Nondetects And Data Analysis:
Reporting & Detection Limits

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Practical Stats

Nondetects

- are "real data" !
- censored data – known only as above or below a threshold
- left- or interval-censored values
- left-censored <1: ← 1
- interval-censored (0 to 1): [0 ⟷ 1]
- contain much of the information present if a single value were reported

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Statistics for Censored Data

- censored data have been used in medical and industrial statistics since the 1950s
- there they usually are “greater-thans”, i.e. >10 , otherwise the issues are the same
- this area of statistics is called "Survival analysis" or "Reliability analysis"
- these methods are used in drug trials, testing equipment and processes, occupational health, astronomy, and in many other fields
- were a few papers in the environmental literature in the 80s and 90s, but these methods became much better known after the publication of my textbook *Nondetects And Data Analysis* in 2005

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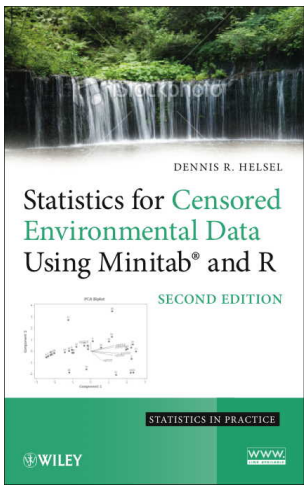
For more detail:

Statistics for Censored Environmental Data
(the second edition)

by Dennis R. Helsel
Wiley (2012)
www.PracticalStats.com/nada



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Reporting Limit

A general term

Calculated in a variety of ways for a variety of purposes

Are two primary types of reporting limits:

- Detection limits
- Quantitation limits

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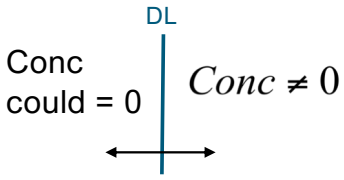
Reporting limits

(standard deviation assumed constant)

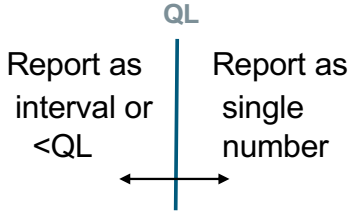
Detection Limit

Values measured above this threshold are unlikely to result from a true concentration of zero



Quantitation limit

Thresholds above which single numerical values (rather than an interval or <QL) are reported.



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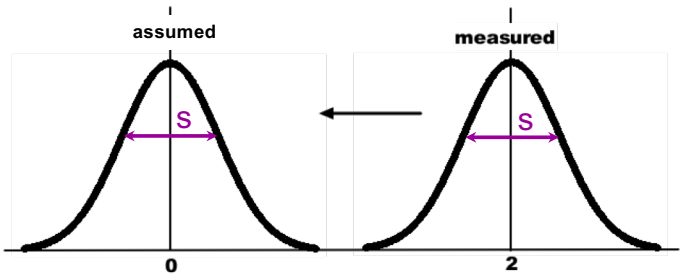
Setting a Detection Limit

Cannot easily measure a 0 signal, so…..

Noise around a standard solution = std deviation (s) assumed equal to noise around 0



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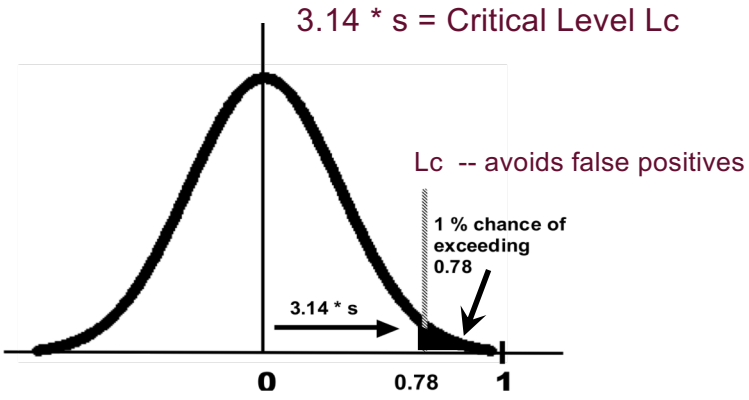
The Critical Level

3.14 * s above 0 should have only a 1% chance of truly originating from conc=0, assuming a normal distribution



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Other names for critical level

- decision level (Currie, 1968)

and infrequently and confusingly,

- method detection limit (MDL)
- limit of detection (LOD)
- Detection limit

Primary concept:
A true zero signal is unlikely to be measured above this threshold.
Avoids false positives, but not false negatives.

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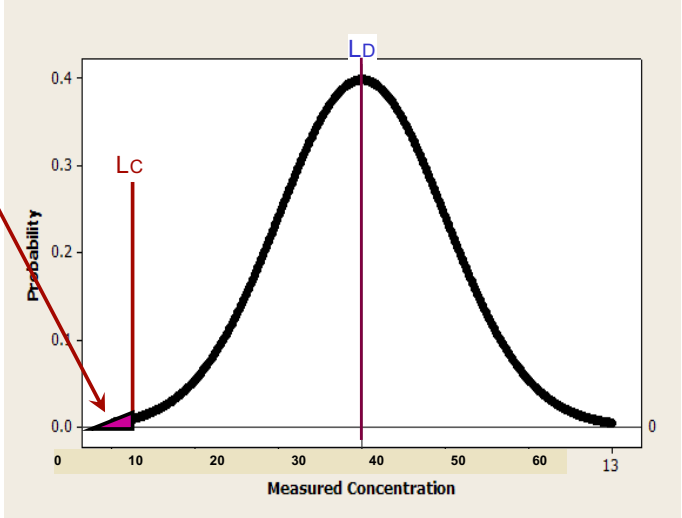
Detection Limit

"To avoid false negatives" ?? set a higher limit, the Detection Limit L_D.

A true concentration at the higher limit L_D has a 1% chance of being measured and reported as <Lc. It still has a 50% chance of being measured and reported as <DL.



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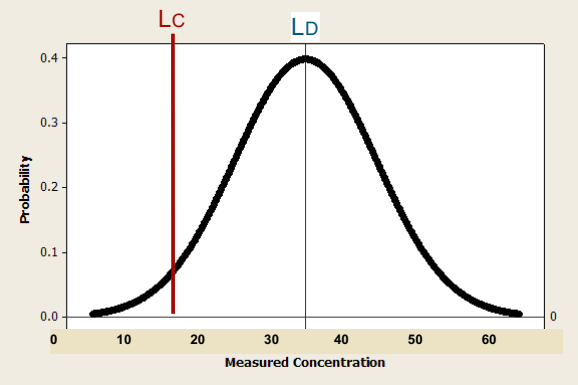
Detection Limit

Standard practice: $\alpha = \beta$, so, $L_D = 2*Lc$

Look at formulae used, not names.



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Other abbreviations for detection limit

- method detection limit (MDL)
- limit of detection (LOD)
- (DL)

Primary concept:

A true concentration at the critical level and therefore at 0, is unlikely to be measured above this detection limit.

Does not avoid false negatives for values above the DL being called <DL.

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Quantitation Limit

- is a higher threshold than L_D
- above the QL a reliable single number is reported
- usually based on a signal to noise ratio

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Setting a Quantitation Limit

- Quantitation limit is set at various values, often = 10 times the noise (signal/noise = 10)

  $10 * s = 3.18 * (3.14 * s) = 3.18 * L_C$

  This is 1.6 * DL. Often rounded to 2 * DL. The most common definition: 2 * DL
- Other multipliers used. 5 * DL, etc. Choice varies with laboratory staff and tradition.

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Other names for Quantitation limits

Limit of determination (Currie, 1968)

Limit of quantitation (LOQ)

Practical quantitation limit (PQL)

Lab reporting level (LRL)

Primary concept:

Above this level the signal is sufficiently larger than the noise to report a reliable single number.

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Data Between the Limits

Between the L_D and QL are observations which are not zero, but are too variable to report as a single number.

Labs differ on how to report them

"J values" "E values" "remarked data"

Primary concept:

One remarked value (4J) cannot be certain to truly be below or above another (5J). Too much noise.

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Data Between the Limits

- Is agreement that data above the QL are reported as single values.
- Most agree that data below the L_D are reported as being between 0 and the L_D (interval) or < L_D.
- There is not agreement on what to do with data between the L_D and QL. Are 3 valid options:

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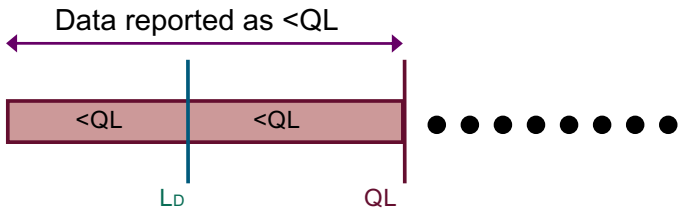
Data Between the Limits

1. Use the quantitation limit as the reporting limit for all values measured below the QL



This has traditionally been done over the years

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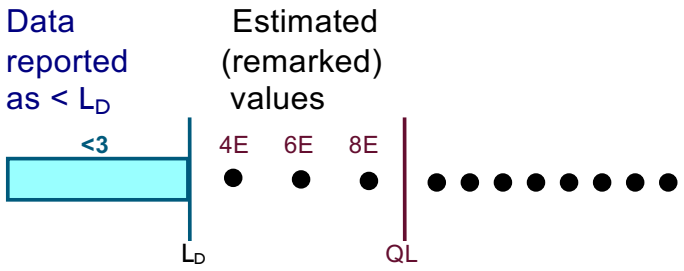
Data Between the Limits

2. Use the detection limit as the reporting limit



Some labs do this today to provide estimates for 'low-level' data

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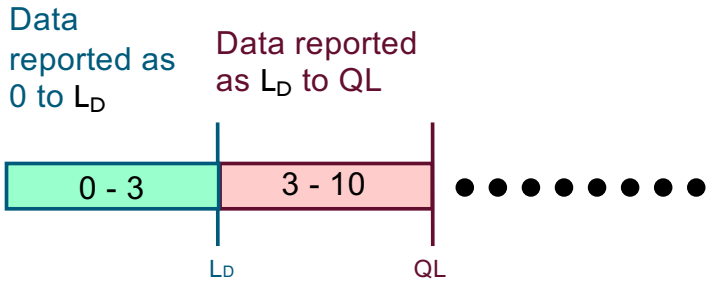
Data Between the Limits

3. Use interval-censored methods



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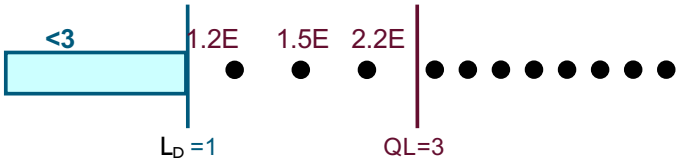
Avoid Insider Censoring!

Data reported as <QL

E's dropped and used as 'detects'. Limit for these is L_D



Problem: The RL used differs depending on the concentration that was measured. This produces upwardly biased estimates for mean and incorrect shape.

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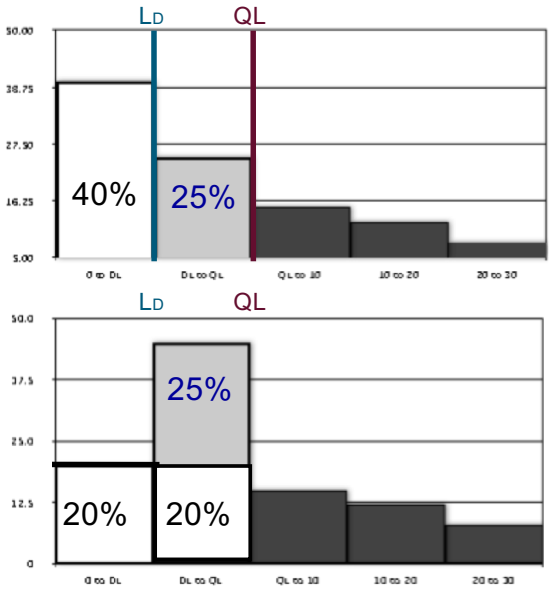
Insider Censoring



Data as measured

Reporting measured <L_D as <QL

Biased data reported

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Insider Censoring

- Adds positive bias to all data, for all subsequent analyses
- Changes shape of distribution
  - Probability plots no longer accurately judge shape of data as measured
- Advocated or mandated (!) by some agencies
- Avoid insider censoring!

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Reporting Limits - Summary

Detection Limit: below might be a zero concentration

Quantitation Limit: below is data with too much noise to report as a single number

Can properly censor data either

- At the quantitation limit
- At the detection limit
- Within the two intervals (0 to L_D) and (L_D to QL)

Do not use insider censoring, or data will be biased upwards with an incorrect cdf. If used by the lab, re-censor all data to QL.

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