Setting standards in analytical science

Measurements for Regulation: Using uncertainty information

S Ellison

The preparation of this paper was supported under contract with the Department of Trade and Industry as part of the National Measurement System Valid Analytical Measurement (VAM) Programme

Introduction

Setting standards in analytical science

- What is Measurement uncertainty?
- International Activity in analytical measurement uncertainty harmonisation
- Problems
- Options

What is Measurement Uncertainty?

Setting standards in analytical science

"A parameter, associated with the result of a measurement, that characterises the dispersion of the values that could reasonably be attributed to the measurand"

(ISO Guide)

The number after the ±

Measurement uncertainty ...

Setting standards in analytical science

- DOES NOT

  ...just include observed precision

- DOES

  ... include ALL POSSIBLE effects

  ... including uncertainties in reference values, environment, method controls....

  ... *try* to say something about where the true value might lie

Problems

Setting standards in analytical science

- “Correct” evaluation
- Impact on compliance assessments
- Correct interpretation
- Communication
- Management
  - of uncertainty
  - of decisions with uncertainty

International activity

Setting standards in analytical science

- Standardisation bodies
- Laboratory organisations
- Accreditation bodies

ISO activity

Setting standards in analytical science

- ISO TAG 4
  - Guide to the Expression of Uncertainty in Measurement (“GUM”)
  - Reformed with advisory remit
- ISO TC/69
  - ISO 5725 (Collaborative study)
  - WG7: ISO TS 21748 - uncertainty using collaborative study data
  - Additional activity on type A methods (TS 21749 - nested designs)

Laboratory organisations

Setting standards in analytical science

- Eurachem (Analytical measurement)
  - Technical guidance on evaluation: QUAM:2000
  - First published international guide using validation data
  - Currently working on interpretation guidance
- Eurolab (non-sectoral)
  - Issued general guidance on evaluation
  - included a PT-based example
  - minimal interpretation guidance*
  - New working group formed 2004

Accreditation bodies

Setting standards in analytical science

- Principal responsibility is general assurance of laboratory competence via ISO/IEC 17025:1999
- Most individual accreditation bodies had their own MU guidance by 1999
- Increasingly adopt expert guidance rather than developing their own
- Harmonise **technical** practices via regional (EA, APLAC) and global (ILAC) guidelines
- Support regulation (mostly!)

EA activity (European Accreditation)

Setting standards in analytical science

- Expert working group on uncertainty (2001)
- Tasked with advising on appropriate methods of assessment
- GUM Compliant
- Included ‘validation’ and collaborative study data
  - With reference to **ISO TS 21748**
  - Included proficiency Test data as basis in very limited circumstances
- Did NOT include guidance on interpretation

Uncertainty evaluation methods

Setting standards in analytical science

- Repeatability assessment
  - Always insufficient...
- ISO Guide approach (“the GUM”)
  - Accreditation
- Validation-based approaches
- Interlaboratory study
  - Traditional in regulatory analysis

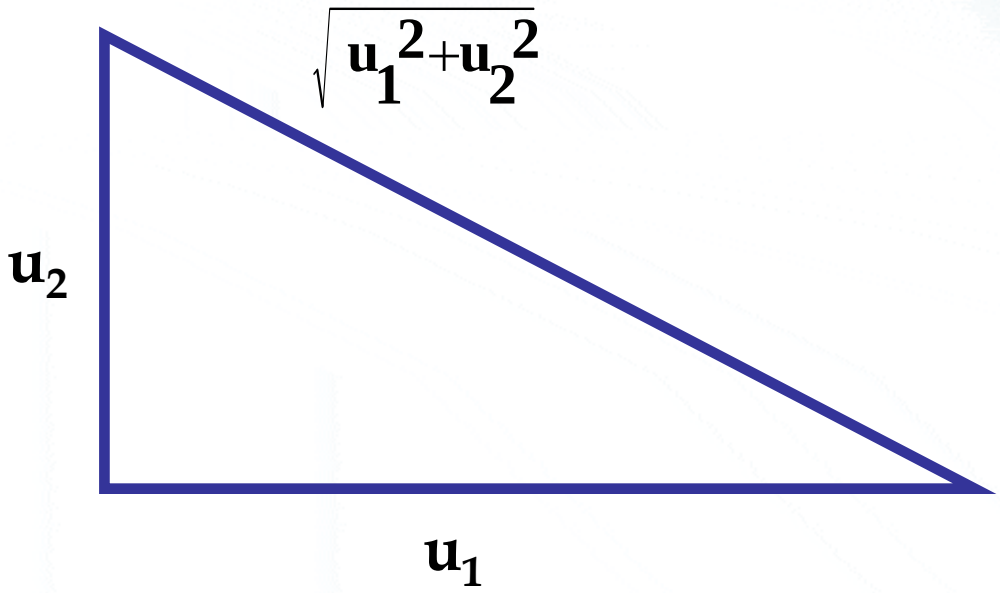
ISO Guide approach

Setting standards in analytical science

- Specify the measurand
  - including complete equation
- Quantify significant uncertainties in all parameters
  - A: from statistics of repeated experiment
  - B: by any other means (theory, certificates, judgement...)
- Express as standard deviation
- Combine according to stated principles
- Multiply by “coverage factor”

Combining uncertainties (ISO)

Setting standards in analytical science



- *Standard deviations*
- *Established error propagation theory*

ISO Guide - Limitations

Setting standards in analytical science

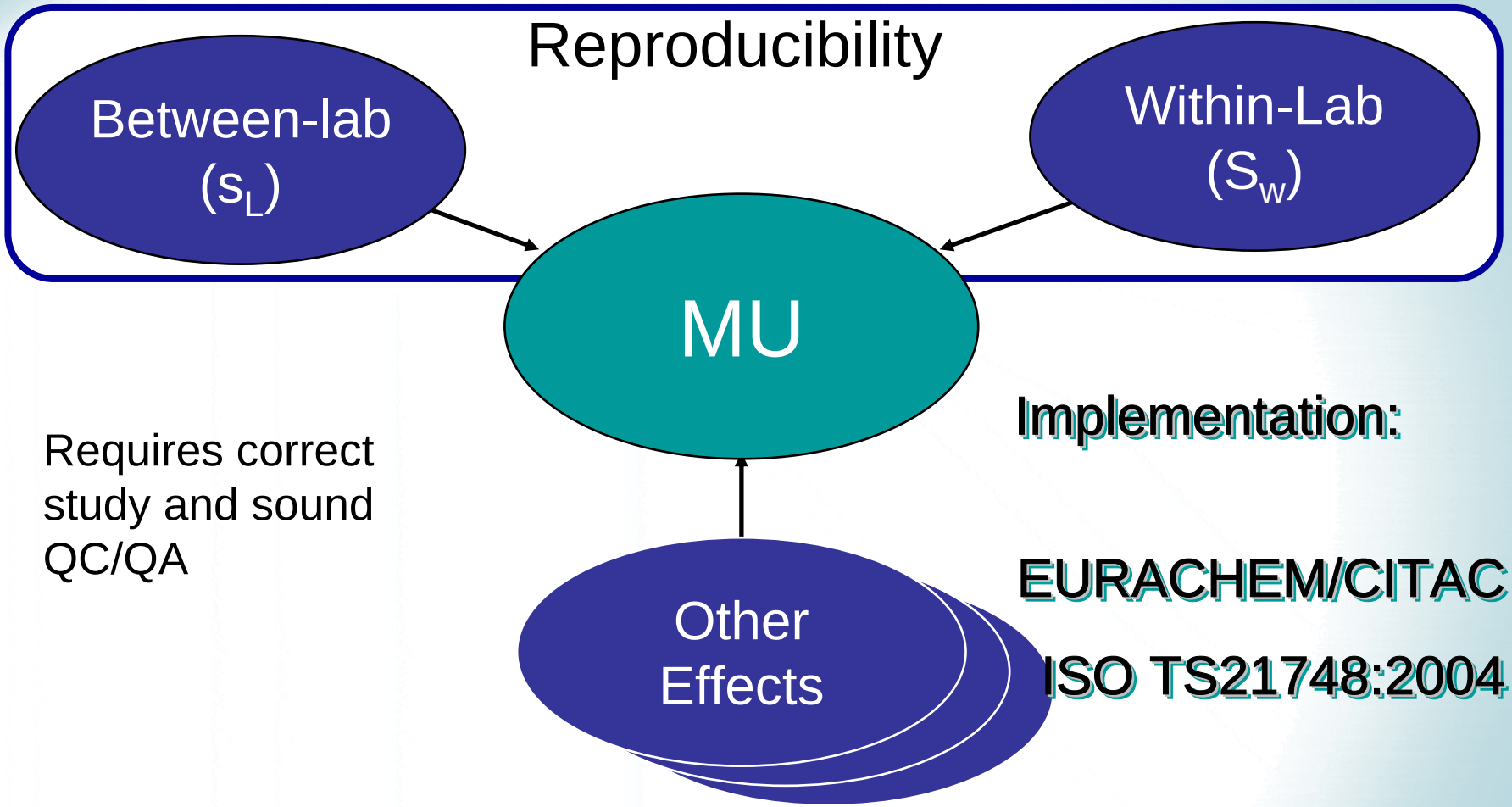
- Basic concepts apply fairly generally
- Detailed procedure is less general:
  - Requires a complete and validated equation with major uncertainties ‘well understood’
  - Assumes that uncertainties are small with respect to the measurement
  - Applies poorly to asymmetric situations

MU based on validation

Setting standards in analytical science

- The best available estimate of precision
  - An effect varied representatively during a precision experiment requires no further study
- The best available estimate of bias and its uncertainty
- Other significant effects evaluated
  - By experiment, or from standing data

Collaborative Study basis



Requires correct study and sound QC/QA

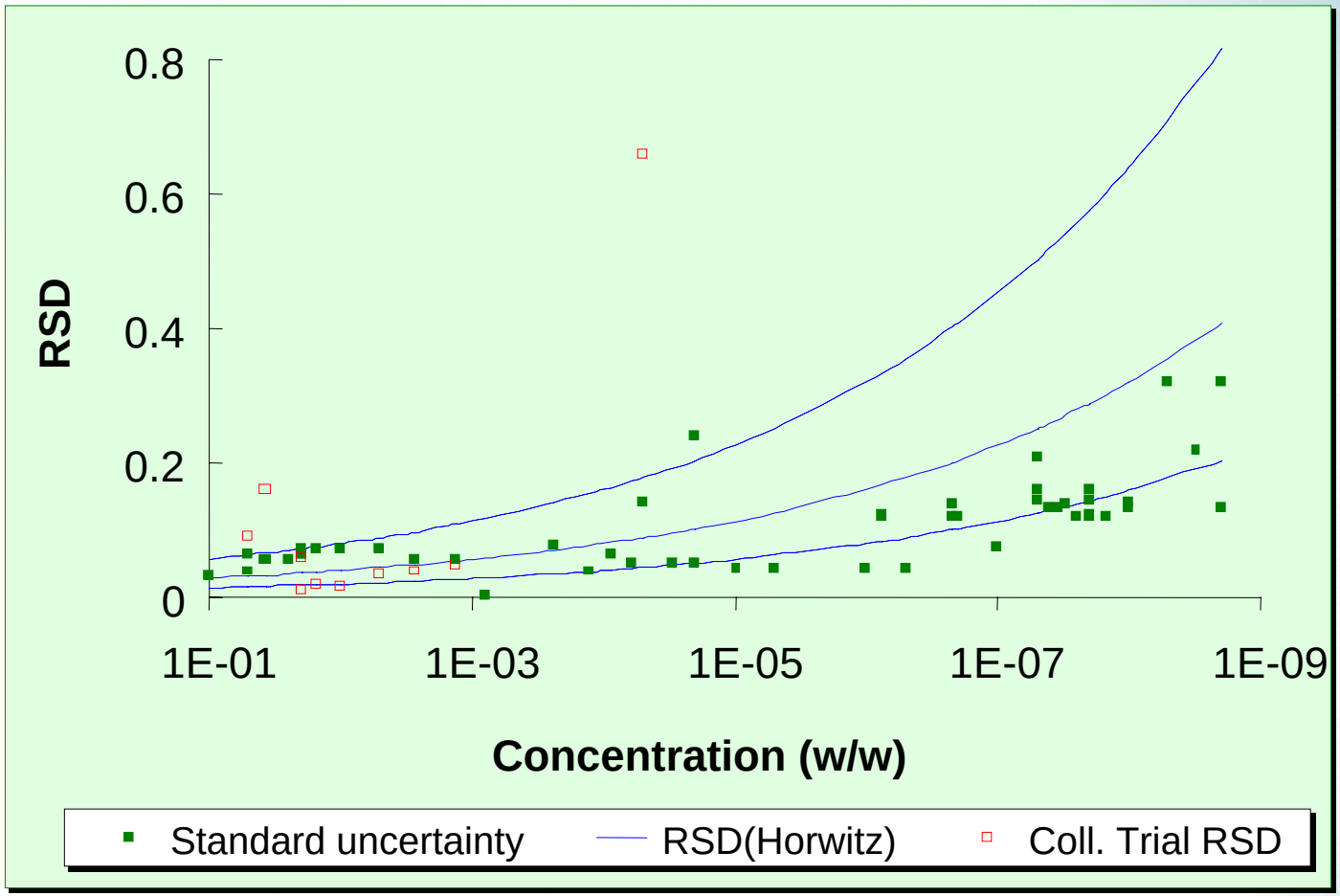
Implementation:

EURACHEM/CITAC

ISO TS21748:2004

Comparing *u* with s_R

Setting standards in analytical science



“Best” Method depends on the problem

Setting standards in analytical science

“Well characterised”
quantified effects, differentiable, continuous, traceable

Poorly characterised;
Unpredictable effects; Input parameters unclear

WELL ← **Measurement model applies** → **POORLY**

POORLY ← **Whole method study applies** → **WELL**

Use both for mutual confidence

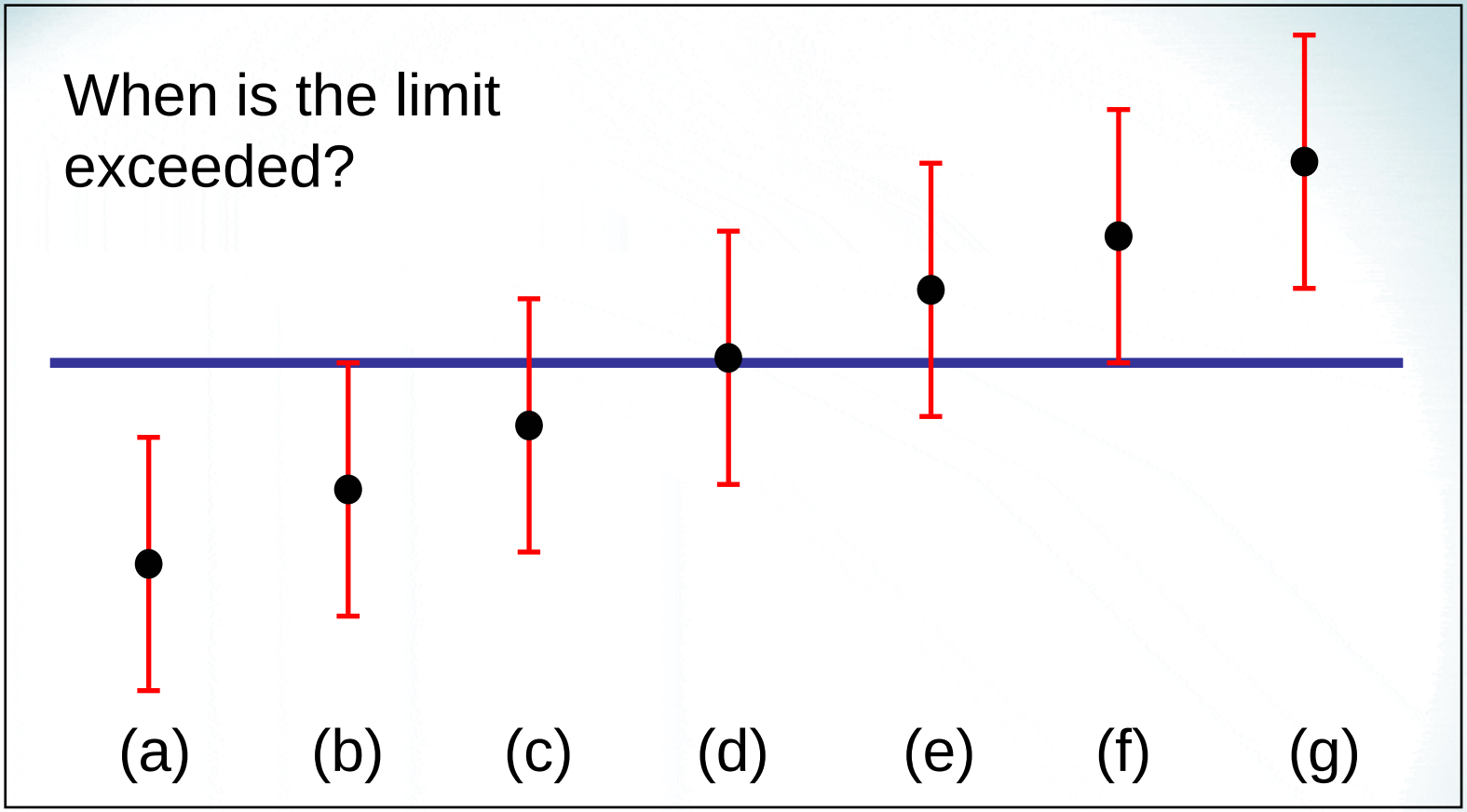
International activity - trends in uncertainty evaluation

Setting standards in analytical science

- Most international bodies recognise interlaboratory study as a valid basis for MU in analytical work
  - Eurachem guide
  - ISO TS 21748
- Some are considering guidance on using PT data for uncertainty estimation
  - Eurolab working group
- Few include definitive rules for interpretation

Interpretation

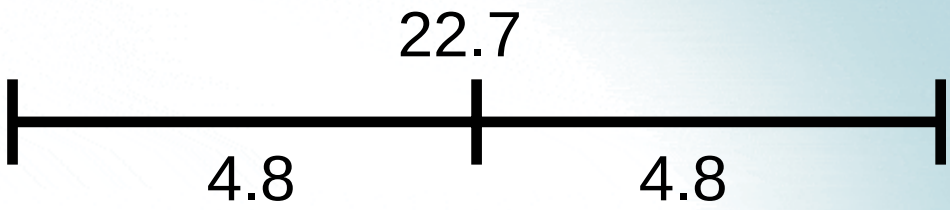
Setting standards in analytical science



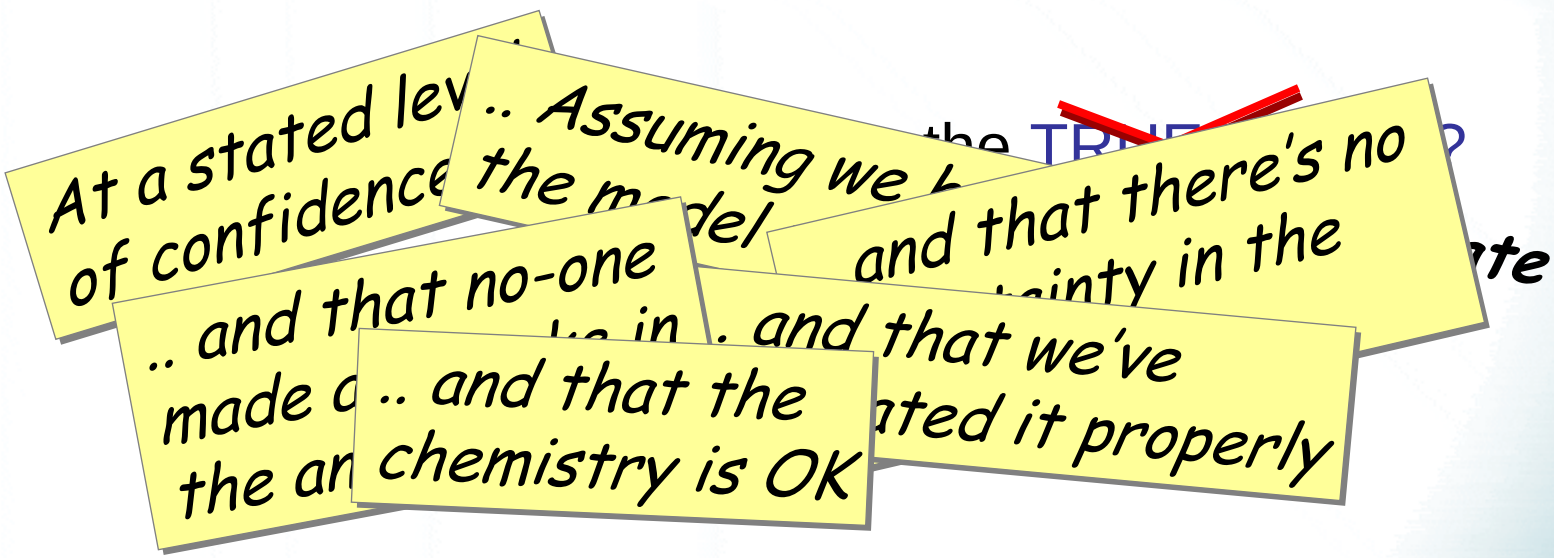
What does Uncertainty mean?

Setting standards in analytical science

22.7 ± 4.8 g



"The amount is between 17.9 and 27.5"

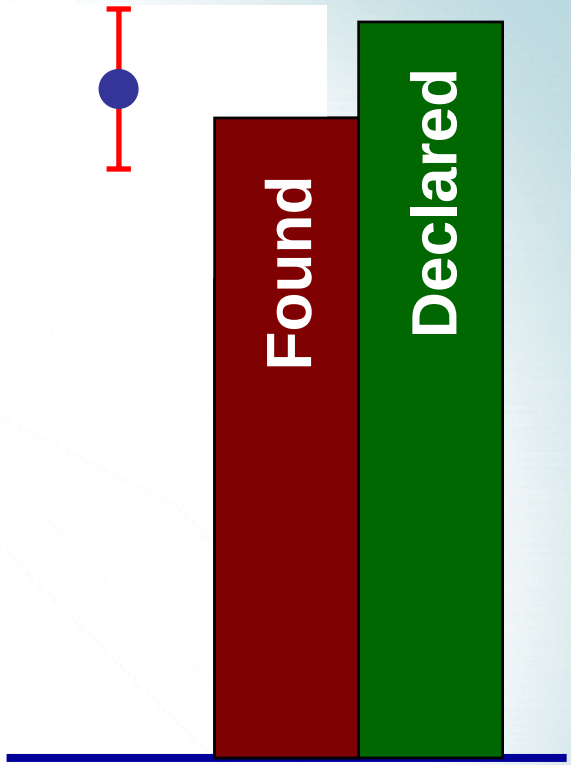


Interpretation: example

Setting standards in analytical science

- Declared Meat Content: 67%
- Public Analyst result: 64%
- Referee result: 65±3%
- Trading Standards officer correspondence:

> This vague answer has prevented a successful prosecution… **has anyone else experienced these ambiguous results ...?**



What does Uncertainty mean?

Setting standards in analytical science

- That the result is uncertain so we can ignore it
- That the analyst doesn't know the answer
- That more crooks will get away with it
- That we need to change the way we interpret results
- That we need to change the law
- ….

Managing uncertainty in regulation

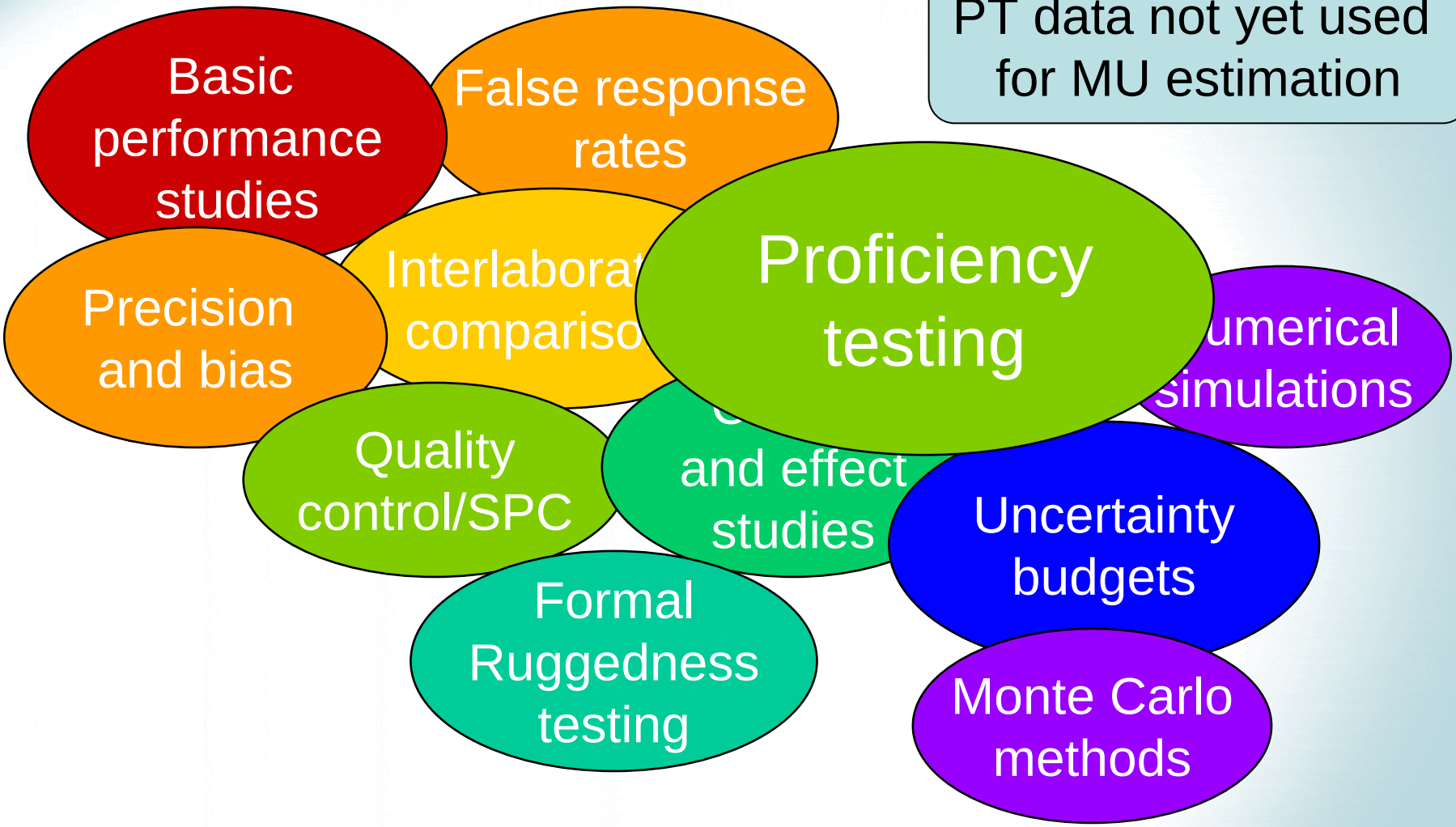
Setting standards in analytical science

- Know and control the uncertainty
- Establish rules for interpretation
  - Whether to use uncertainty
  - How to evaluate
  - Positive compliance versus positive non-compliance

Controlling uncertainty

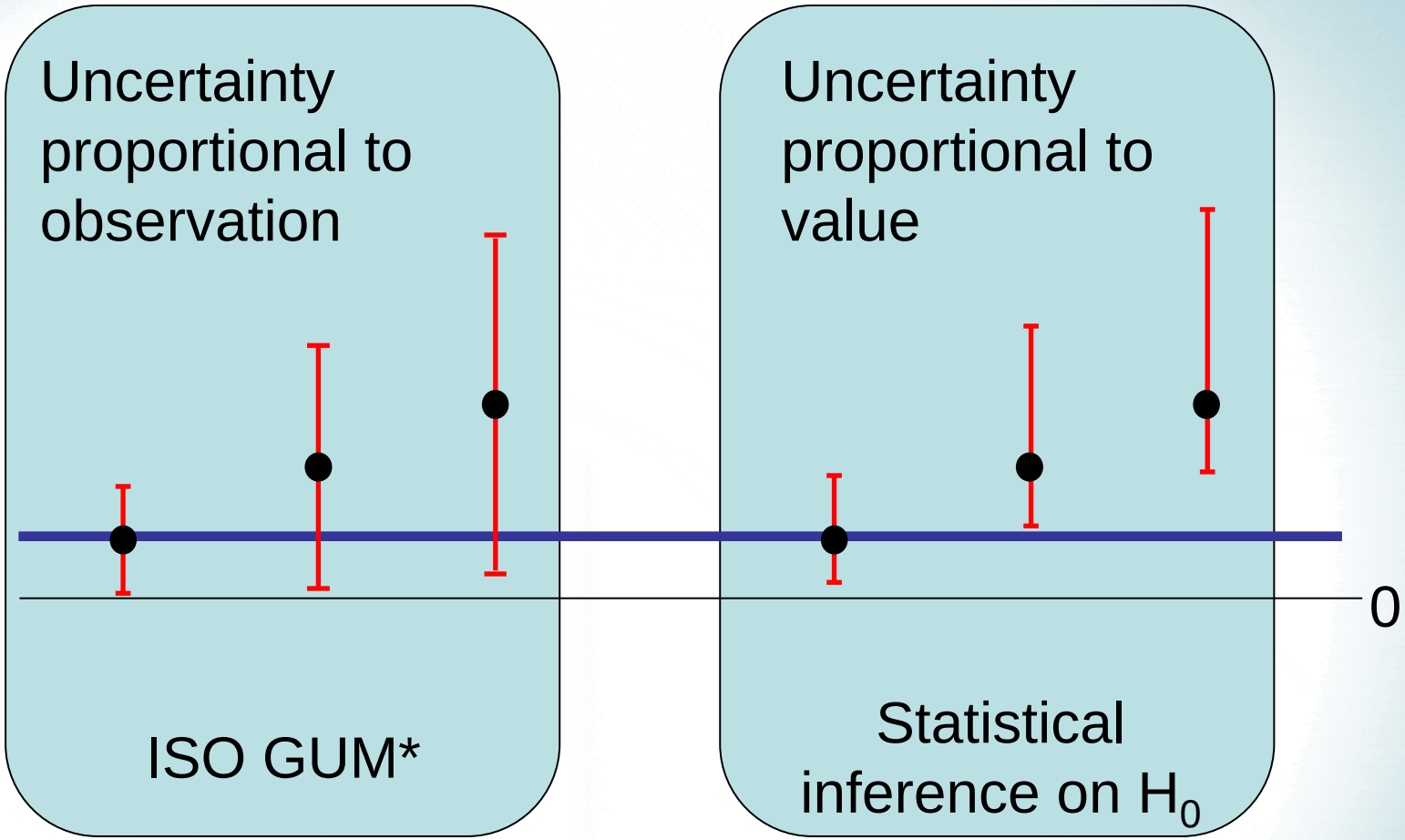
Setting standards in analytical science

PT data not yet used for MU estimation



Proportionality

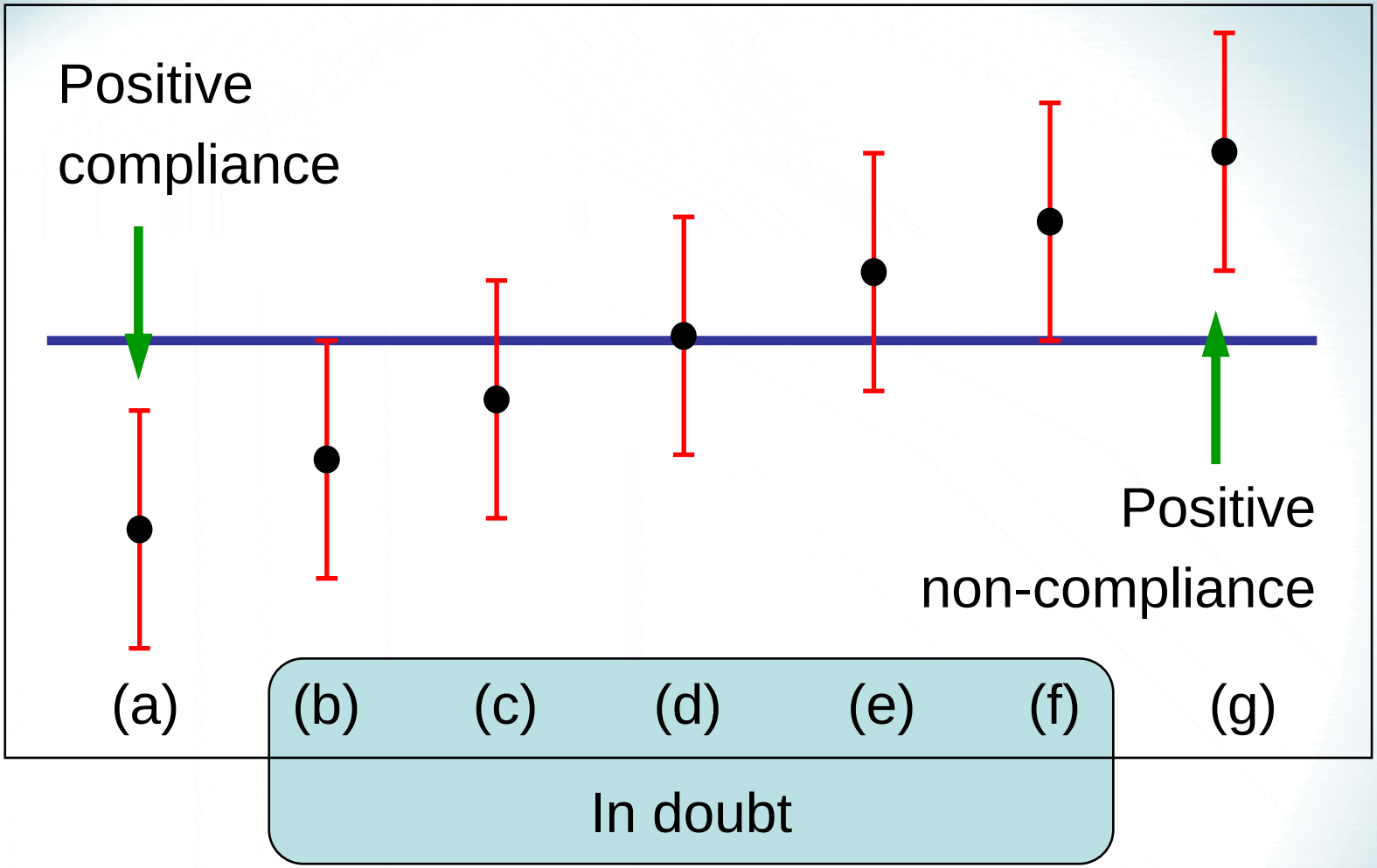
Setting standards in analytical science



Uncertainty must be *very* well understood

Typical Current guidance

Setting standards in analytical science



Features of current guidance

Setting standards in analytical science

- Divides the region into sharp ‘comply/non-comply/in doubt’ regions
- Does not specify level of confidence
- Generally assumes uncertainty is small and constant
- Requires additional information (e.g. contract review) to handle the ‘grey area’
  - Typically client-led
  - Allows for regulatory statements

Regulators' behaviour*

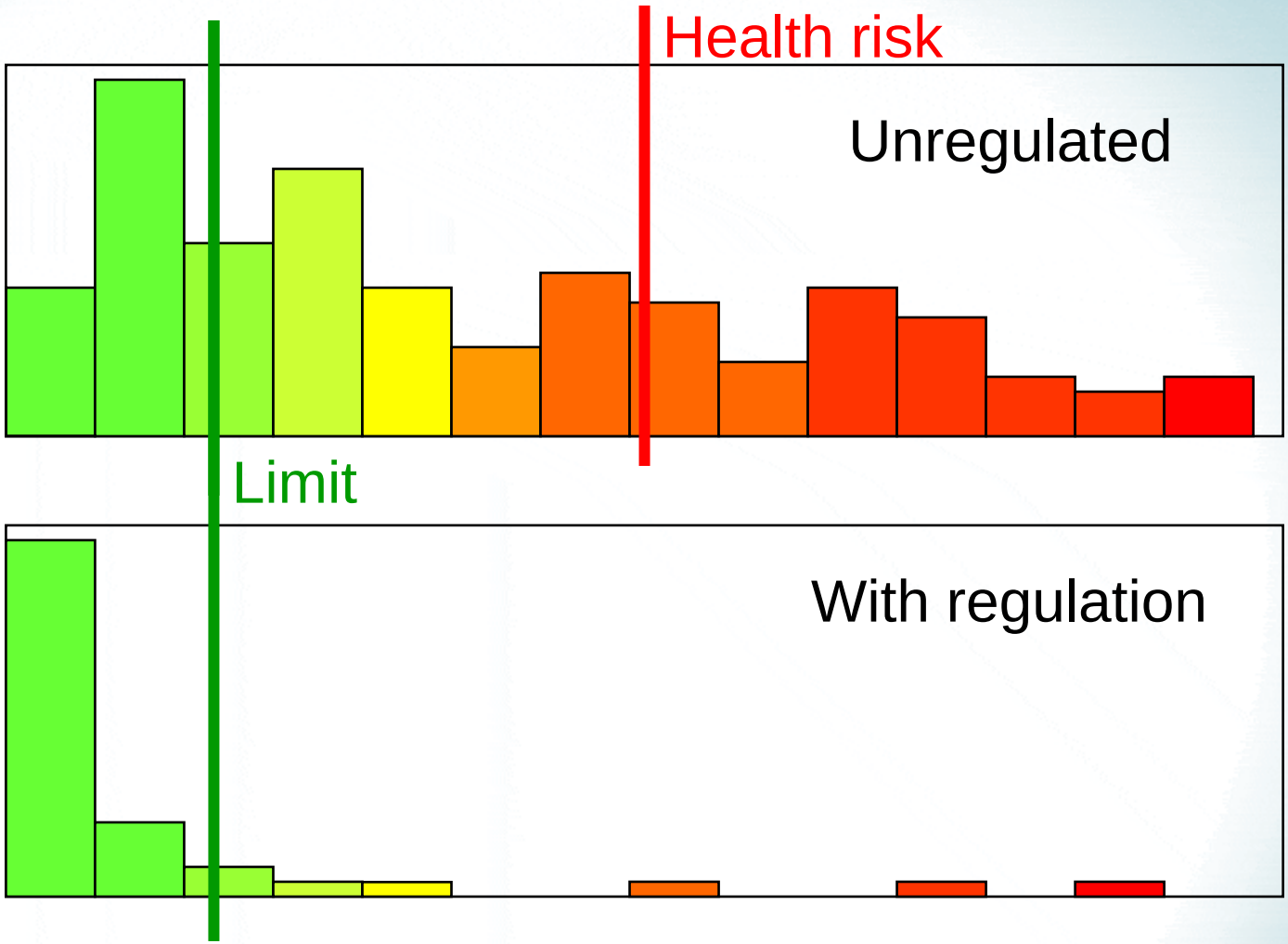
Setting standards in analytical science

- Set regulations to achieve aims
  - allow experts, courts and industry to establish methods of policing and compliance detection
- Do not assume measurement is the only enforcement method
- Set limits such that 'borderline cases' are not very important
- Act further if disagreement undermines regulation

**Inferred from observation*

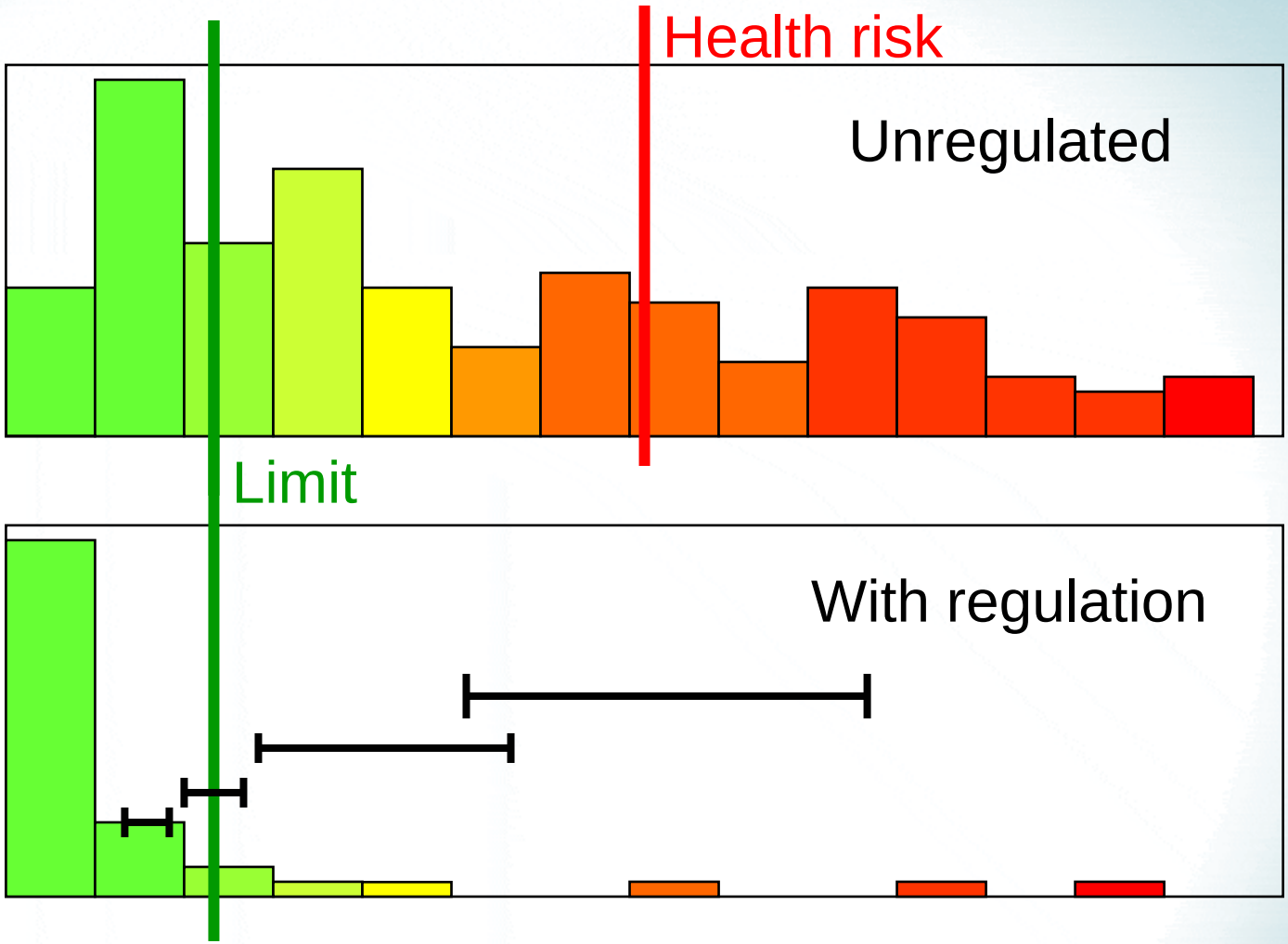
“Reasonable assurance”

Setting standards in analytical science



“Reasonable assurance” and uncertainty

Setting standards in analytical science

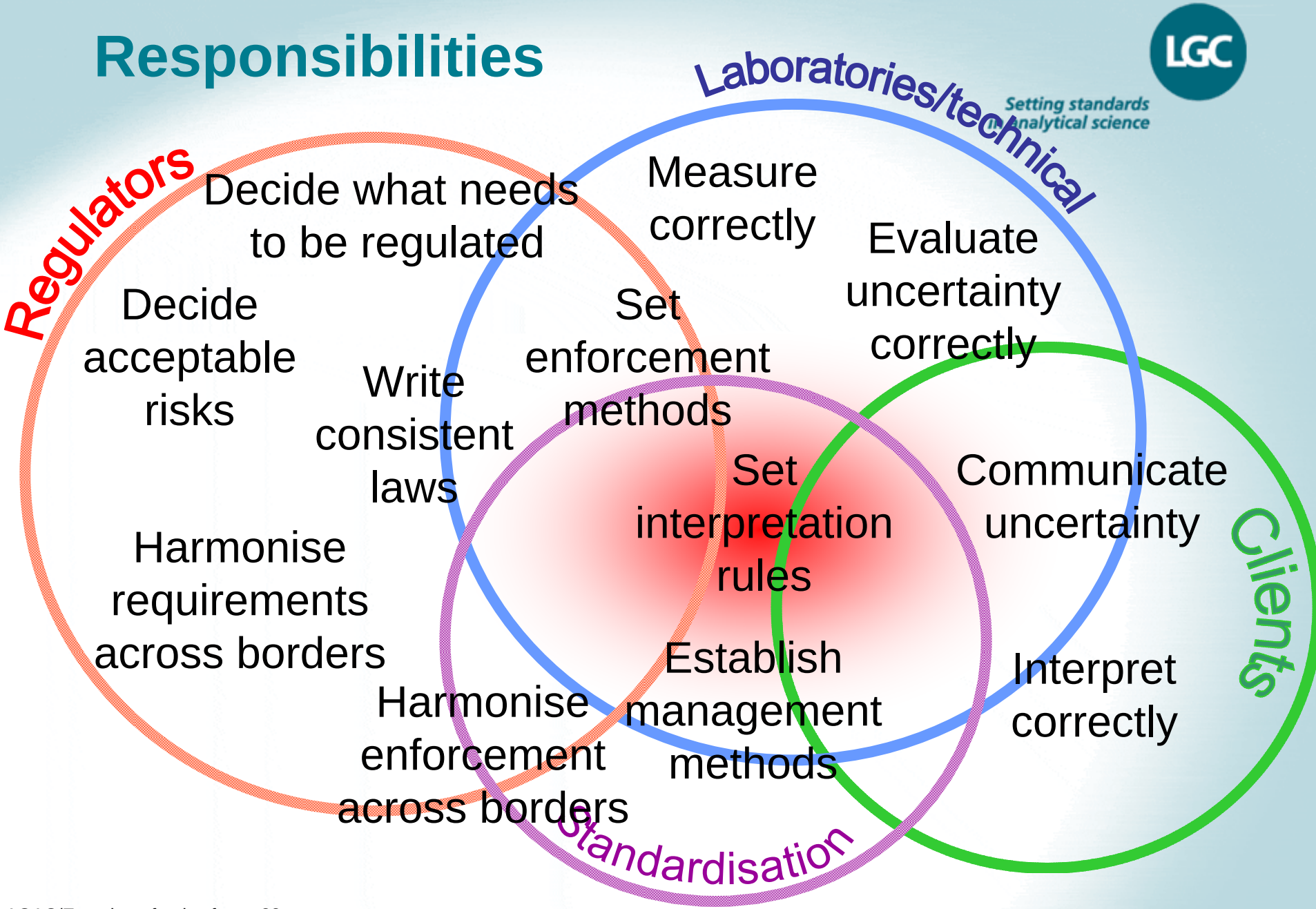


Managing uncertainty in regulation
Options for interpretation

Setting standards in analytical science

• Ignore uncertainty • Incorporate uncertainty in limit	Regulators and tech experts must establish acceptable uncertainty and demonstrate it
• Require uncertainty reporting	Labs estimate uncertainty; regulators/experts decide how and set interpretation rules
• Require expert interpretation	Labs must become experts; usually includes knowledge of MU

Responsibilities



Conclusions

Setting standards in analytical science

- Measurement uncertainty guides interpretation
- Interlaboratory study tends towards higher uncertainties
- Some technical issues still unclear
  - Using PT data; effect of proportionality
- Setting interpretation rules simplifies matters for enforcers
  - .. and should be a co-operative activity