Beyond the dot-and-bar plot: Graphical methods for interlaboratory data analysis

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LGC Teddington

Why use graphical methods?

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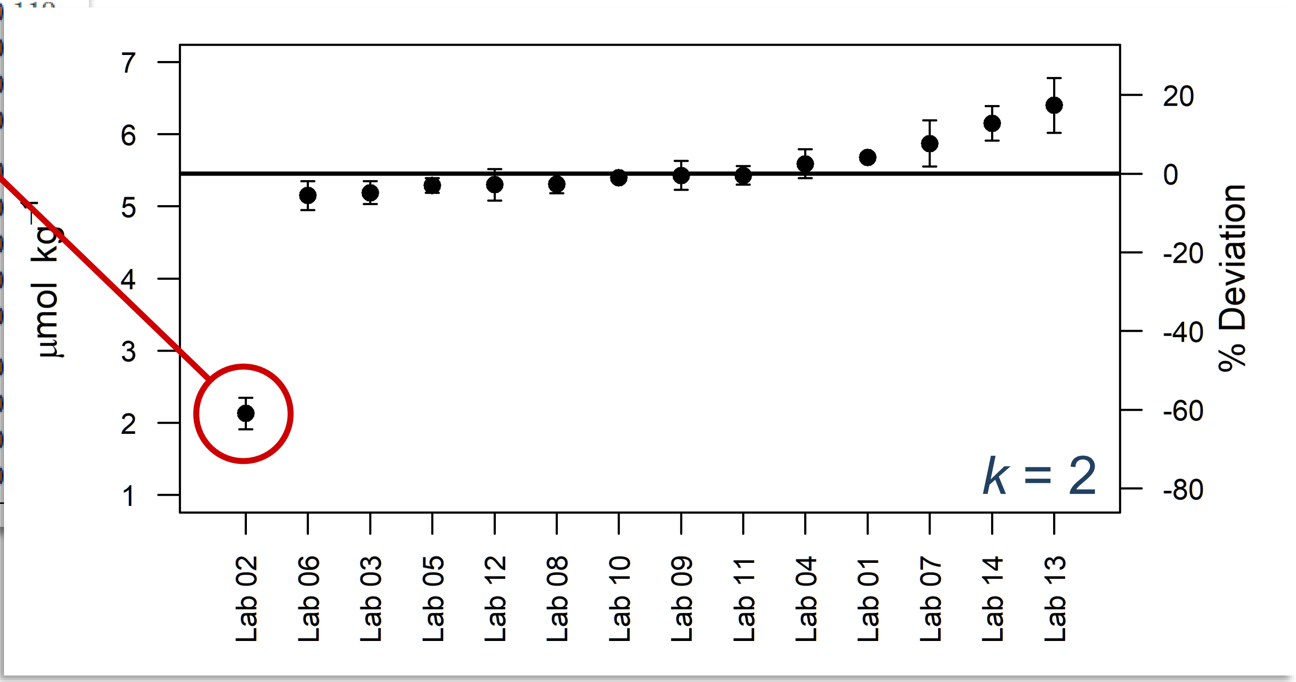
Institute	x / µmol kg^{-1}	u / µmol kg^{-1}
Lab01	5.681	0.029
Lab02	2.130	[illegible]
Lab03	5.190	[illegible]
Lab04	5.590	[illegible]
Lab05	5.290	[illegible]
Lab06	5.150	[illegible]
Lab07	5.870	[illegible]
Lab08	5.310	[illegible]
Lab09	5.430	[illegible]
Lab10	5.397	[illegible]
Lab11	5.430	[illegible]
Lab12	5.300	[illegible]
Lab13	6.400	[illegible]
Lab14	6.150	[illegible]

CCQM-K13
Cadmium in sediment



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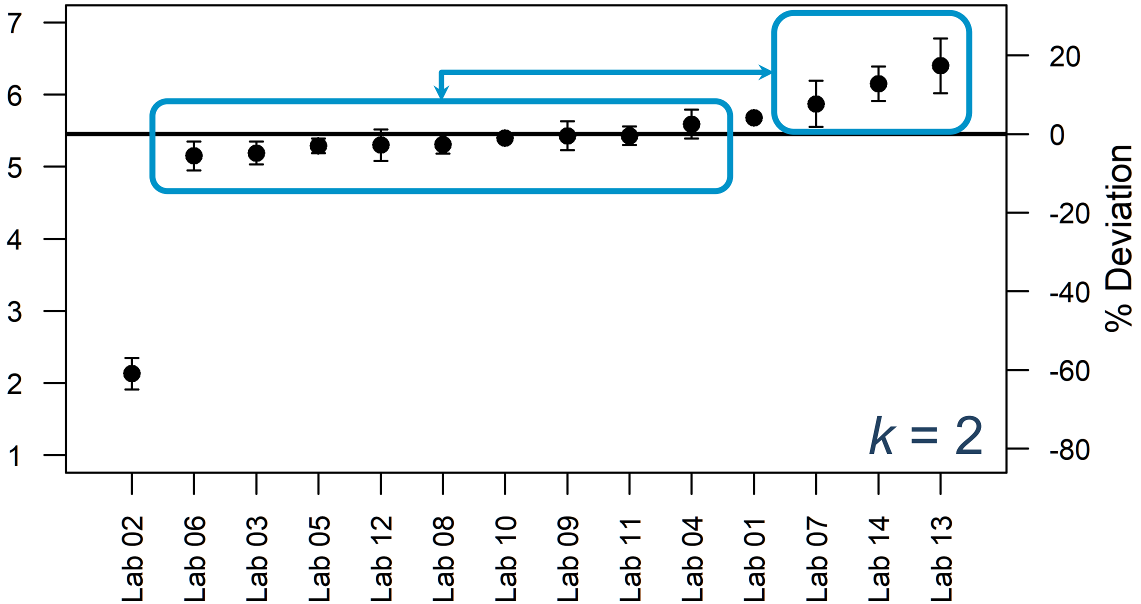

CCQM-K13
Cadmium in sediment

The purpose of visualisation is insight, not pictures

– Ben A Shneiderman

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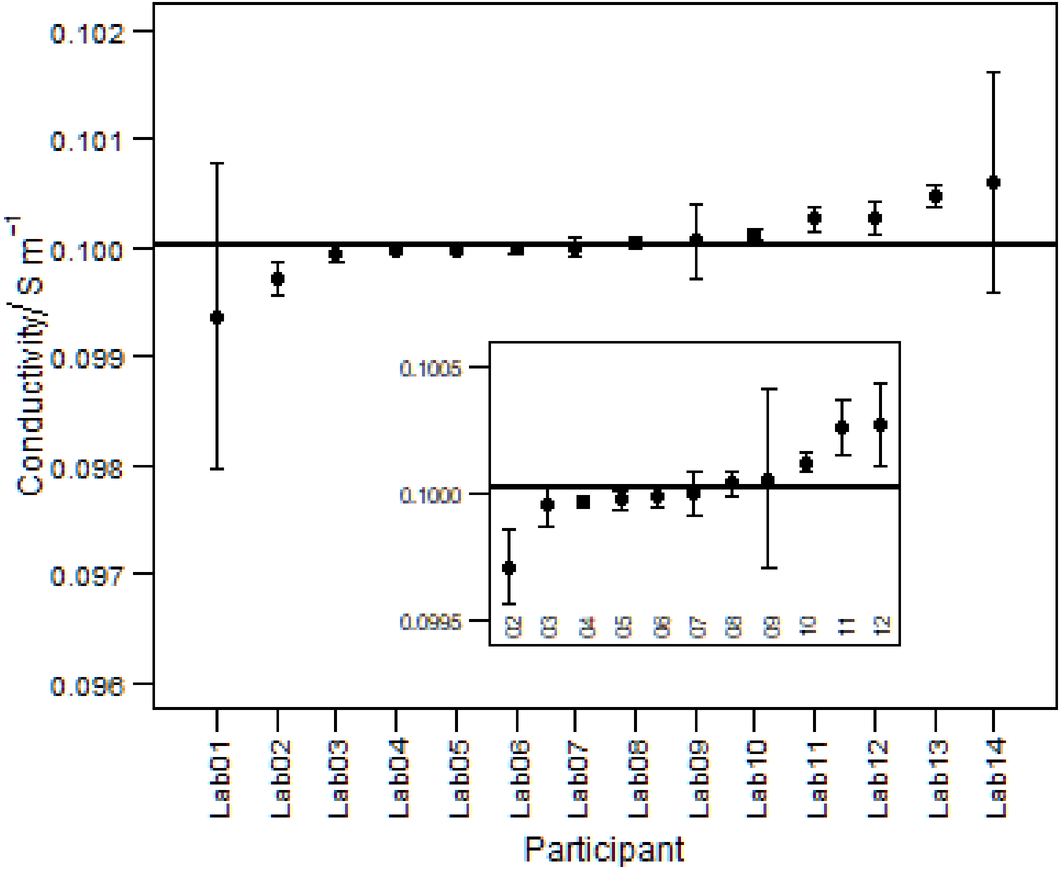
The dot-and-bar plot

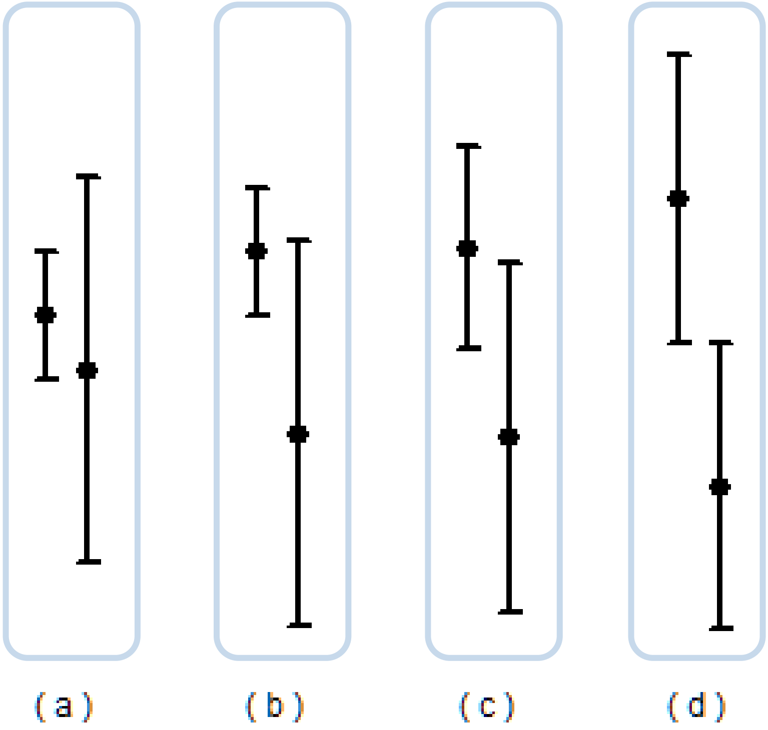
The dot-and-bar plot



Conductivity results from CCQM-P22, on conductivity of standard buffer solutions.

Error bars show expanded uncertainties at *k* = 2.

Inference from dot and bar plots
i) Interpreting overlap



All bars at 95% confidence

a) Both points within others' interval;

b) One point within another's interval:

Never significant at 95% level

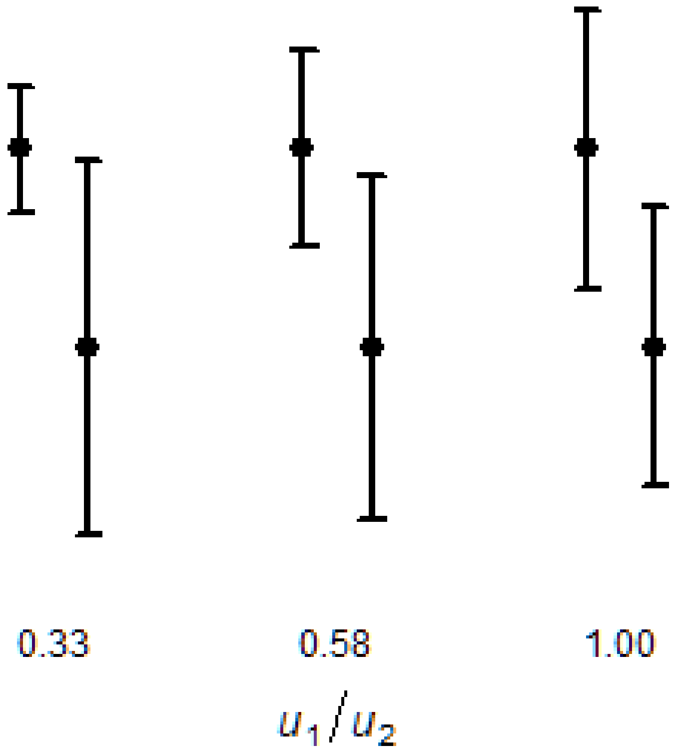
c) Partial overlap

No simple interpretation

d) 95% bars in contact

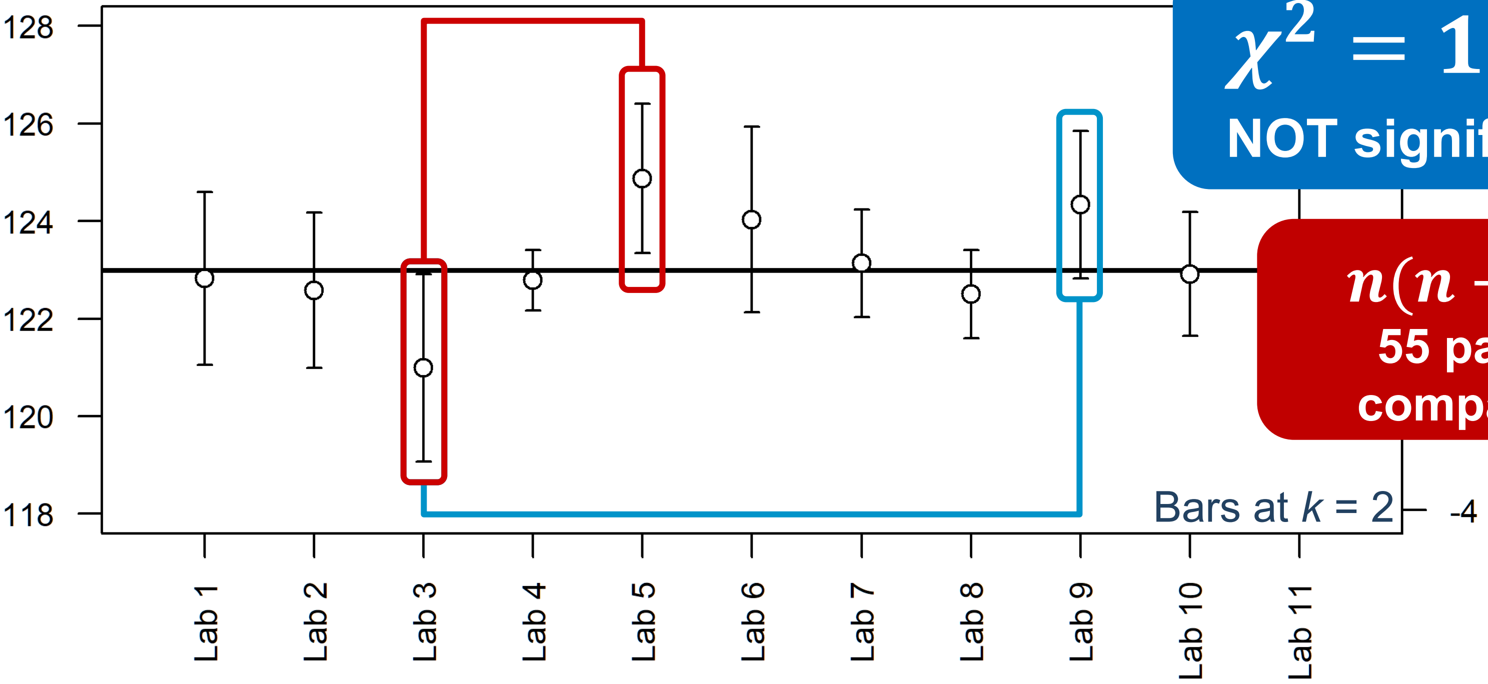
Significant at c. 99% level

Inference from dot and bar plots
ii) Overlap and significance



All pairs show significant difference at exactly 95% confidence

Inference from dot and bar plots
iii) Multiple comparisons



$$\chi^2 = 16.9$$

NOT significant

$$n(n-1)/2$$

55 pairwise comparisons

Dot-and-bar plots
summarise well
but are
easy to misinterpret

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Other graphical tools

1. With a reliable reference value

Example data set: CCQM K13 Cadmium in a sediment

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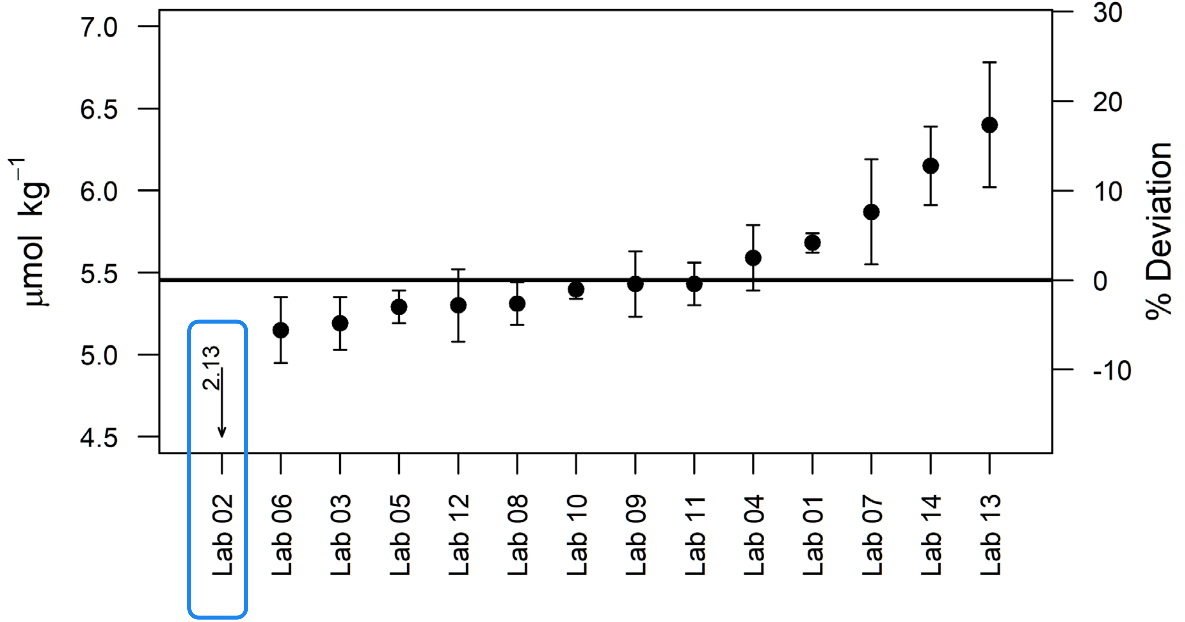
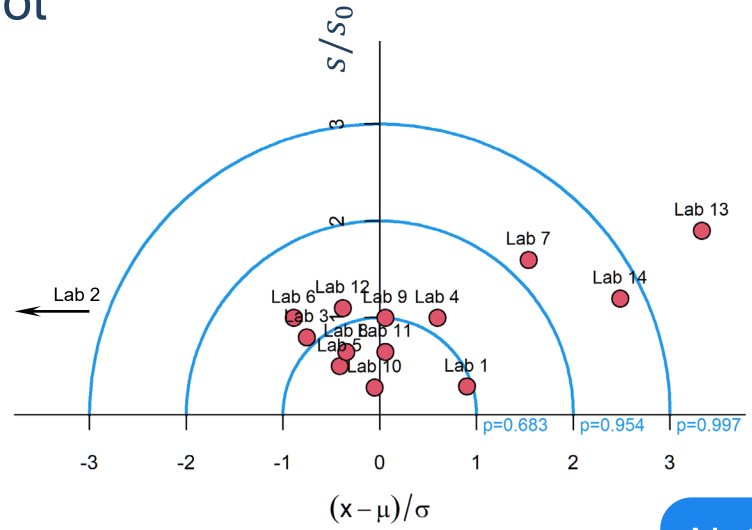


Extreme value off scale

Separating value and uncertainty - a common theme

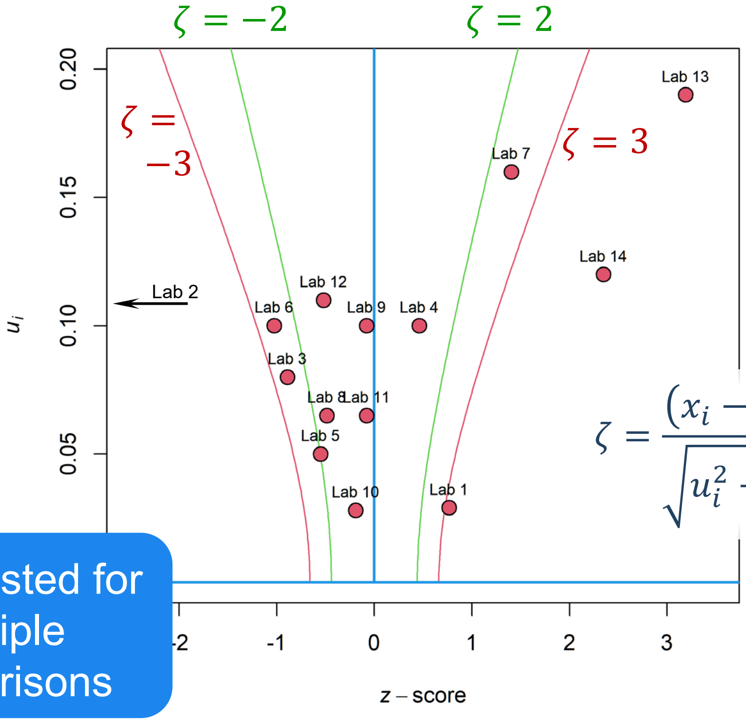
Duewer concordance/precision plot



Uncertainty

Value

Naji 2 plot



$$\zeta = \frac{(x_i - x_{ref})}{\sqrt{u_i^2 + u_{ref}^2}}$$

Not adjusted for multiple comparisons

Additional graphical tools

2. Without a reliable reference value

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Pairwise comparisons don’t need a reference value

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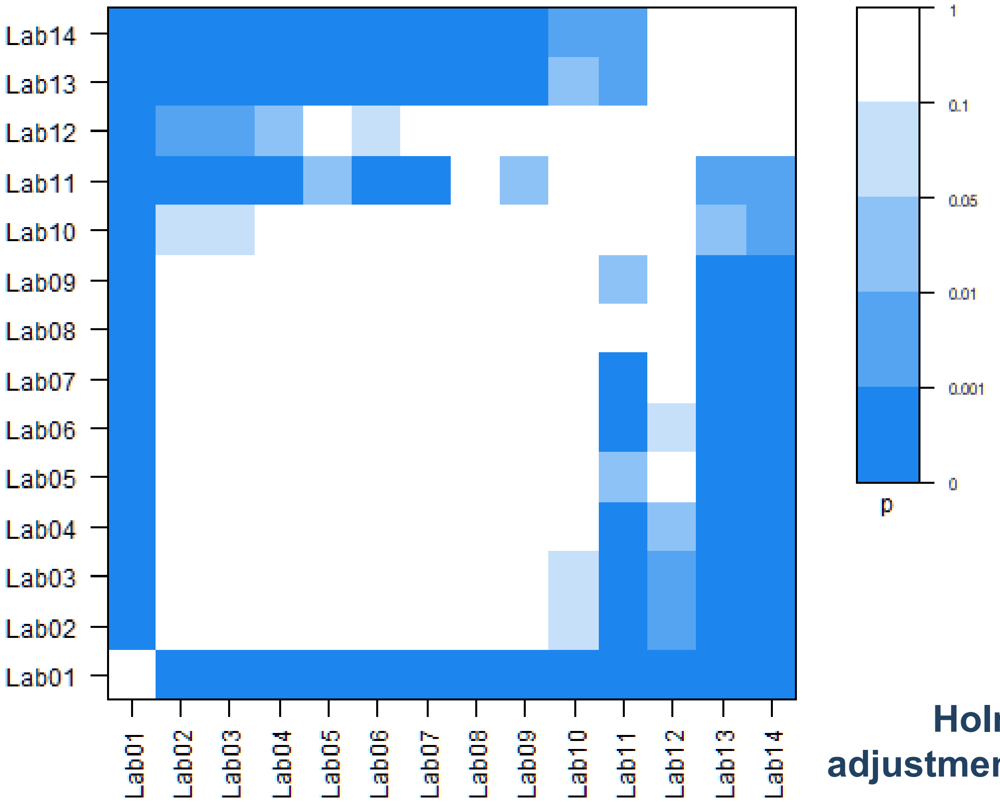
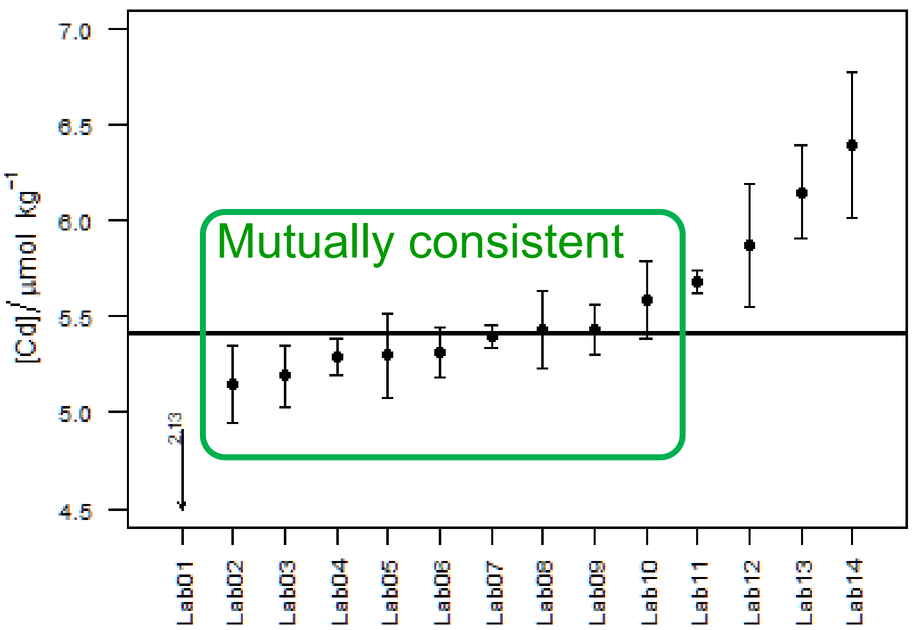
"Consistency plots" – a pairwise summary

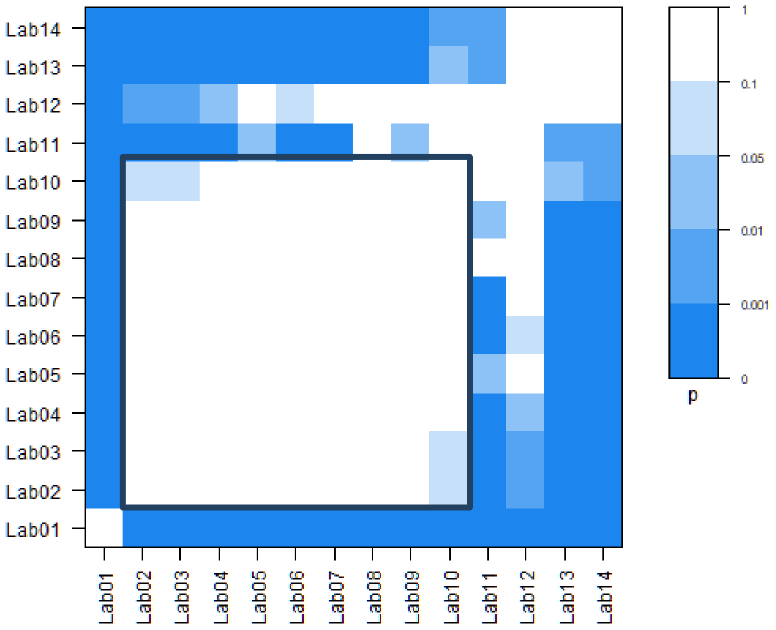
1. Calculate z_{ij} for pairwise differences
$$z_{ij} = \frac{|x_i - x_j|}{u(x_i - x_j)}$$
2. Determine probability (*z*- or *t*-test)
3. Adjust for multiple comparisons
4. Plot as pairwise display



Holm adjustment

“Consistency plots” – interpretation





“Consistency plots” – interpretation

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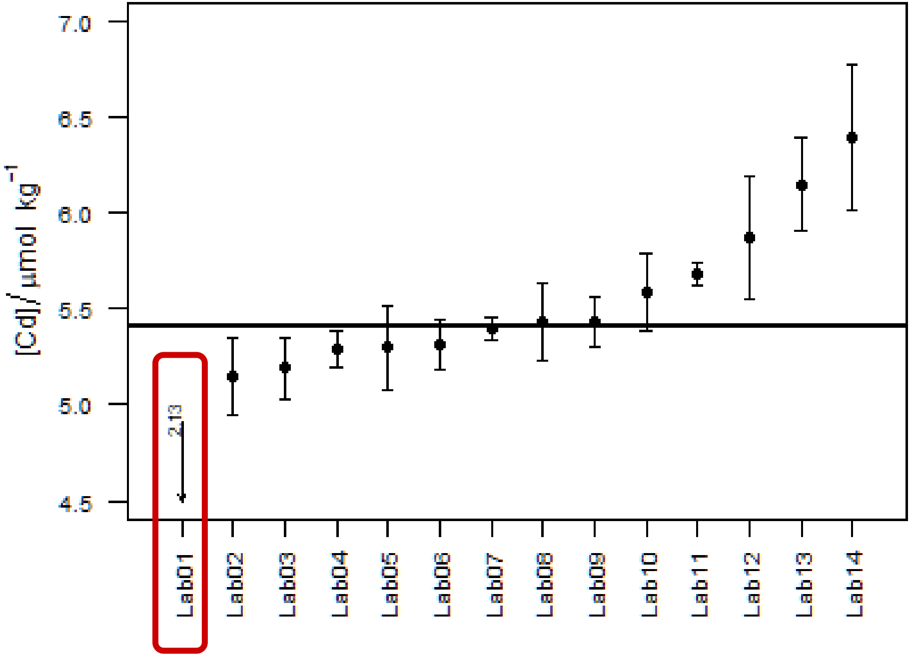
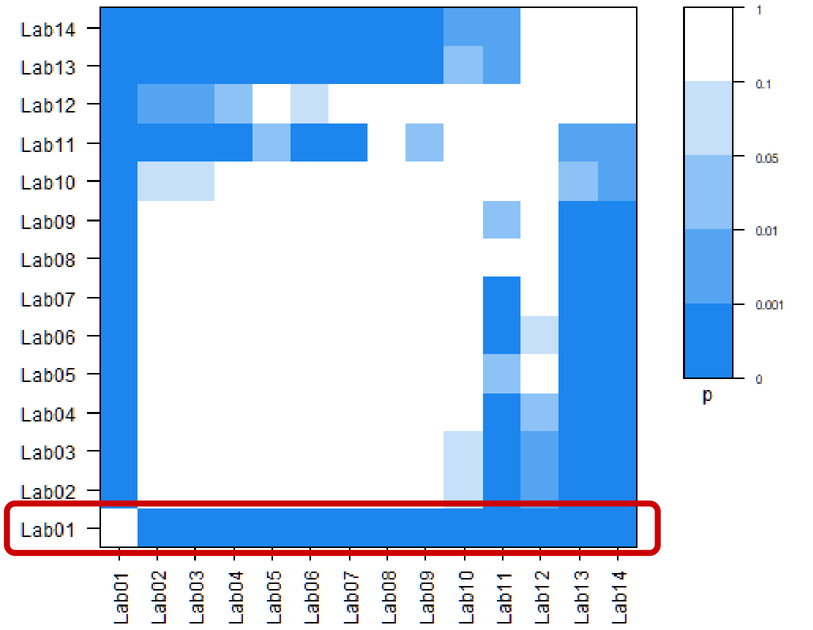
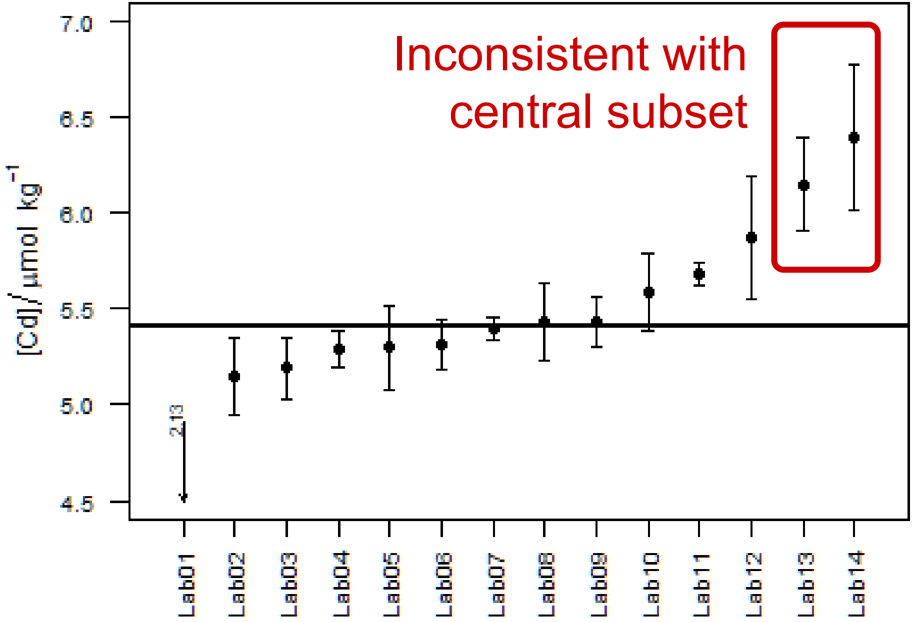


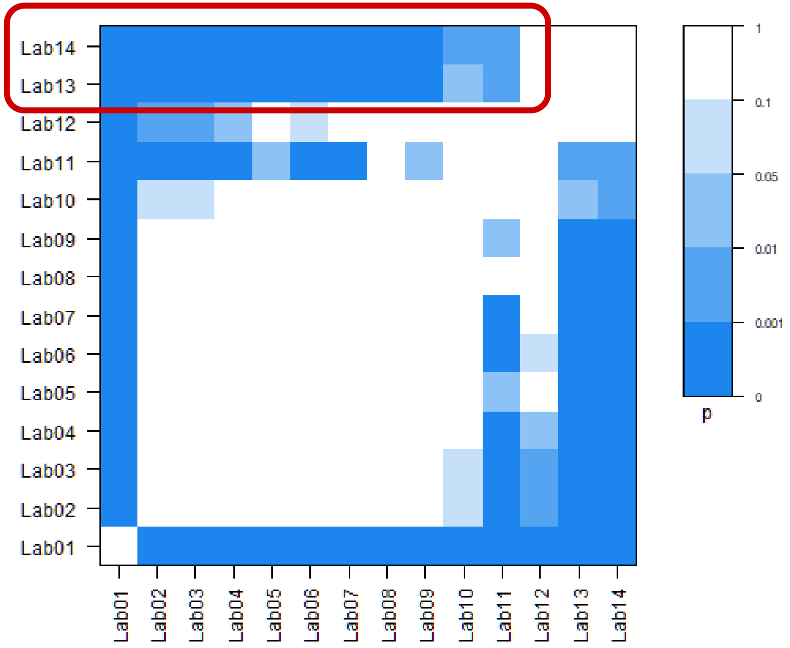


Extreme outlier

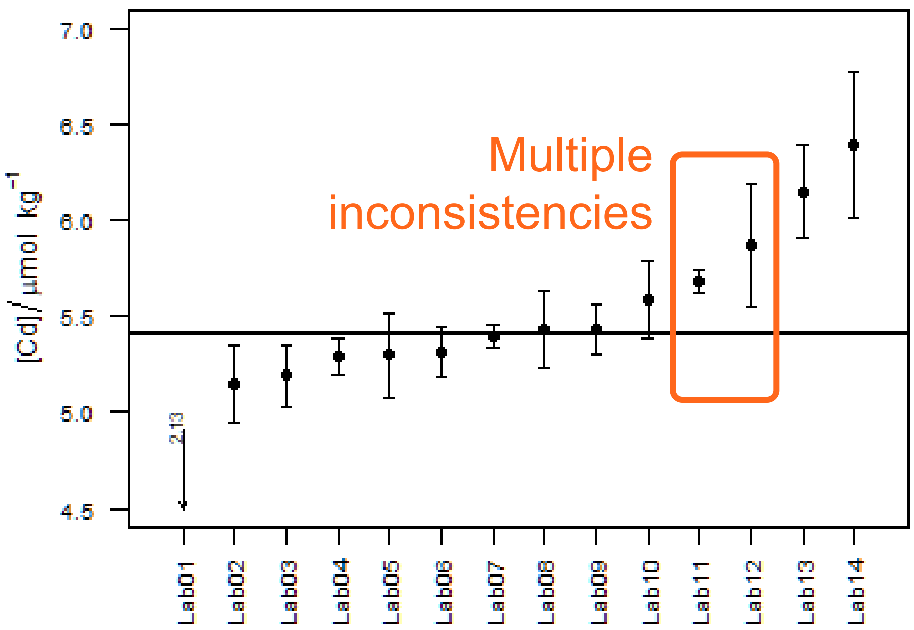
LGC

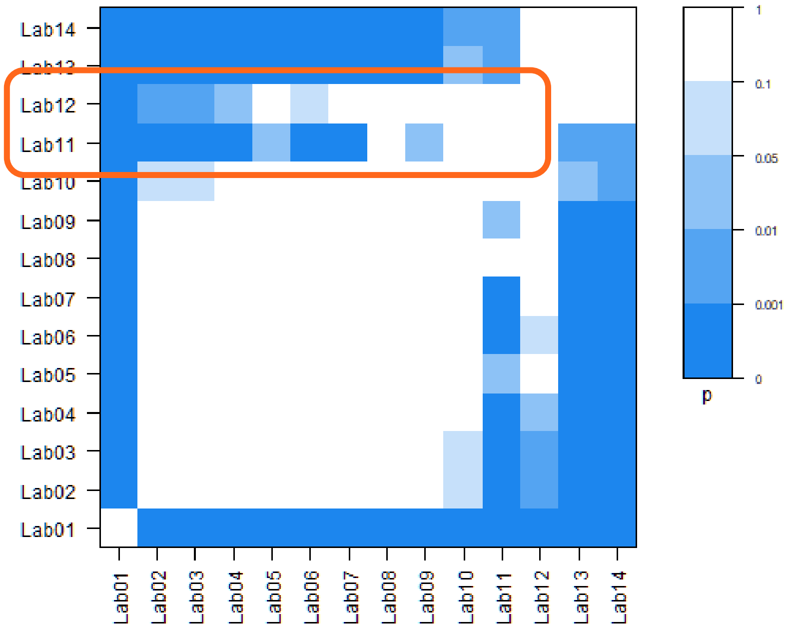
"Consistency plots" – interpretation





"Consistency plots" – interpretation

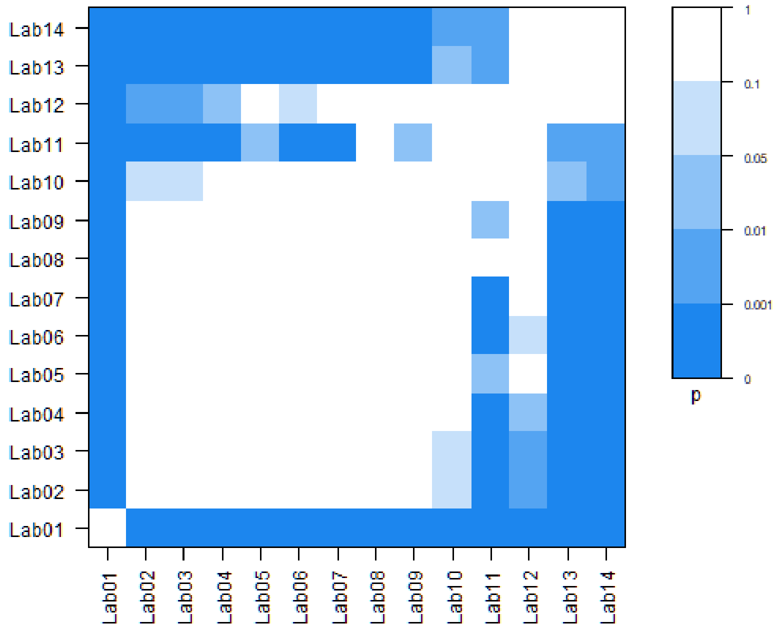




"Consistency plots" – Pros and cons

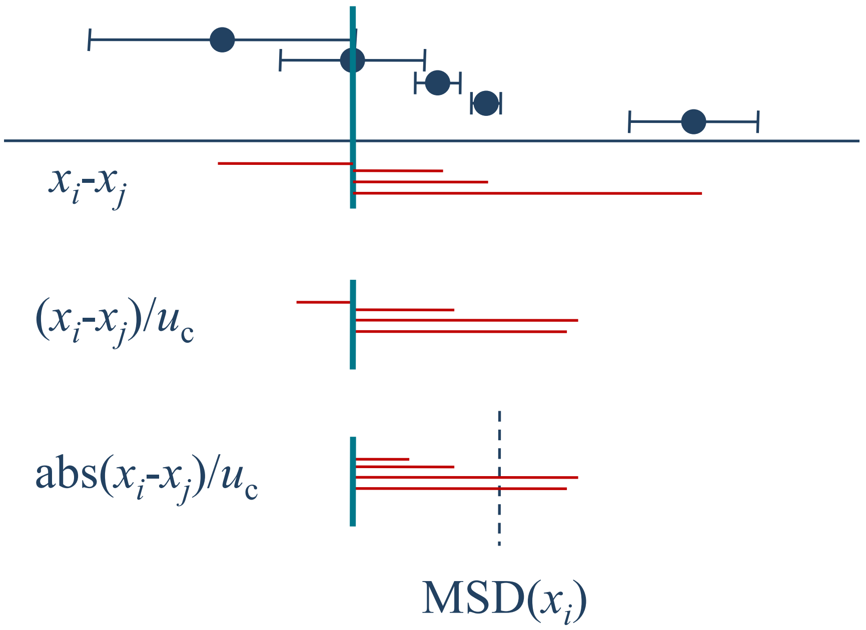
- **Pro**
  - Not reliant on a particular estimator
  - High information content
  - Unambiguous interpretation
    - Adjusted p-values correct for implicit multiple comparisons
  - Relatively easy to explain

- **Con**
  - Adjustment method is a choice
    - Strong adjustment reduces power
  - Not a 'summary'

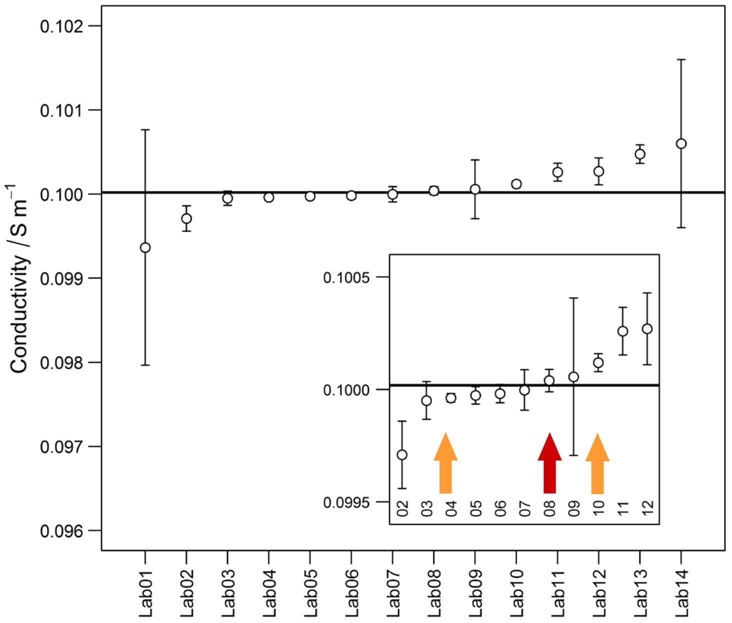


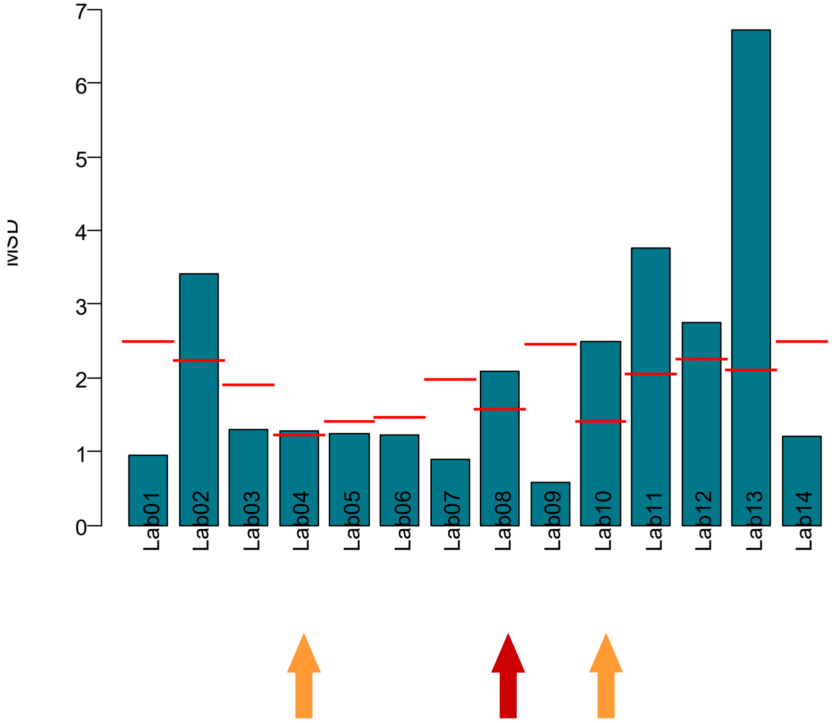
A pairwise summary indicator: Median scaled difference

$$\mathrm{MSD}_i = \operatorname*{med}_{j,i\neq j}\left(\frac{\left|x_i - x_j\right|}{u\left(x_i - x_j\right)}\right)$$



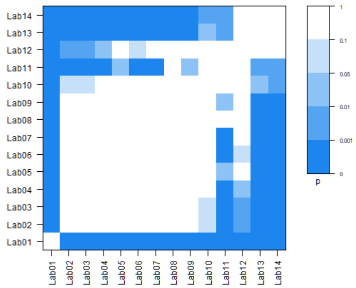
MSD example:
CCQM-P22 - Non-IID bootstrap quantiles

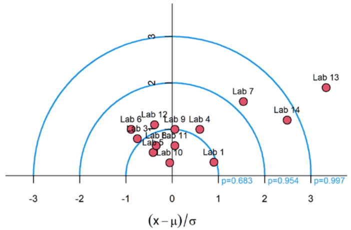


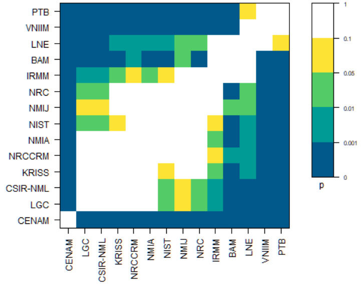


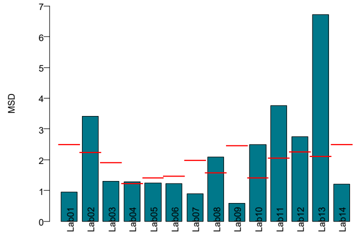
SUMMARY

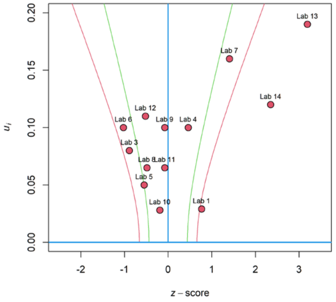
There's more to interlab graphics than dot-and-bar plots











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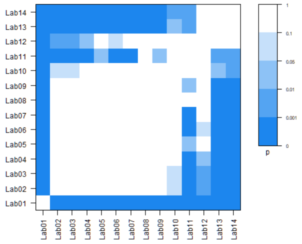
References



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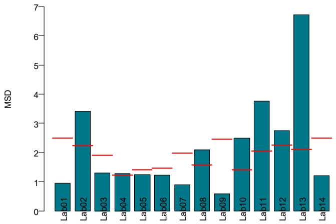
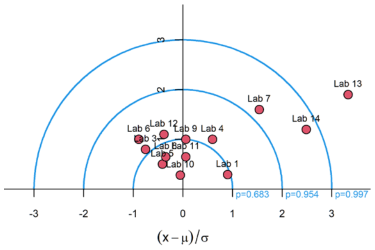


Ellison, S.L.R. An outlier-resistant indicator of anomalies among inter-laboratory comparison data with associated uncertainty *Metrologia* 55 840 (2018)

https://orcid.org/0000-0002-3008-6656

References



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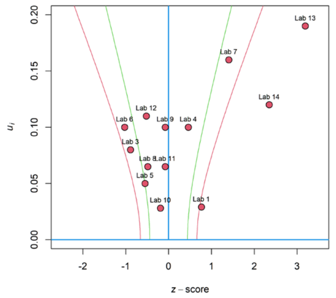

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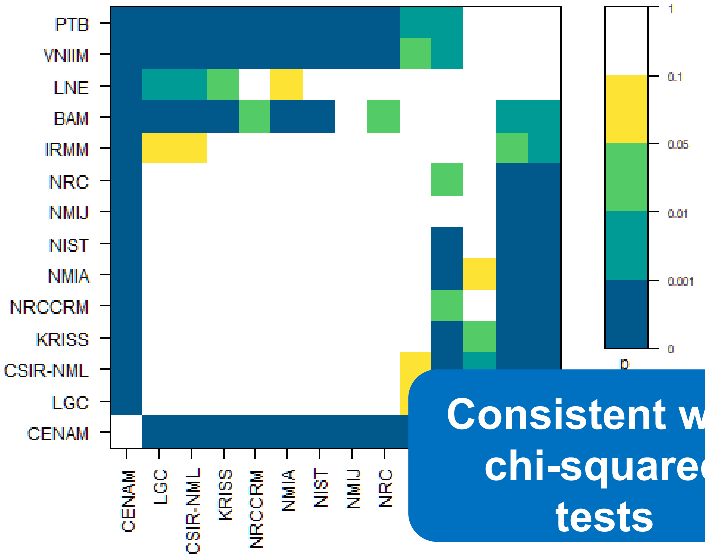
Accred Qual Assur 27, 145–153 (2022).
https://doi.org/10.1007/s00769-022-01496-w

Comparing adjustment methods

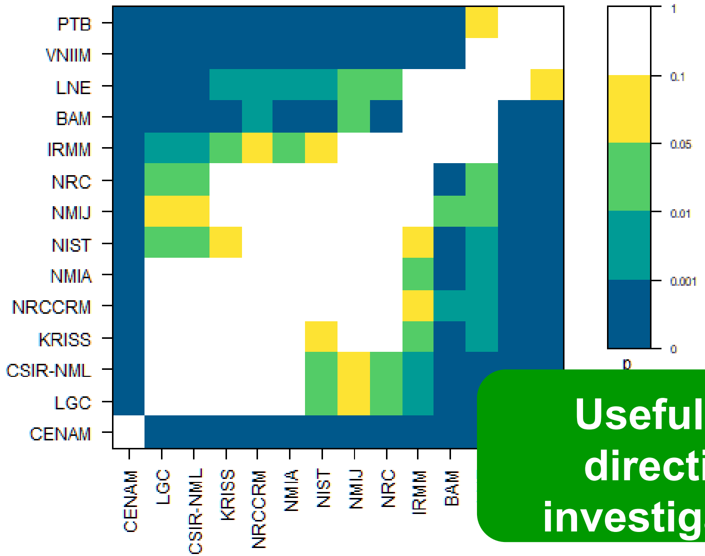
Holm



Consistent with chi-squared tests

Preserves family-wise error rate α

Benjamin-Hochberg

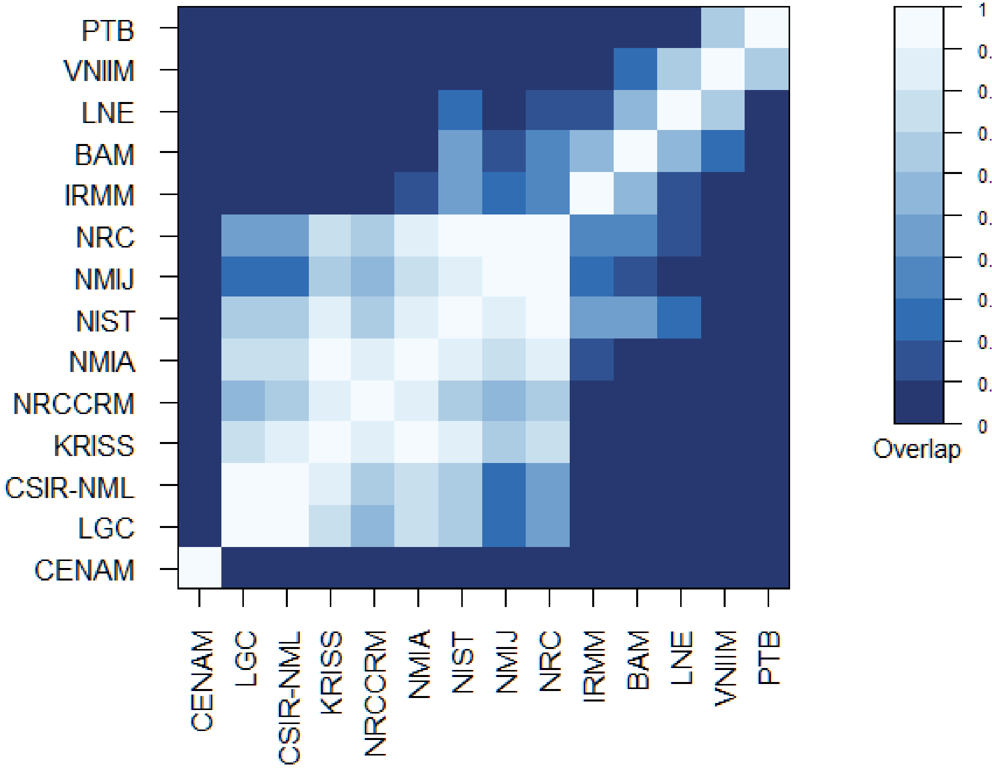


Useful for directing investigation

Controls false discovery rate

Pairwise overlap

- **Plot of mutual distribution overlap**
  (Following Cofino/Quasimeme*)



*See, for example:
Burrell S, Crum S, Foley B, Turner AD (2016), Proficienc
testing of laboratories for paralytic shellfish poisoning toxins in shellfish by QUASIMEME: A review,
Trends in Analytical Chemistry, 75, 10-23,
https://doi.org/10.1016/j.trac.2015.09.004.