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Detection limits

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Literature

L.A. Currie: Anal. Chem. 40(3):586-593 (1968)

L.A. Currie: Anal. Chimica Acta 391: 127-134 (1999)

L.A. Currie: Appl. Rad. Isot 61: 145-149 (2004)

ISO 11929-3 “Determination of the detection limit and decision threshold for ionizing radiation measurements – Part 3: Fundamentals and application to counting measurements by high resolution gamma spectrometry, without the influence of sample treatment

D.J. Strom, J.A. MacLellan: Health Physics 81(1):27-34(2001)

Literature

New International Standard that uses Bayesian statistics

ISO 11929-7 “Determination of the detection limit and decision threshold for ionizing radiation measurements – Part 7: Fundamentals and general application

http://www.iso.org/iso/home/store/catalogue_ics/catalogue_detail_ics.htm?csnumber=31070

Concepts

- Critical limit (L_C)
- Upper limit (L_U)
- Detection limit (L_D)
- Determination limit (L_Q)
- Minimum Detectable Activity (MDA)

- **“a priori detection limit” (now Detection Limit, L_D)**
- **“a posteriori upper limit” (now Decision Threshold, L_C),**

Lloyd A. Currie: “Limits for Qualitative Detection and Quantitative Determination” Anal. Chem. Vol.40, No.3, 1968

Hypothesis test

ERROR TYPE I

α

Hypothesis test

ERROR TYPE II

β

EXERCISE

At an above ground laboratory a gamma-ray peak at 662 keV is found. It is concluded that the peak is above decision threshold.

Later at an underground laboratory no sign of the peak was found when the same sample is measured.

Which type of error was made in the above ground laboratory? (Type I or Type II)

How do we know that it was not a Type II error of the underground laboratory?

DECISION THRESHOLD

There was nothing in the sample
What is the maximum amount that could be present?

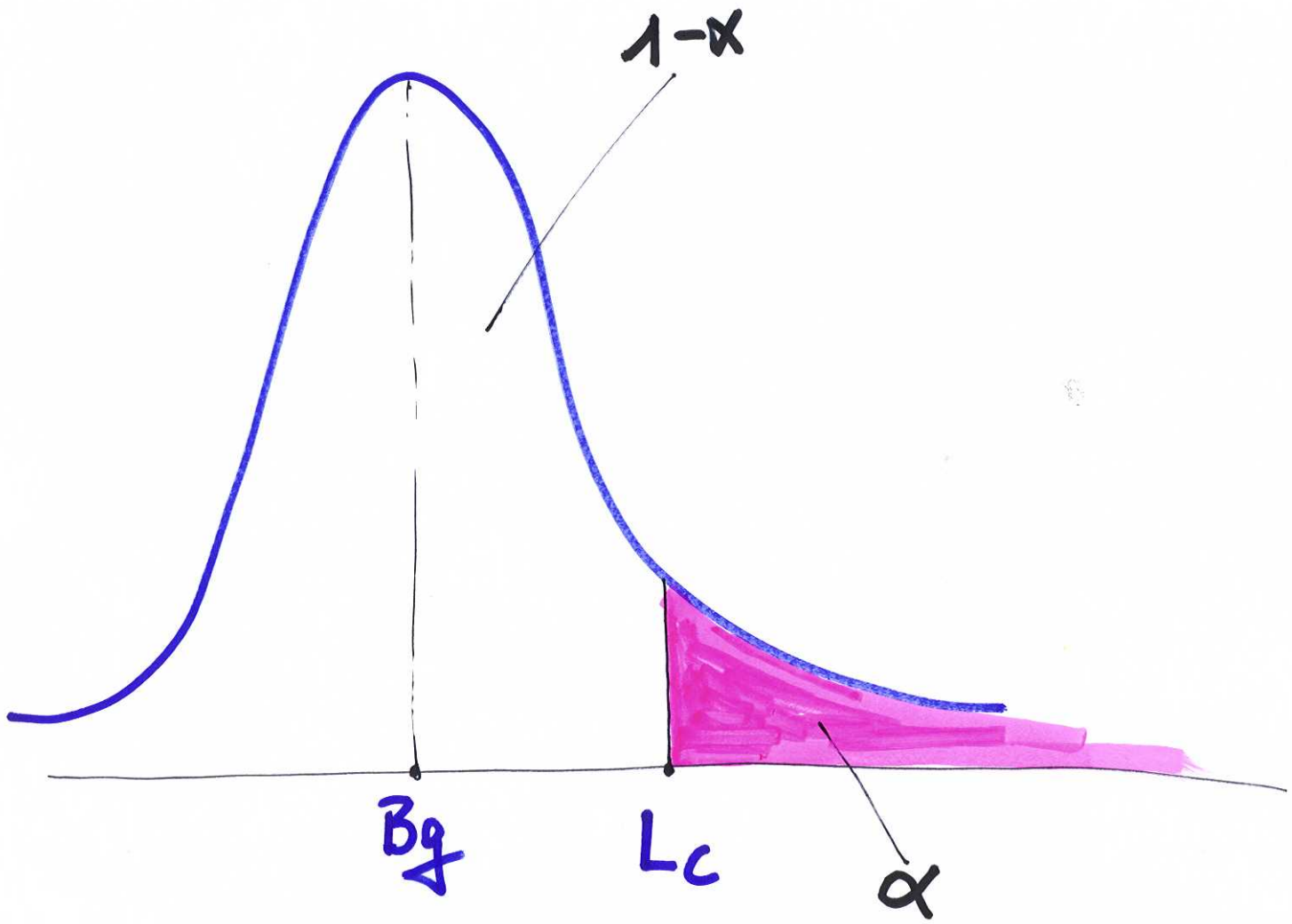
Is the net count significant?

Significance Level

$\alpha = 0.05$ **(IUPAC recommended)**

$\alpha = 0.01$

Significance Level



DETECTION LIMIT

What is the <u>minimum</u> amount this instrument can detect?

Power

$1 - \beta = 0.95$ **(IUPAC recommended)**

$1 - \beta = 0.99$

QUANTIFICATION LIMIT

$= L_Q$

= Determination limit

Minimum quantifiable value

How many counts would I have to have to achieve a particular statistical uncertainty?

RSD_Q = Relative Standard Deviation

IUPAC recommendation = 0.10

→ $L_Q = k_Q \sigma_Q$, with $k_Q = 1/RSD_Q$

Working expression: $L_Q = 10\ \sigma_0$

Also a priori

WHEN IS OUR RESULT DIFFERENT ENOUGH FROM THE BACKGROUND VALUE?

Working Expressions

$$L_c = 2.33\ \sigma_b$$

$$L_d = 4.65\ \sigma_b$$

Decision Threshold – general case

$$L_C = k_{1-\alpha}\sqrt{\sigma_s^2 + \sigma_b^2} =$$

Common error in many software to take too short region for background determination

$$= 1.645\sqrt{2\,\sigma_b^2} =$$

$$= 2.33\,\sigma_b$$

FOR $\alpha = 0.05$

AND $\sigma_s^2 = \sigma_b^2$

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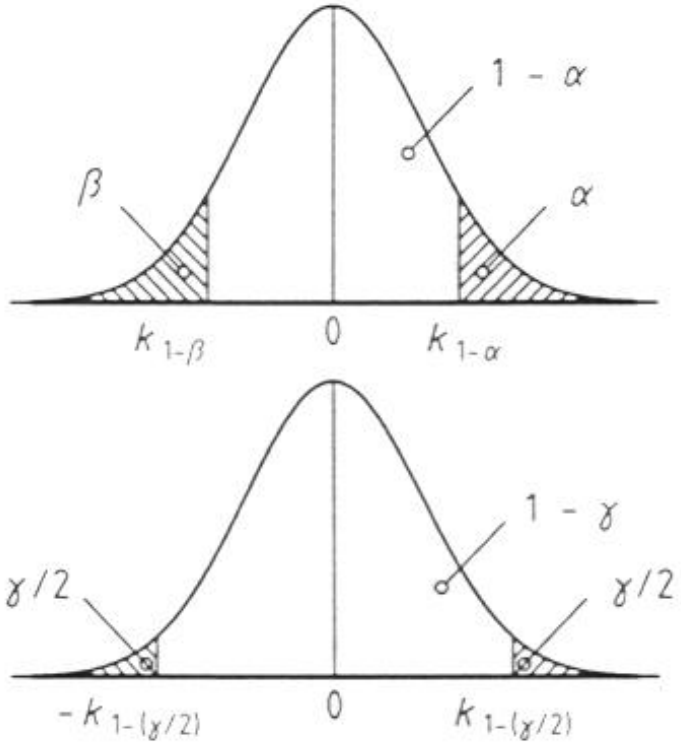
k-values from tables

ISO 11929-3:2000(E)

Table 2 — Values $k_{1-\alpha}$, $k_{1-\beta}$, $k_{1-(\gamma/2)}$ as a function of the error probabilities α and β and of the confidence level $1-\gamma$ (quantiles of normal distribution)

Error of probability α or β	Confidence level $1-\gamma$	$k_{1-\alpha}$, $k_{1-\beta}$, $k_{1-(\gamma/2)}$
0,1586	0,682	1,000
0,1000	0,800	1,282
0,0500	0,900	1,645
0,0250	0,950	1,960
0,0228	0,955	2,000
0,0100	0,980	2,326
0,0050	0,990	2,576
0,0014	0,997	3,000
0,0010	0,998	3,090



Detection Limit – general case

$$L_d = L_C + k_{1-\beta}\sqrt{\sigma_s^2 + \sigma_b^2} =$$

$$= (k_{1-\alpha} + k_{1-\beta})\sqrt{\sigma_s^2 + \sigma_b^2} =$$

$$= (1.645 + 1.645)\sqrt{2\,\sigma_b^2} =$$

$$= 4.65\,\sigma_b$$

FOR $\alpha = \beta = 0.05$

AND $\sigma_s^2 = \sigma_b^2$

Regions for determination of a peak (ISO 11929-3)

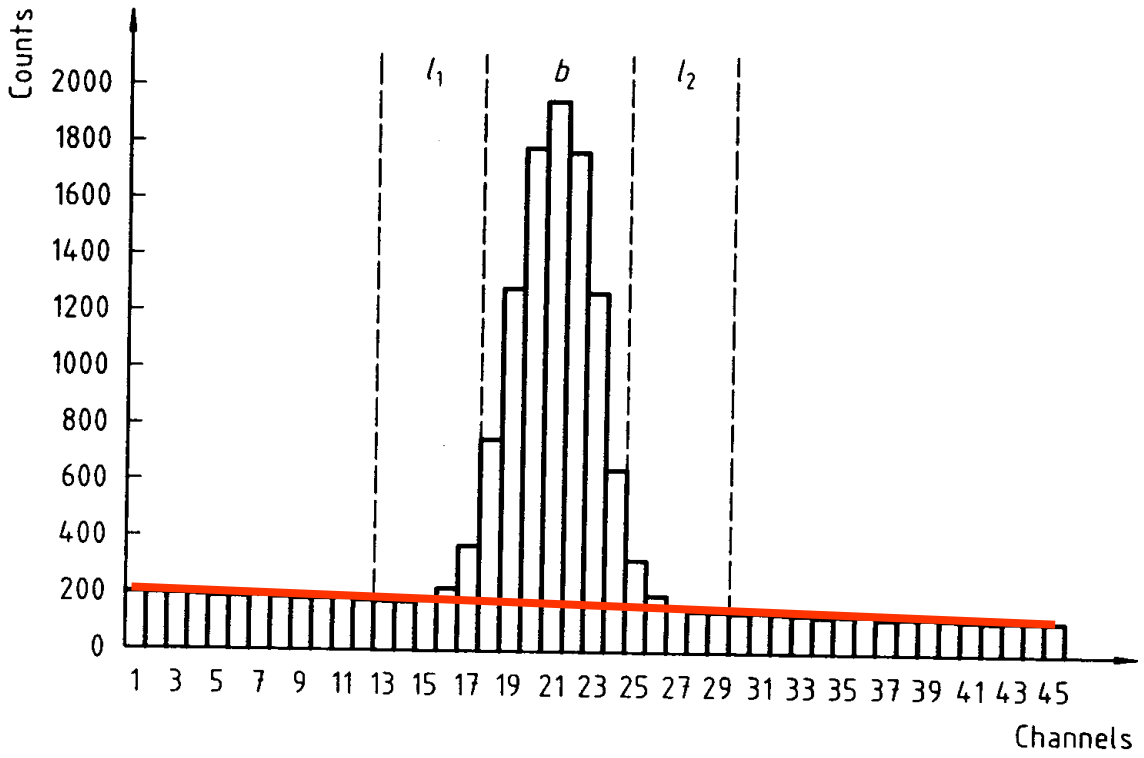


Figure 1 — Specification of regions on a peak

Peak / background

ISO 11929-3:2000 The number of background counts in the region of interest can be determined from channels of the regions A_1 and A_2 on both sides of the region of interest by the trapezoid rule:

$$N_0 = (N_1 + N_2)\frac{b}{2l}$$

with: FWMH ≤ b ≤ 2.5 FWHM and b ≥ 4 channels

and $b \le 2l \le 10b$

Other procedures which give similar results for the background can also be used.

The Detection Limit
(with a certain power value)
defines your
measuring system

The Decision Threshold
(with a certain significance level)
defines your
result !

“The difference between using the decision threshold and using the detection limit is that measured values are to be compared with the decision threshold while the detection limit is to be compared with the guideline value”

ISO 11929-3:2000

Decision threshold

	Approximated formula (more exact)	Simplified formula
ISO 11929-3	$R_n^* = \frac{k_{1-\alpha}^2}{2t}\frac{b}{2t}\left[1+\sqrt{\frac{4R_0 t}{k_{1-\alpha}}\frac{2l}{b}\left(1+\frac{2l}{b}\right)}\right]$	$R_n^* = k_{1-\alpha}\sqrt{\frac{R_0}{t}\left(1+\frac{b}{2l}\right)}$
DIN 25482-5	$R_n^* = \frac{k_{1-\alpha}^2}{2t}\frac{b}{2l}\left[1+\sqrt{1+\frac{4R_0 t}{k_{1-\alpha}^2}\frac{2l}{b}\left(1+\frac{2l}{b}\right)}\right]$	$R_n^* = k_{1-\alpha}\sqrt{\frac{R_0}{t}\left(1+\frac{b}{2l}\right)}$

R_n^*	Net effect counting rate, difference between gross and background effect counting rates
R_0	Background effect counting rate
α	Probability of wrongly rejecting the hypothesis (error of the first kind)
$k_{1-\alpha}$	Quantile of normal distribution for error of the first kind

Recommendations

- **Distinguish between Detection limits and Decision Thresholds**
- **State which formula you use**
- **Give (at least check) the actual false detection rate for blanks**
- **Give upper limit instead of "non-detects"; or even better give value + uncertainty even if value is lower than L_C (provided you state L_C)**

Recommendations (2)

- Current formulas are bad < 100 counts
- Current formulas yield too many false positives
- Keep your eyes open for alternative approaches (Strom and MacLellan Health Phys. 81(1)27-34, 2001)
- Distinguish between “sensitivity” and “detection limit”