Values and uncertainties near the detection limit

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The Edge of Reason

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The preparation of this paper was supported by Department for Business, Energy & Industrial Strategy under the National Measurement System Chemical and Biological Measurement Programme
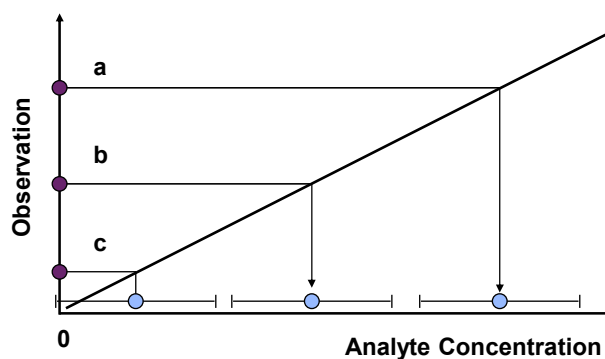
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Introduction

- **The detection limit – a brief history**

- **Measurement Uncertainty near the detection limit**

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Detection limits

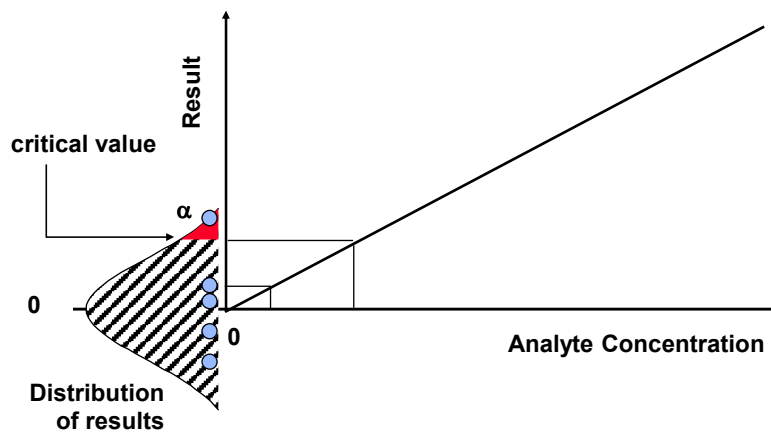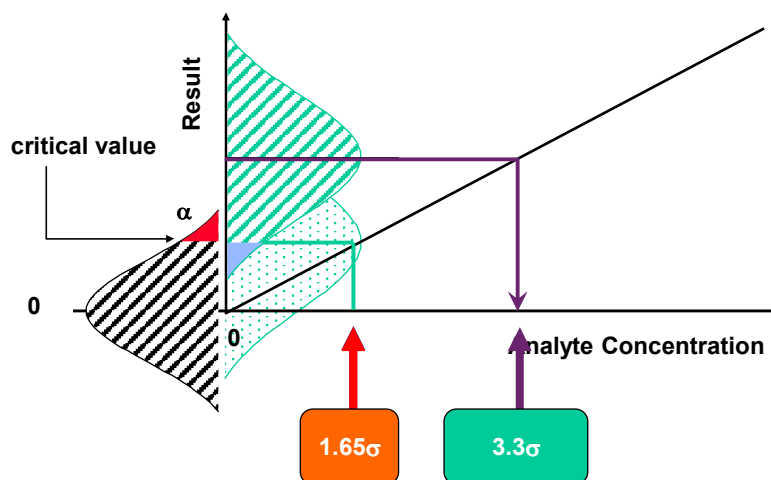**Calculated concentration with uncertainty**

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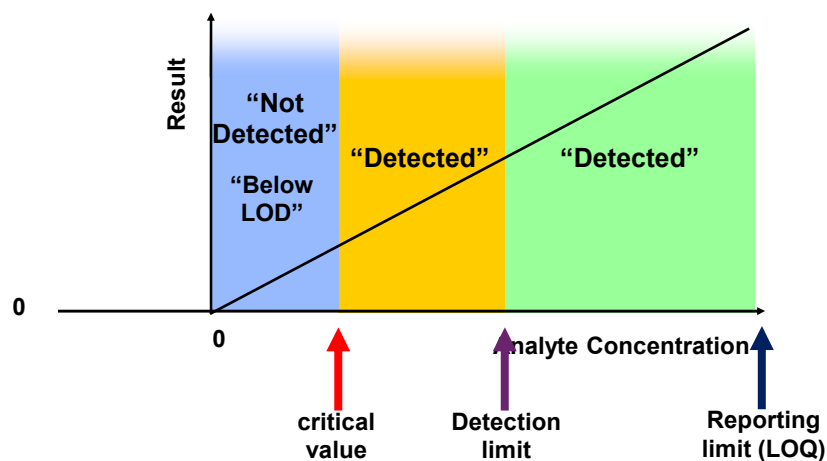# The detection limit: Part 1

The detection limit: Part 2
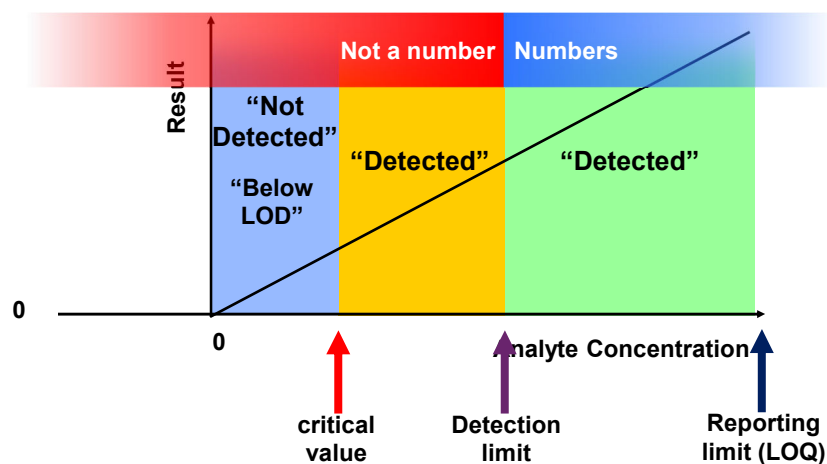

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The detection limit: Part 3

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Results above the critical value and BELOW THE LOD are POSITIVE

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The detection limit: Common (mis)interpretations

All numerical results are valid estimates – even those below the LOD

Using sub-LOD data

- **"Less than" cannot* be averaged**
- **"Less than" cannot* be scored in PT**
- **"Less than" cannot be added**
  - except to form a bigger "less than"
- **... or subtracted.**

> **Report the raw observation and uncertainty if at all possible**

- **... but "-0.2 mg/kg $\pm$ 0.3 " can...**

*Maximum likelihood and approaches excluded

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And there shall be...

> **Measurement**
>
> **Uncertainty**

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Uncertainty near zero/100%

±2σ

0

Impossible values

±2σ

0

What is the 'best estimate'?

Should the uncertainty change?
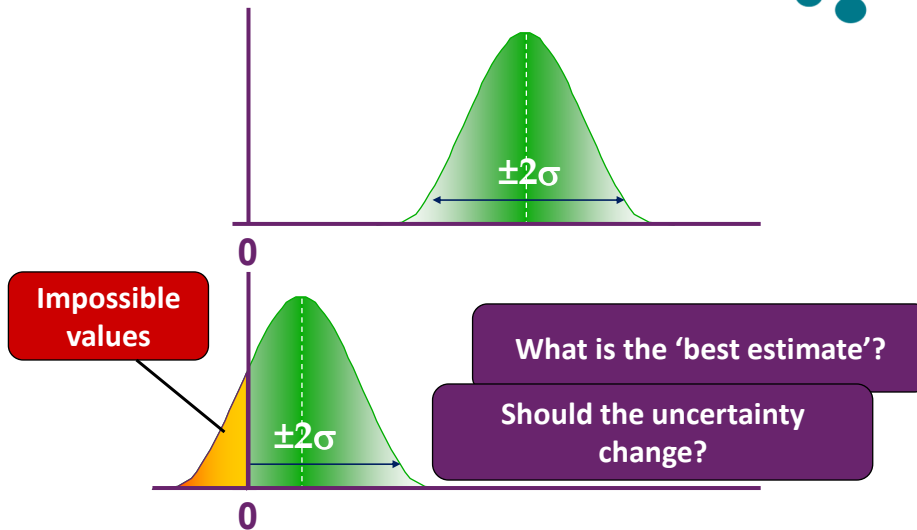
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Truncation provides accurate coverage

±t.u

Retain mean value

Asymmetric interval:
0 < x < x+t.u

0
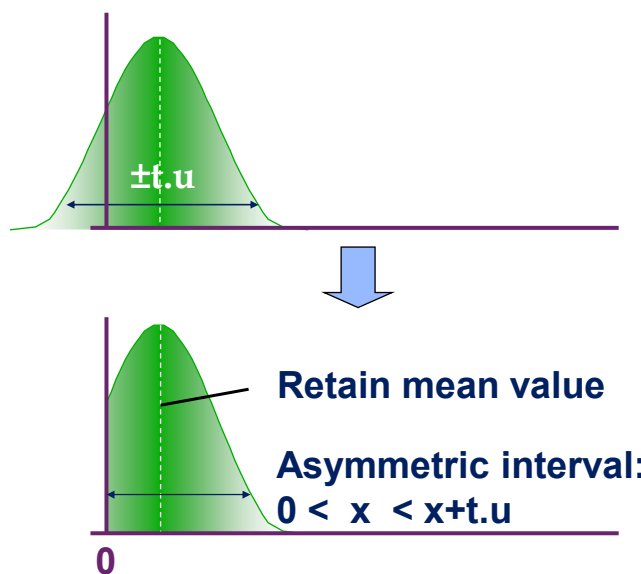
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Truncated interval near zero
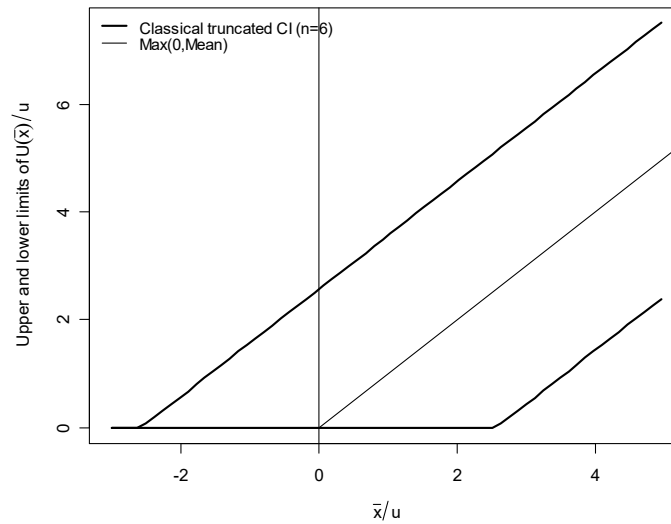
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Bayesian approach

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Bayesian interval

95% of posterior distribution
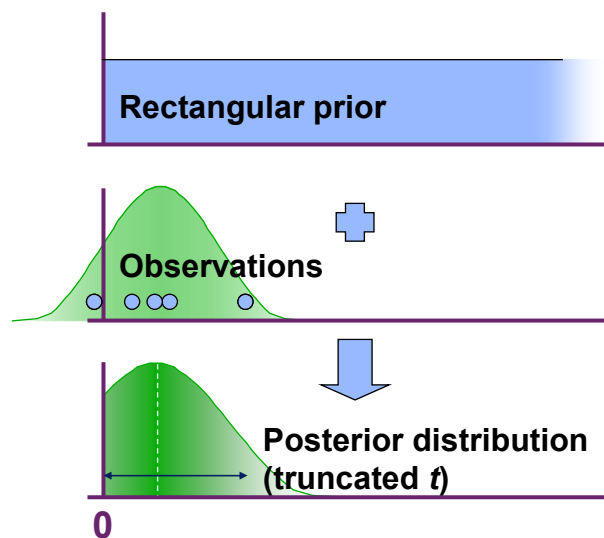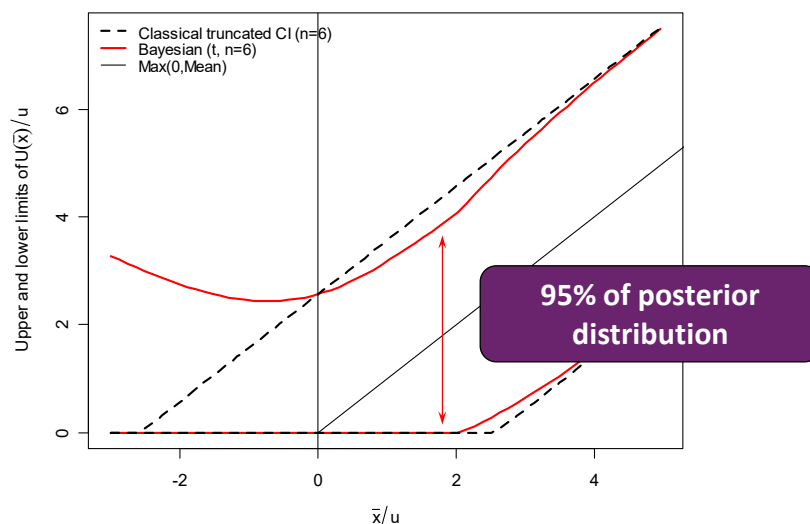
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Reporting measurement uncertainty on values near zero

- **Truncated interval retains exact coverage properties**
  - Standard uncertainty unchanged
  - Minimally biased mean
  - Convergence to zero width implies probable measurement failure
- **Bayesian interval more general but more complex to calculate**

- **Essential to truncate AFTER ALL OTHER CALCULATIONS**
  - Truncating interim values leads to increased bias

"Handling undetected and low-level components in purity determination".
S Cowen, S L R Ellison, Accred. Qual. Assur. 12, 323-328 (2007)

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"Less than LOD" does NOT mean "invalid result"

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Can MU replace LOD?

Advantages

- No arbitrary cut-off
  - Everything is a number
- Decision could be specific to the particular test item
  - Uncertainty for *that* result

Challenges

- MU does not give information about the measurement procedure
- MU is complicated near zero
  - Traditional MU limits may include zero
  - Many useful Bayesian approaches could exclude zero
- MU should be about the test item
  - But often isn't
- An MU interval is two-sided
  - A detection decision is one-sided

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Measurement uncertainty is not the same as detection capability

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Conclusions and recommendations

- **Detection limits are based on statistical reasoning**
- **Detection limits are not decision limits**
- **Reporting limits are beyond the limit**

- **Report raw values if you can**
- **Reasonable uncertainty intervals are possible**
  - and may even replace 'limits'?

- **MU and detection capability give different information**
  - We may continue to need both, for different purposes

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