U-Th-Pb geochronology in Iolite

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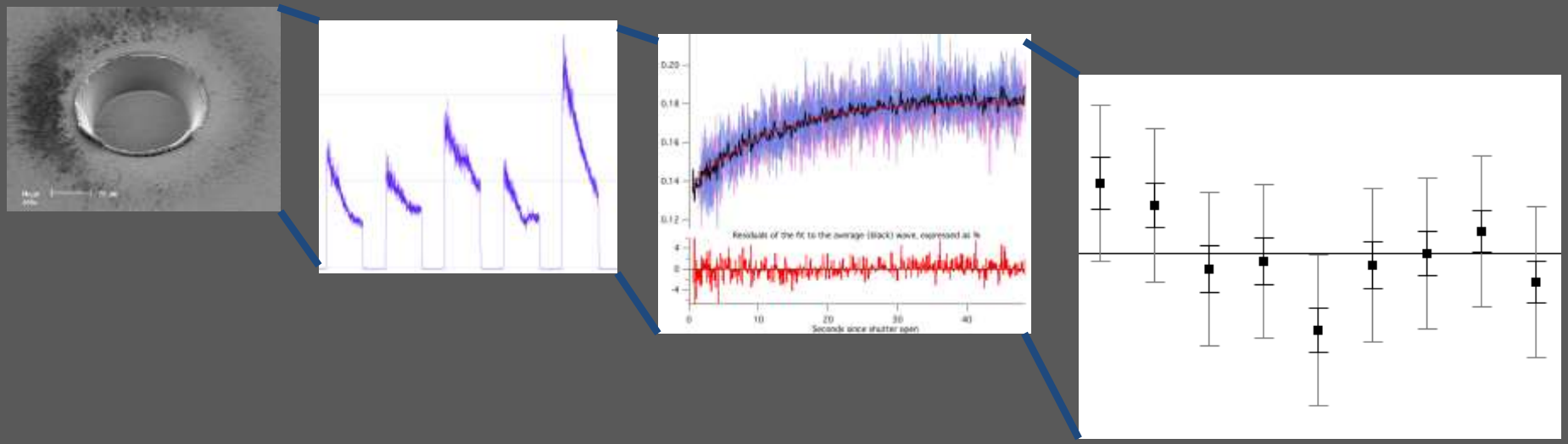
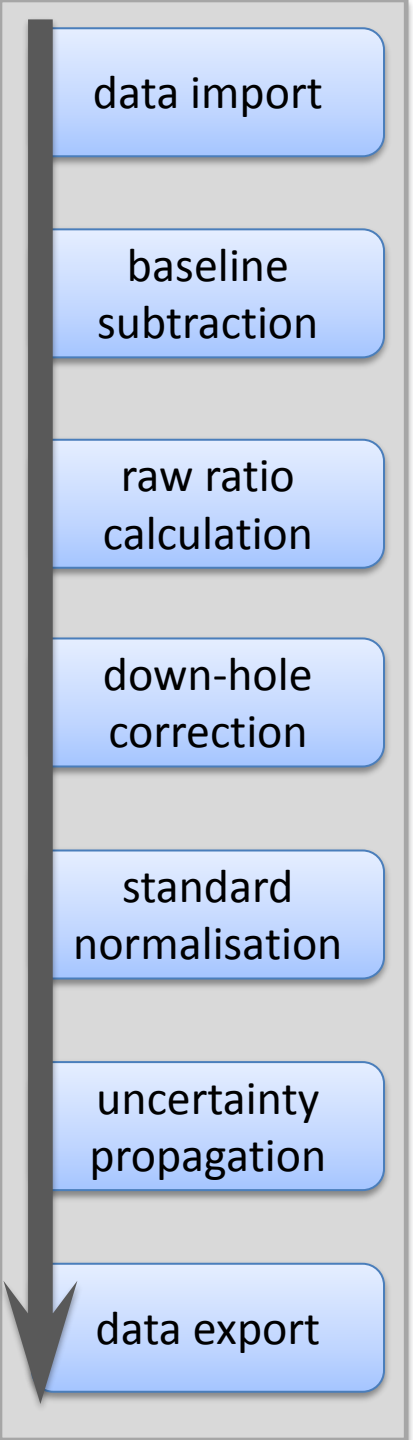
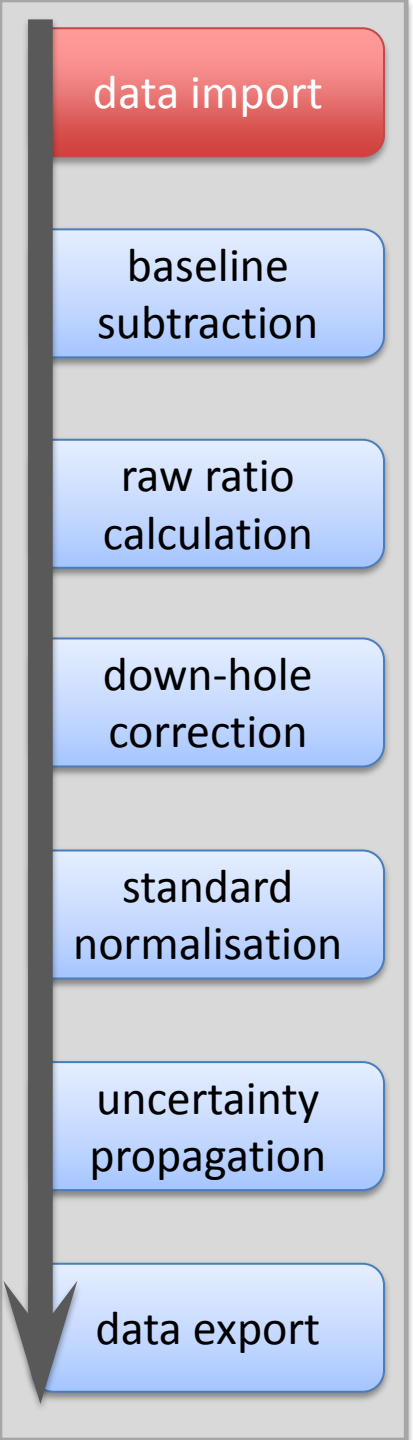
www.iolite.org.au



Outline:

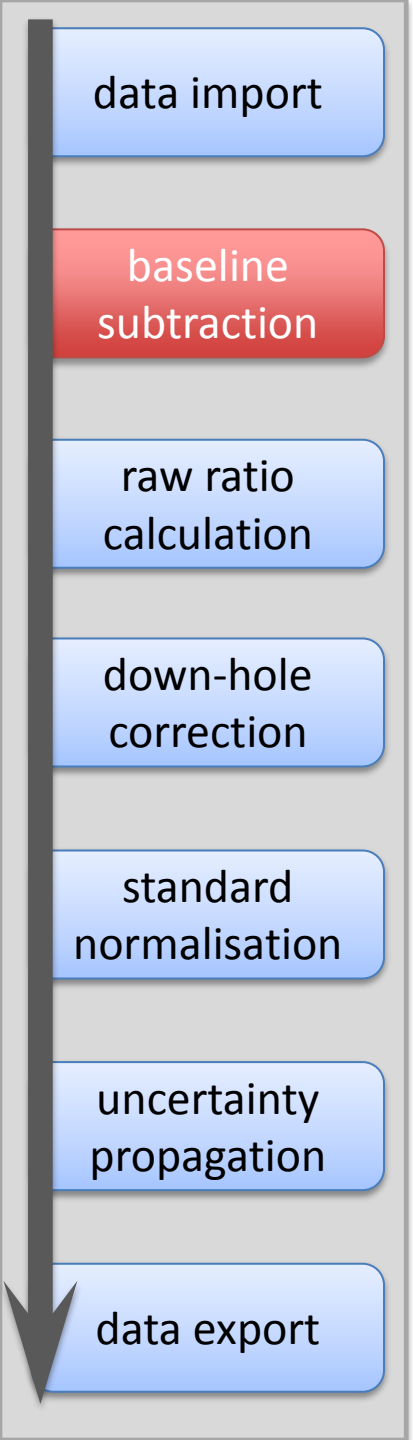
- Illustrate general workflow of data reduction
- Provide details of specific stages of interest
- Highlight some strengths and weaknesses


data import
baseline subtraction
raw ratio calculation
down-hole correction
standard normalisation
uncertainty propagation
data export



Data import:

- Import data from most mass spectrometers into a standardised format within the software
- This allows identical treatment of data, regardless of its source
- Imported as individual time-slices, and all subsequent data reduction is per timeslice



Baseline subtraction:

- Time periods of baseline (blank) are selected, either automatically or manually
- From these selections the baseline of each measured isotope is interpolated throughout the session

data import

baseline subtraction

raw ratio calculation

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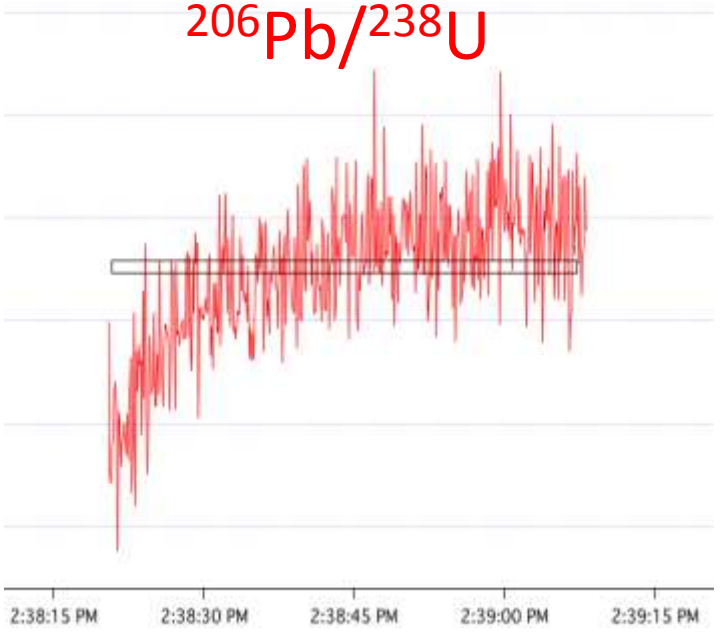
Raw ratio calculation:

- Baseline-subtracted intensities of each isotope are used to calculate raw (i.e., measured) ratios
- Ratios are calculated for every timeslice of data



data import

baseline subtraction

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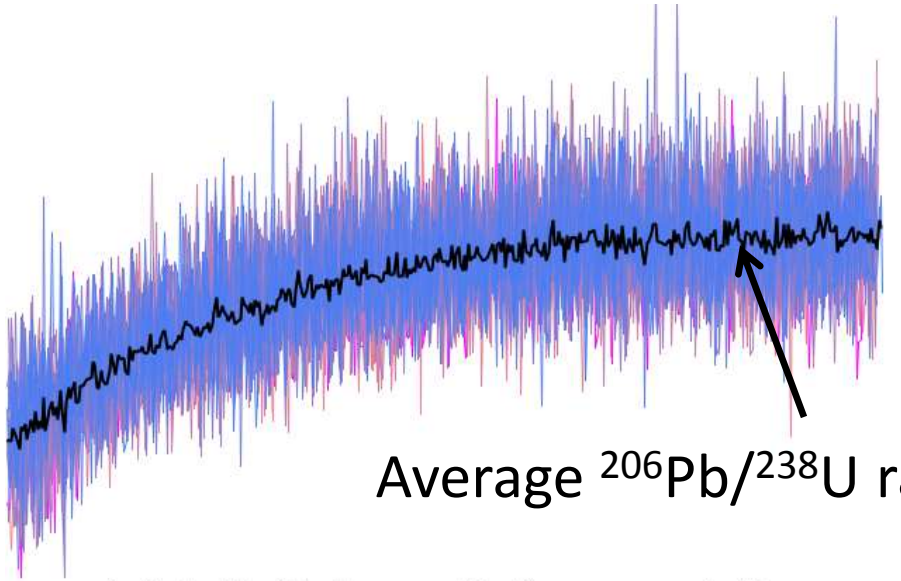
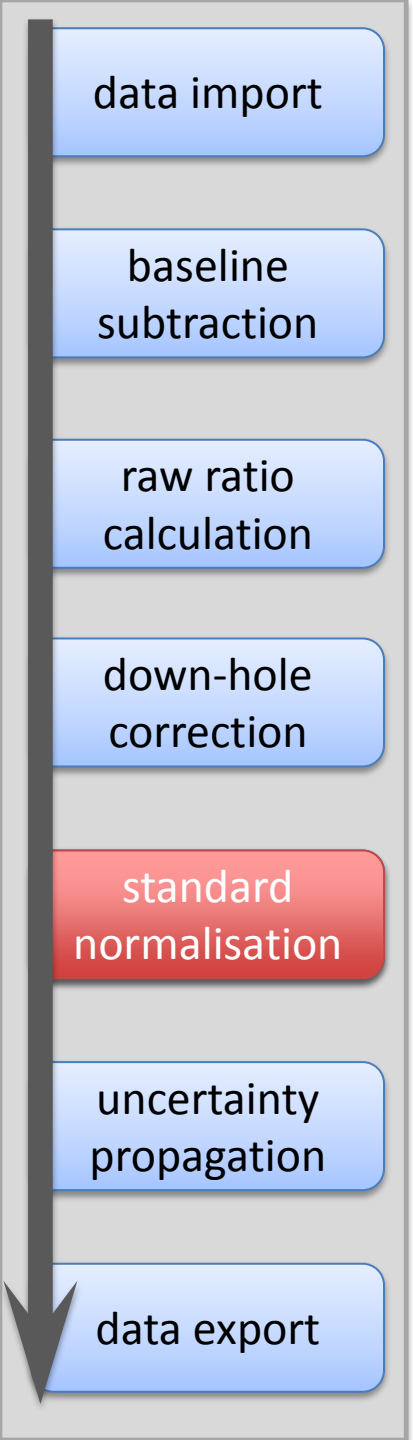
Down-hole correction:

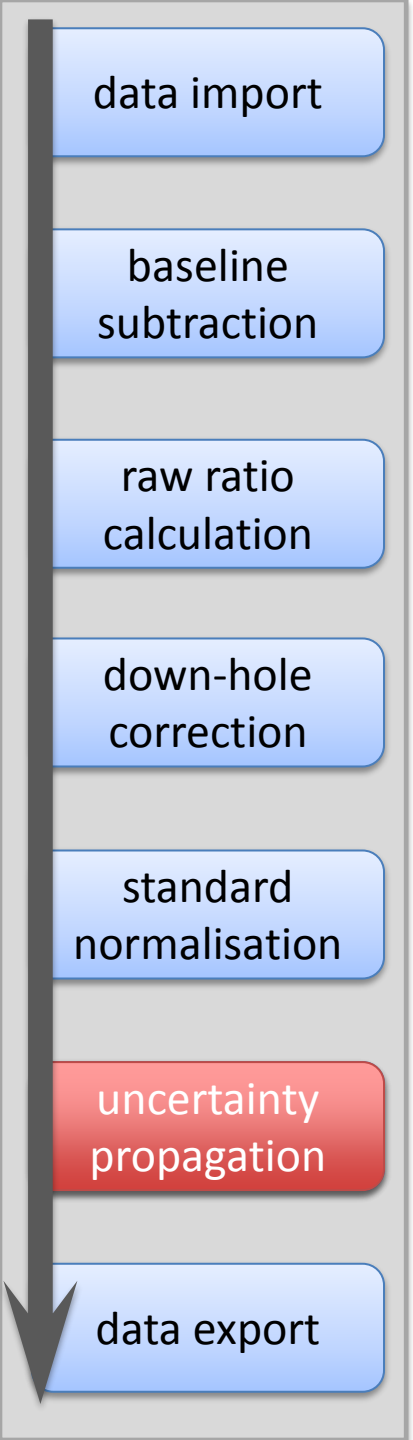
- Correction of elemental fractionation induced by laser - time since laser shutter opened is used as a proxy for pit depth
- All analyses of the reference standard are combined to model the effect – each analysis is then “flattened” using the model
- No attempt to correct to “true” ratio, only to flatten each analysis





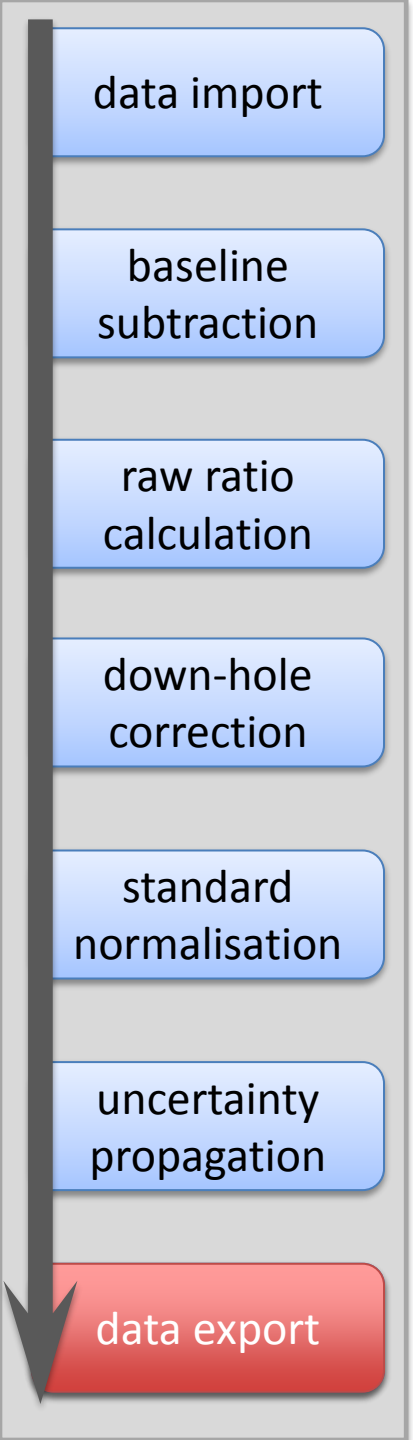
Standard normalisation:

- Normalisation to the reference standard is treated separately to down-hole fractionation
- After down-hole correction, ratios are flattened, but still not adjusted to the accepted values of the reference standard
- This is done using a spline that interpolates the correction factor through the session
- Fully corrected ratios are now available



Uncertainty propagation:

- Use analyses of the reference standard to estimate the propagated uncertainty of analyses
- This is done by individually removing each analysis and treating it as an unknown – this results in a population of pseudo-secondary standards
- Does not address sources of bias (e.g., non-matrix matched standards, or the infamous measurement biases between zircon standards)
- Requires >15 analyses of the reference standard to work reliably



data export:

- Data can be exported from Iolite for use in other software (e.g., Excel and Isoplot)
- Can also export a PDF report of population statistics (e.g., weighted average of multiple analyses)

Some strengths and weaknesses of the approach

MOR vs. ROM

- Iolite data is built to be processed timeslice-by-timeslice
- Therefore mean-of-ratios (MOR) by default
- Ratio-of-means (ROM) is currently not straightforward.
- ROM less biased for very low counts

Down-hole fractionation

- Modelling the nature of fractionation versus depth allows detection of variation within an analysis (e.g., zoning, common-Pb)
- Assumes reference standards and unknowns have identical behaviour
- Assumes that fractionation does not vary within the session
- Allows down-hole fractionation (short-term) to be treated separately from long-term drift in elemental fractionation

Session-based reduction

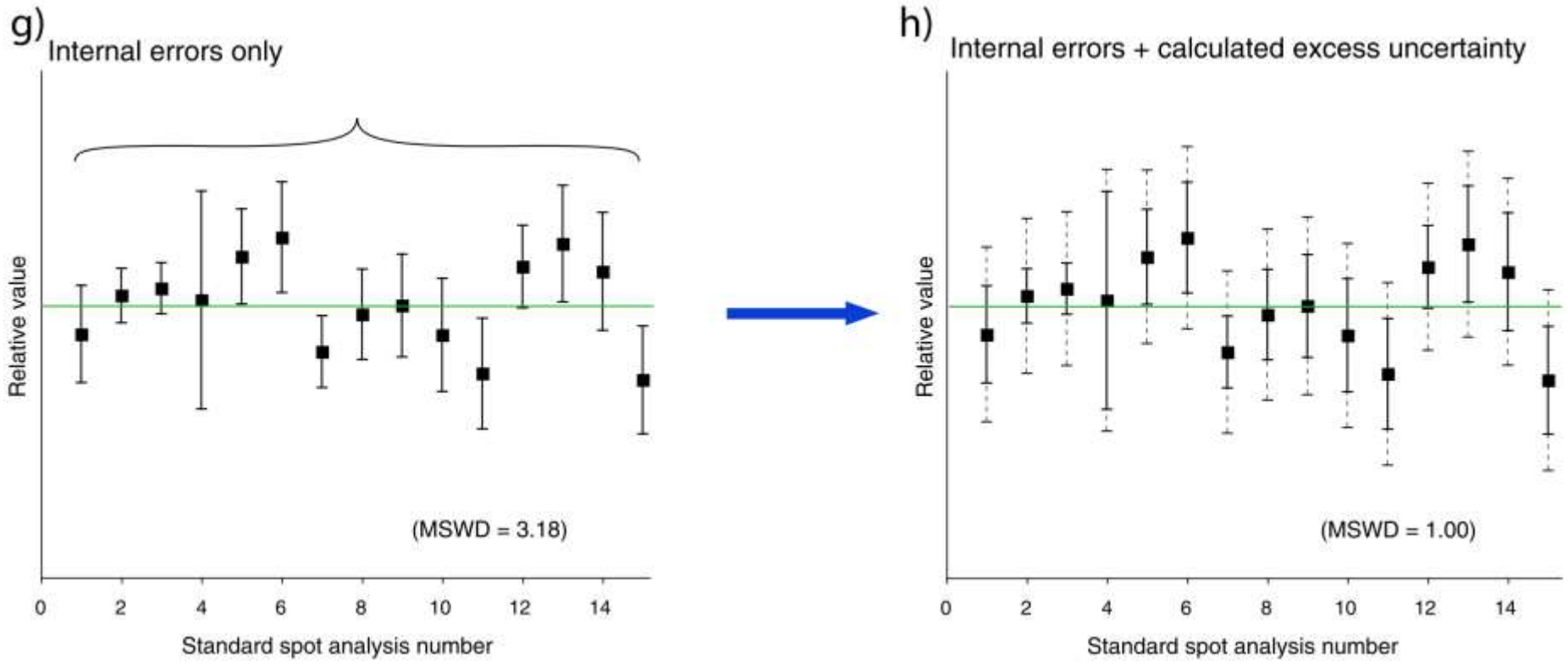
- Treat an entire session of data at once – can be hundreds of analyses
- Large numbers of analyses have advantages:
  - Values that vary with time (e.g., baselines) can be interpolated as a group using splines
  - Larger number of reference standards allows better normalisation through the session
  - Uncertainty propagation using pseudo-secondary standards

More on the method of uncertainty propagation

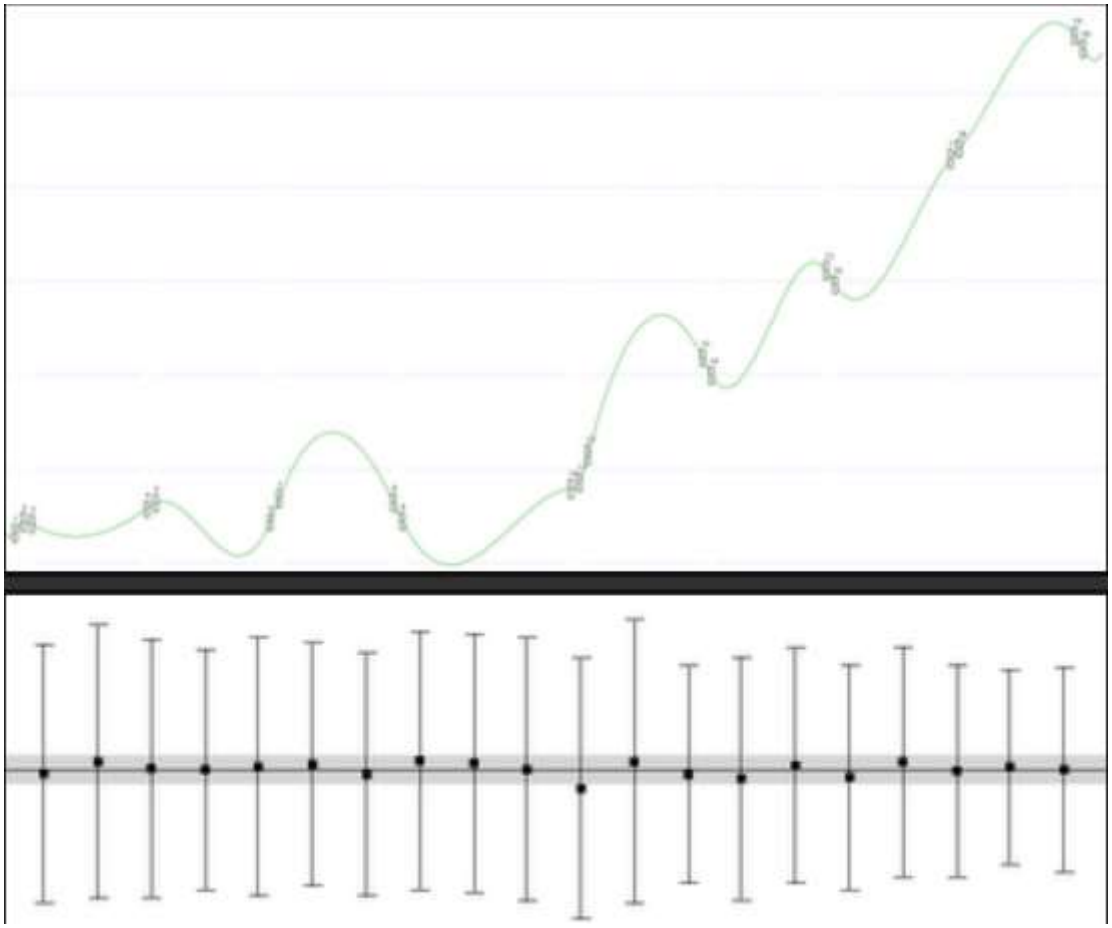
Basic concept:

- Idea is to assess whether the calculated 2 s.e. internal precisions of analyses are a realistic estimate of the total uncertainty
- Do this by assessing whether scatter in the reference standard analyses can be explained by the internal precision 2 s.e.
- If not then there must be an additional source of uncertainty – this is estimated and propagated into all analyses

- If internal uncertainties are insufficient to explain scatter then assume there is an additional source of “excess scatter”
- Iteratively determine how much excess scatter is required
- The excess scatter is combined in quadrature with the internal precision



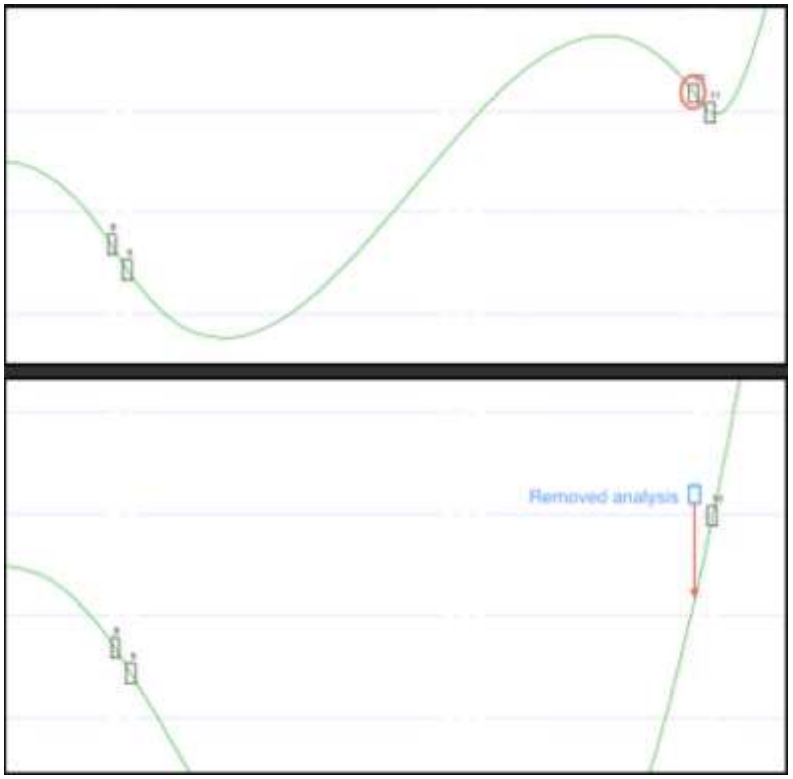
Splines cause some complications

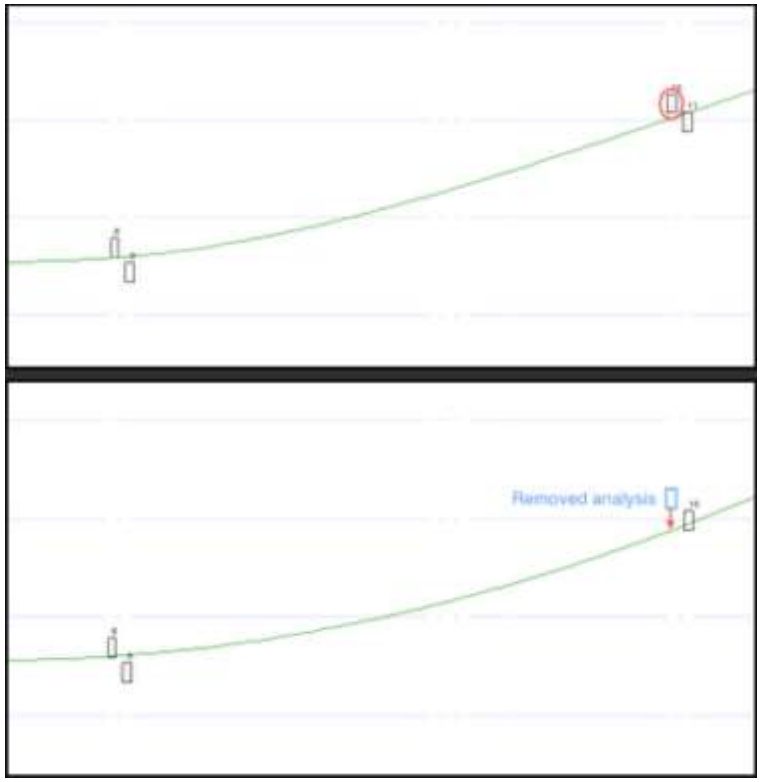


Unsmoothed spline results in no scatter in corrected analyses

Use “odd man out” approach

- Remove each analysis in turn and process it as an unknown
- This results in a group of pseudo-secondary standards (requires a sufficiently large pool of analyses)





Comparison to other packages

Uncertainty propagation protocol/workflow:

– Pseudo-secondary standards using “odd man out”. Doesn’t detect bias, only scatter.

Common-Pb correction:

– Currently only available using the VizualAge add-on

Inter-element fractionation correction:

– Down-hole correction modelled from average of reference standards. Separate normalisation of residual elemental fractionation using splines

Weighted Mean/Linear regression support:

– Weighted mean of final ratios supported. Concordia plotting supported using VizualAge add-on

Rejection criteria:

– Can be set to none/2 s.d./3 s.d.

Handling/storage of reference values:

– All values of reference standards are stored in text files and are readily viewed/edited

Key differences from other available packages:

– Method of down-hole fractionation correction

– Interpolation of values using splines

– Uncertainty propagation method