The median scaled difference:

An outlier-resistant indicator of anomalies for inter-laboratory data with reported uncertainties

Stephen L R Ellison

LGC Limited, Queens Road, Teddington, Middlesex TW11 0LY

Introduction

When inter-laboratory studies return data with different uncertainties, it is hard to determine whether a given point is anomalous given its associated uncertainty. Difference from an estimate helps but results depend – sometimes strongly - on the particular estimator chosen, and multiple outliers 'mask' one another.

This paper introduces the median scaled difference, a simple-to-calculate indicator that does not depend on choice of estimator, is effective for detecting anomalous value/uncertainty points, and that is resistant to multiple outlying values

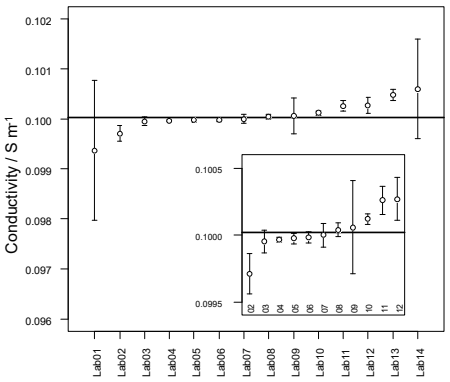
Using pairwise comparison

Dependence on a particular location estimator can be removed by focusing on pairwise differences; a lab that consistently disagrees with most other labs is worth further investigation.
A pairwise chi-squared statistic [1] achieves this but is badly affected by outlying values [2].
A median of scaled differences (MSD), defined as

$$\mathrm{MSD}_i = \underset{j,l\neq j}{\mathrm{med}}\left(\frac{|x_i - x_j|}{u(x_i - x_j)}\right)$$

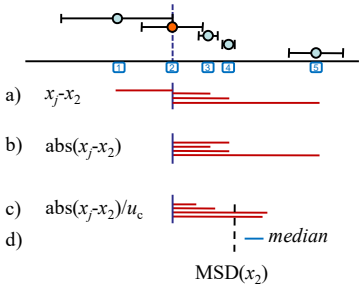
combines the estimator-independence of pairwise comparisons with the very strong outlier resistance of a median.

Figure 1 – Example



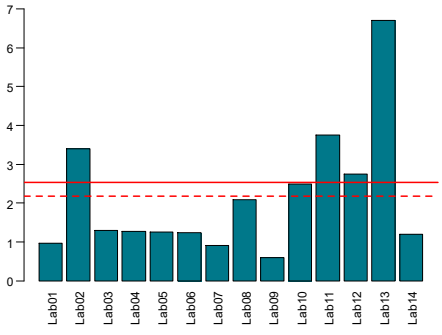
Data from CCQM-P022 - conductivity. Error bars show expanded uncertainty. The horizontal line is the median.

Figure 2 – Calculating the MSD



The MSD is calculated for a data point (point 2, above) by a) taking differences for each other point; b) taking the absolute value, c) dividing each by the uncertainty of the difference (which can include covariance) and d) taking the median of these scaled absolute differences

Figure 3 – Calculated MSD for CCQM-P022



Calculated MSD values for all labs in CCQM-P02. The solid horizontal red line is the upper 99% critical value for a single lab (roughly 2.5 in this case).

Example

Figure 1 shows data from CCQM-P022, an early conductivity study. Ordinary outlier tests might identify Lab01 as extreme. However, Lab01 clearly agrees well with all other results after considering the reported uncertainty.

The inset shows that Lab02 agrees with far fewer labs once uncertainties are considered, with labs 11 and 12 also far from the median line.

Other estimators would potentially show different values as "extreme"; for example, Lab04 is far from the median compared to Lab 4's uncertainty, but would be very close to a weighted mean.

Interpretation

The distribution for the MSD has been established for the equal uncertainty case. As a guide for whole data set inspection:

MSD > 2.5 indicates an anomalous value/uncertainty pair.

For more exact inference, critical values are available [2]. Figure 3 compares calculated values with critical values.

Unequal uncertainties

The guidelines above work well but for the more important case of very different uncertainties, which require different critical values for each data point, a simulation approach is recommended [2].

What has the MSD told us?

In this case, the calculated MSD values (Figure 3) tell us:

- The most extreme values in Figure 1 are **not** anomalous compared to their uncertainties
- Lab 13 **does** disagree substantially with a majority of other labs; it is a high value with small uncertainty.
- Labs 2, and 10-12 also merit investigation.

Individual critical values from simulation support these quick conclusions, but also show that lab 4's small uncertainty could be worth investigation despite the relatively central location [2].

Conclusions

- The MSD is a simple and powerful indicator of location/uncertainty anomalies in interlaboratory data with uncertainties.
- The MSD can be calculated without first choosing a particular location estimate ("KCRV").
- Performance evaluation [2] shows that individual MSD values are not strongly influenced by other anomalous results

A complete software implementation of the MSD calculations, including critical values, is available [3]

References

1. Douglas RJ, Steele AG: Pair-difference chi-squared statistics for Key Comparisons. *Metrologia* 2005, **43**, 89-97
2. Ellison, SLR: An outlier-resistant indicator of anomalies among inter-laboratory comparison data with associated uncertainty. *Metrologia* 2018, **55**, 840-854
3. Ellison, SLR: metRology: Support for Metrological Applications. R package version 0.9-29-1. https://r-forge.r-project.org/projects/metrology/