recommended robust algorithms (Algorithms A and S)

Comparison of Mean, sr, and sR



Mean comparison
sr comparison
sR comparison

Summary of Comparison

- The means were very similar.
- Repeatability standard deviations (sr's) tended to be larger using the standard calculation.
- Reproducibility standard deviations (sR's) differed on individual comparisons, but on average were similar.

Statistical Efficiency of Estimators

- Efficiency is generally compared under ideal circumstances: simulated data set with normality and no outliers.
  - This shows the trade-off between robustness and efficiency when robustness is not necessary.
- Comparison was made using simulation with p=10 simulated labs and nr=3 simulated reps.
- In the simulation, $\mu = 0$, $\sigma_r = 1$, $\sigma_L = \sqrt{3}$, $\sigma_R = \sqrt{\sigma_r^2 + \sigma_L^2} = 2$.
- Efficiency was estimated as the ratio of the standard deviations $\frac{SD\ Standard\ Estimate}{SD\ Robust\ Estimate}$.

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Simulation Results

Parameter	Std. Est. Avg.	Rob. Est. Avg.	Std. Est. SD	Rob. Est. SD	Estd. Eff. of Robust Estimator
Mean	0.00	0.00	0.575	0.583	98.8%
Within Lab SD (sr)	0.99	1.00	0.158	0.170	92.6%
Lab-to-Lab SD (sL)	1.68	1.76	0.457	0.532	85.8%
Reproducibility SD (sR)	1.97	2.05	0.389	0.455	85.6%

- There is very little loss of efficiency in the mean value estimator.
- There is a small efficiency loss (~7% within lab and ~14% between labs) with the robust estimators of the standard deviations and a small offset in the estimated between laboratory standard deviations.

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Summary

- The robust estimation procedure for the analysis of collaborative studies (ISO 5725-5) provides a good alternative to the standard procedure (ISO 5725-2).
  - The results do not show large discontinuities and are less dependent on analyst choices.
  - A comparison shows generally similar results (on average).
  - The efficiency loss is acceptable using the robust estimation procedure.

Thank you

Questions?

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Michael.J.Morton@altria.com