Practical Aspects of the Concept “Lower Limit of Detection”

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A sample's "true" count rate

from N atoms of interest is:

$R(s) = N*\lambda$ ...

Any "actual" count rate includes background:

$C(s+b)/t = C(s)/t + C(b)/t$

Unfortunately, often C(b) >> C(s) … !

What to do about correcting background?

- Measure a background or "blank" count rate C(b)/t

$$R(b) = C(b)/\ t(b)$$

- Measure a gross sample count rate

$$R(s+b) = C(s+b)/\ t(s+b)$$

- Calculate the net count rate from

$$C(s) = C(s+b) - C(b), \quad R(s) = C(s)/\ t(s)$$

- Test the "significance" of the net count (or rate)

  to decide if there is any activity > background…

Significant compared to what …the background ?

The objective here is to compare the gross sample activity against a reference value – the background – to test the hypothesis that the sample contains net activity (or not) …

The trick is to invoke a statistical model to relate actual observed net counts (or count rate) to what would be the "true" counts – or "true" mean count rate - of the radionuclide in a model distribution … then generate estimates and likelihoods …

A probability model for decay of radioactive atoms ….

The Poisson probability density distribution:

$$P(C;u) = u^C e^{-u} / C!$$

Where P(C;*u*) = probability of observing C counts in time t when the mean count is *u* and the "true" count rate is R: *u* = R t .

The standard deviation $\sigma = \sqrt{u}$

This is only a one-parameter model….

If the number of events (samples) is “large”,

The probability of observing n counts can be approximated by

$$P(n) = \frac{1}{\sigma\sqrt{2\pi}}\exp(-(n-u)^2/2\sigma^2)$$

… the Gaussian probability model where σ is the standard deviation of a normal distribution…

Reasonable assumptions about the ‘normality’ of the distribution of counts and the number need to be made …

What is a ‘large’ count for practical purposes ?

Suppose the mean u ~ n= 40

the prob. of observing exactly 40 counts is

$$P(Poisson) = \frac{40^{40} * e^{-40}}{40!} = 0.0629$$

….while by the Gaussian (normal) approximation it is

$$P(Gauss) = \frac{1}{\sigma\sqrt{2\pi}} * \exp(-0) = \frac{1}{\sqrt{40} * \sqrt{6.28}} = 0.0631$$

This looks pretty good … but how many counts are really needed …30, 50, ...? Some say at least 50

The ‘background interference’ problem is …

Find a small signal in the presence of a lot of noise …

Detection is easy if the radionuclide signal rate R(s) is >> R(b)…

What if it is not ?

Hypothesis testing using Normal Statistics models …

Use Bayesian inference including ‘prior’ information …

Start with determining net counts and their standard deviation …

We measure a net count rate including background:

R(net) = R(gross) – R(b) = C(g)/ t(g) – C(b)/ t(b)

The standard deviation of the net count rate, s(n) is

$$s(n) = \sqrt{R_g / t_g + R_b / t_b}$$

which is a measure of precision of the measurement

If $R_b >> R_g$, background dominates s(n)

Addressing the problem by Hypothesis Testing….

* Formulate a 'null hypothesis' : that the distribution of net counts represents the 'blank' (mean count = 0), and determine if this hypothesis can be rejected – i.e., if the alternative hypothesis (mean count >0) is true

* Assume data approximate a Gaussian Distribution

* Apply a Decision Rule to decide to accept or reject the null based on its likelihood …

Hypothesis Testing (I) …Nulll & Alternative

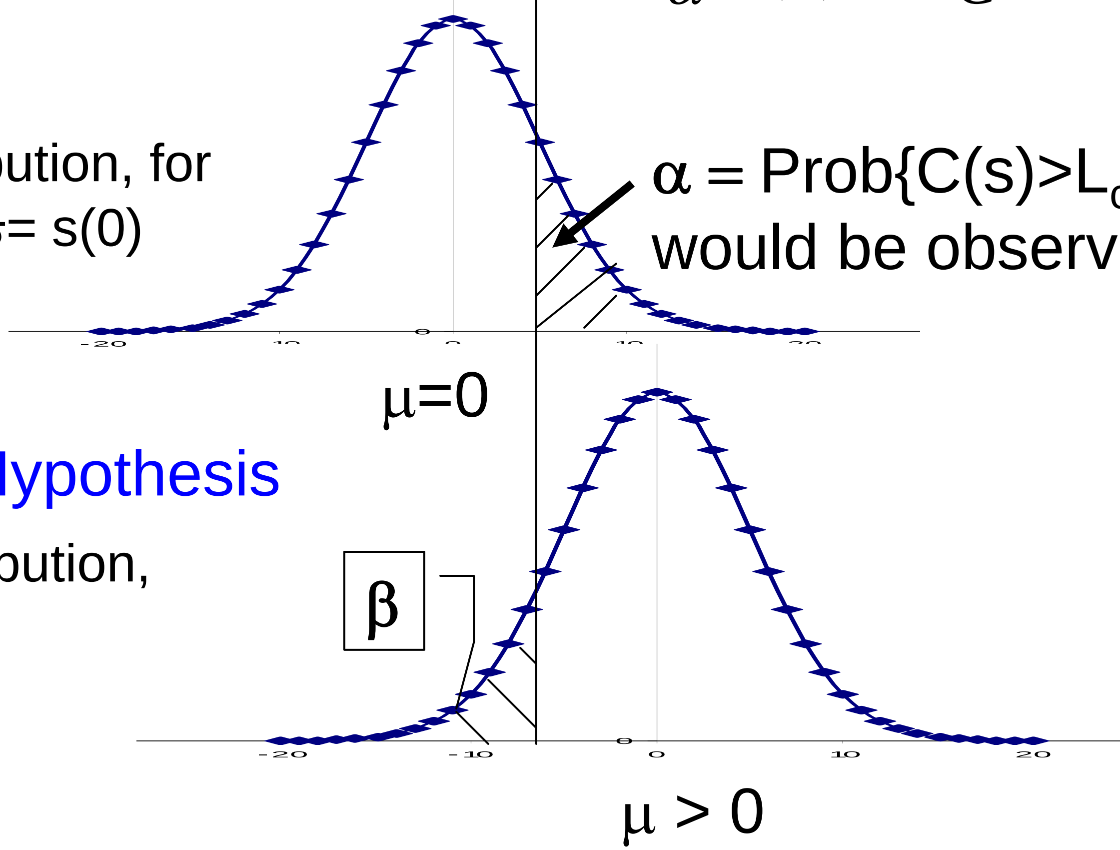
The Null Hypothesis : count distribution has mean = 0,

Std. Dev.= $\sigma(0) \approx s(0) = \sqrt{\{C(s)+C(b)\}+C(b)} = \sqrt{2*C(b)}$

Define decision level: $= k_\alpha \sigma(0) = L_C$

A. Normal distribution, for mean μ = 0, σ= s(0)

α = Prob{C(s)>L_c would be observed}



The Alternative Hypothesis

B. Normal distribution, mean μ > 0

Hypothesis Testing (II) … decision rule

Here’s the decision rule: if C(s) > L_C , accept that μ>0

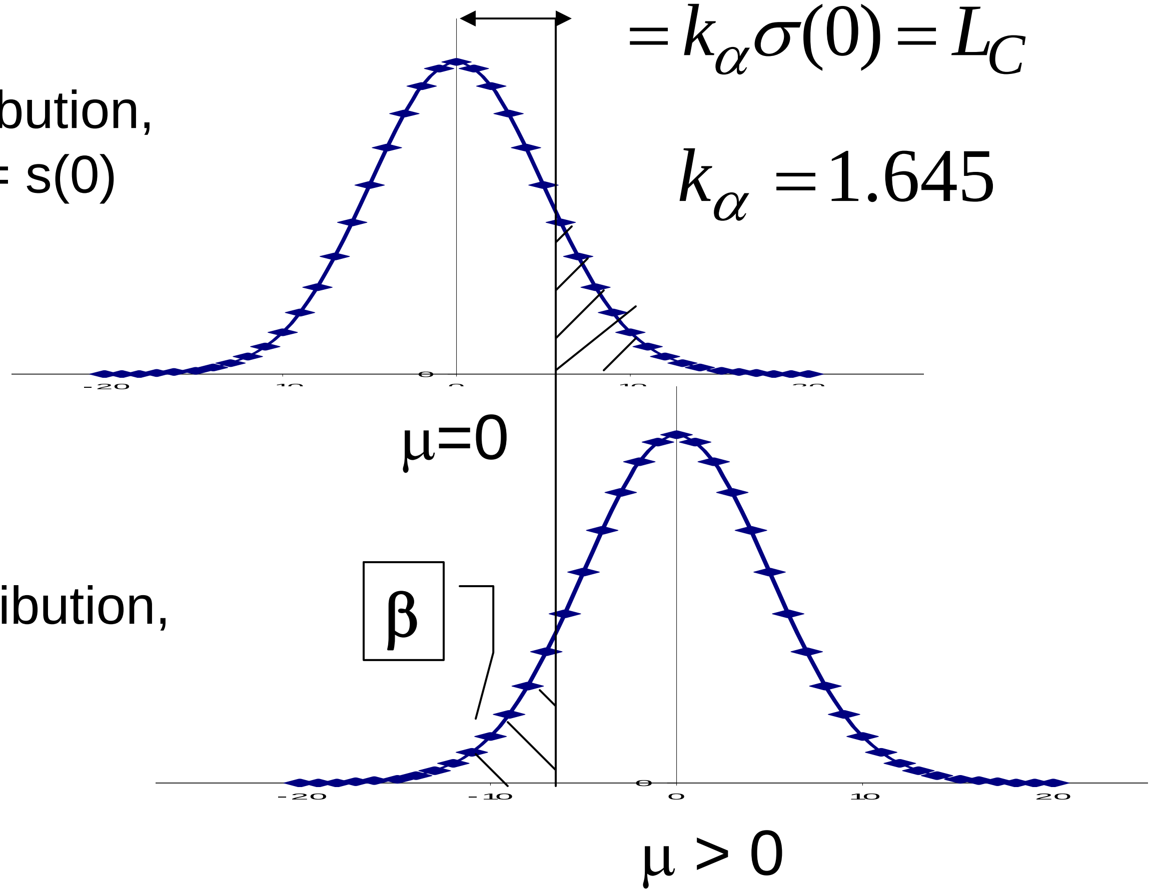
(α= prob. of “false positive” error, typ.= 5%), else accept μ =0.

$$= k_\alpha \sigma(0) = L_C$$

$$k_\alpha = 1.645$$

A. Normal distribution, mean = 0, σ= s(0)

B. Normal distribution, mean μ > 0



We estimate $\sigma(0)$ by s(n) evaluated at R(n) = 0 …
i.e., when R(gross) = R(background) :

$$\sigma(0) \approx s(0) = \sqrt{2R_b / t_b},$$ for the paired observation case

Define $L_C = k(\alpha)\ \sigma(0)$, for α = 5% , $k(\alpha)$=1.645

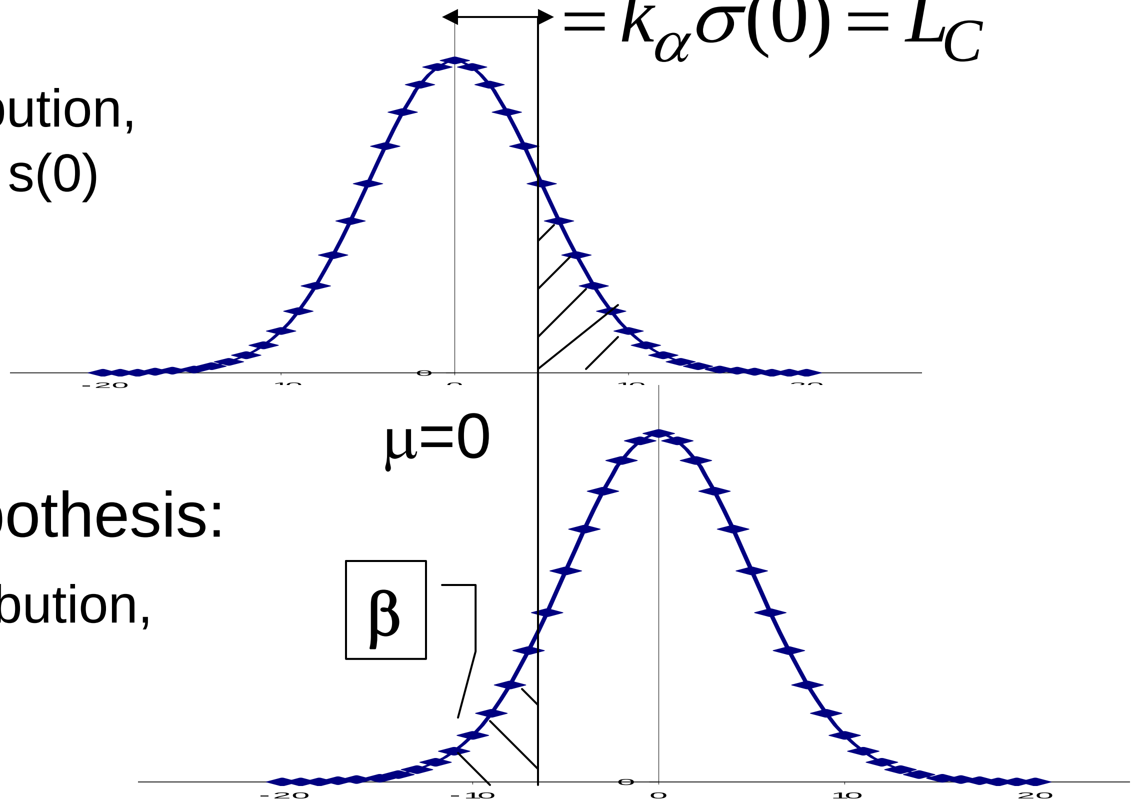
$$L_C = k(\alpha)\sqrt{2R_b / t_b} = 1.645 * \sqrt{2R_b / t_b} = 2.33\sqrt{R_b / t_b}$$

Note: as μ_s->0 for fixed μ_b an increasing fraction of net count observation fail to yield evidence of activity in the sample !

Hypothesis Testing (III) … the "false negative"

$$= k_{\alpha}\sigma(0) = L_C$$

A. Normal distribution, mean = 0, σ= s(0)



Alternative hypothesis:

B. Normal distribution, mean μ>0

μ > 0

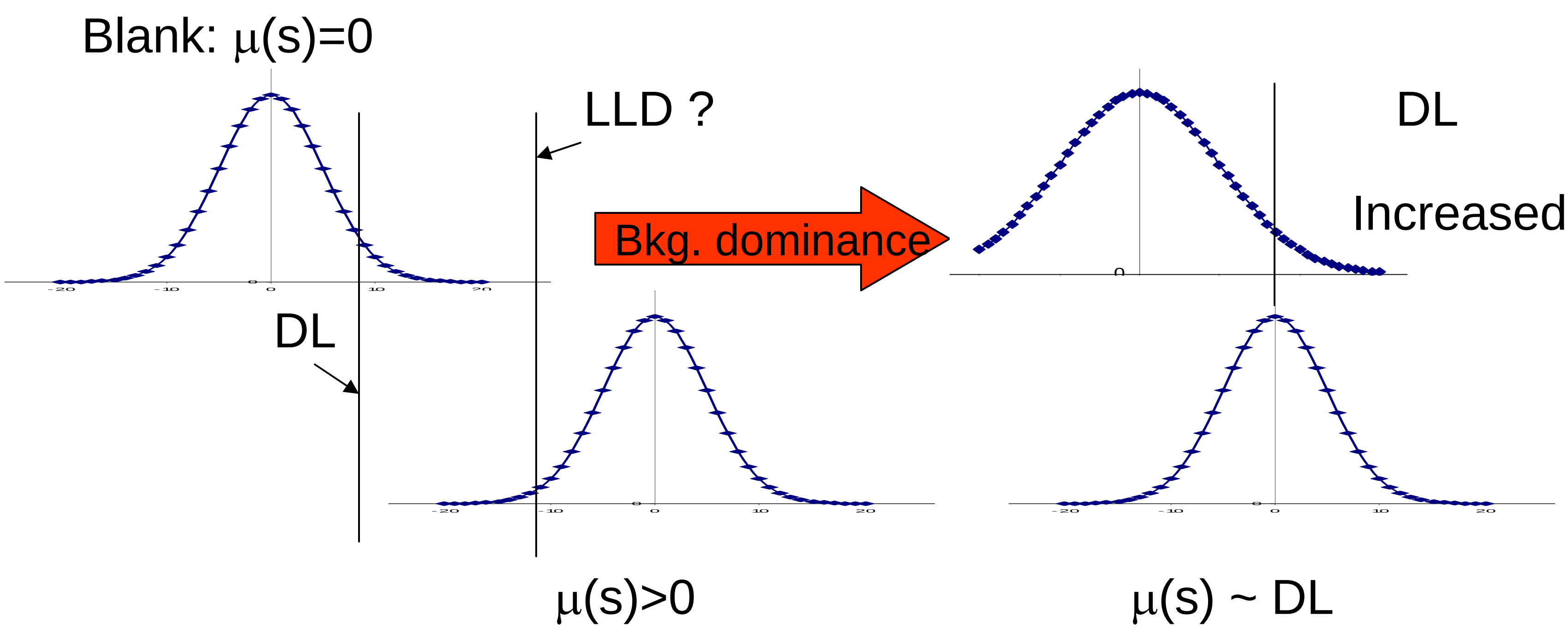
β = Prob { C(s) < L_C would be observed when μ(s) >0}

… the chance a net positive count will produce the wrong decision !

The 'Power' of the Decision Rule …

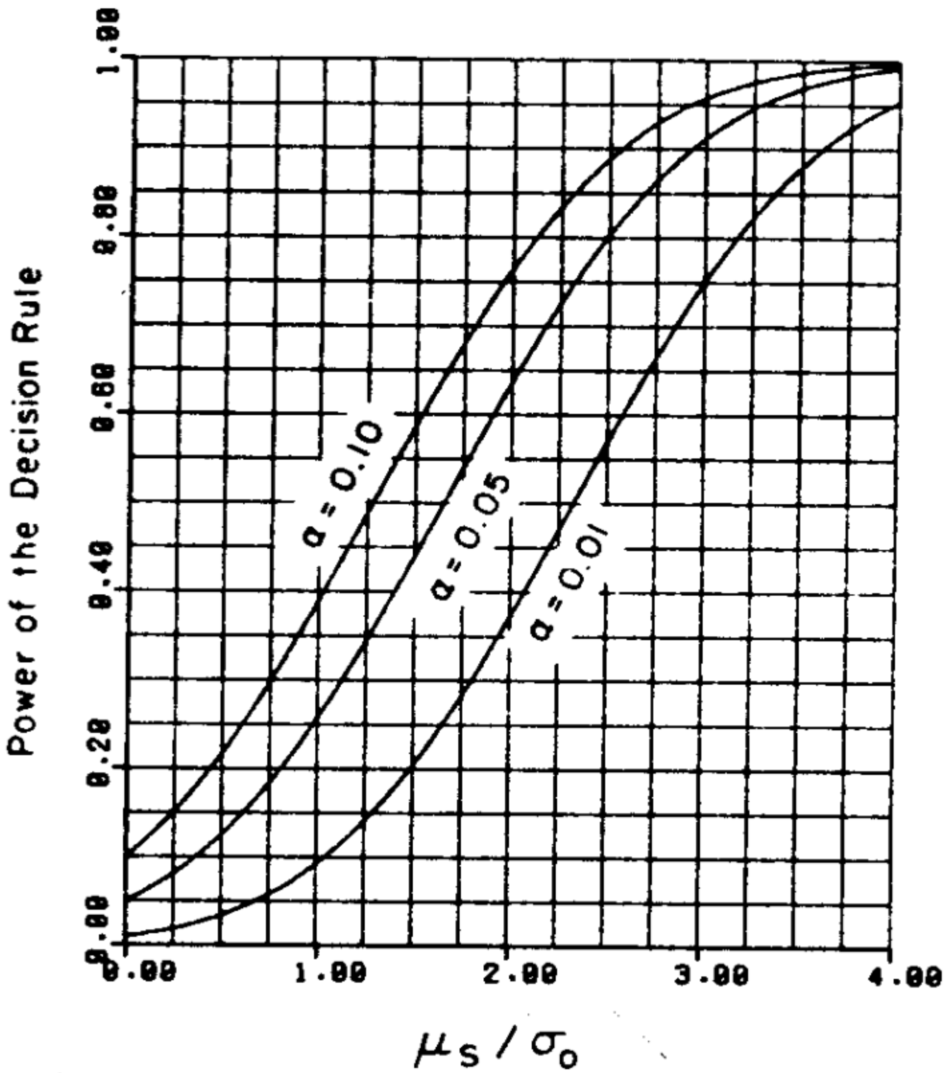
If β = 5%, then (1-β) = 95%, which is the probability that when μ(s)>0, a correct decision is made based on finding a net positive count (C(s) > 0).

The quantity 1-β is called the 'power' of the decision rule[1].



(1) Donn & Wolke, Health Phys. (32),1977

Power of the decision rule vs ratio of 'true' net count μ_s to the standard deviation of well-known blank σ_0



μ_s/σ_0 may be thought of as a signal to noise ratio – or a measure of background dominance…check the case when ratio is 1.645 … (!)

(From Donn & Wolke, Health Phys.,(32) 1977)

The “Lower Limit of Detection” - LLD

LLD is the smallest concentration of radioactive material in a sample that will yield a net count above the blank that will be detected with at least 95% probability, with no greater than 5% probability of falsely concluding that a blank observation represents a “real” signal.

Thus, LLD is the lowest $\mu(s)$ for a given $\mu(b)$ which will ensure 95% power …”

For paired measurement LLD = 2 *L_C = 4.65 $\sigma(0)$

Some observations about the Decision Rule …

• For net counts (count rates) > L_C , the chances of "false positive" results are low – report "detected"

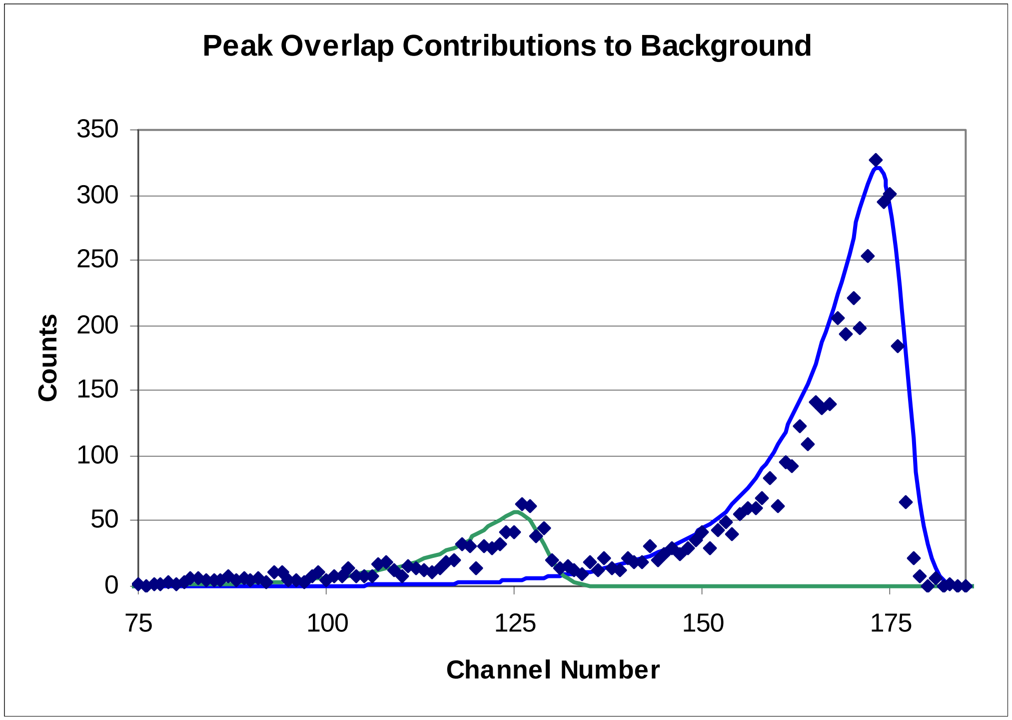
• As mean of the net C(s) get larger (relative to σ_0), the "power" of the decision increases – more confidence in reporting "detected"

• If "false negative" decisions are unwanted, increase required counts for the decision … do this by improving the procedure (e.g., longer counts, sigma multiplier ?)

• L_C is the "alert level"… "action level"…. "alarm level", **not** LLD (or MDA) !

• LLD is the level against which the capability of a system to reliably detect a given quantity is assessed !

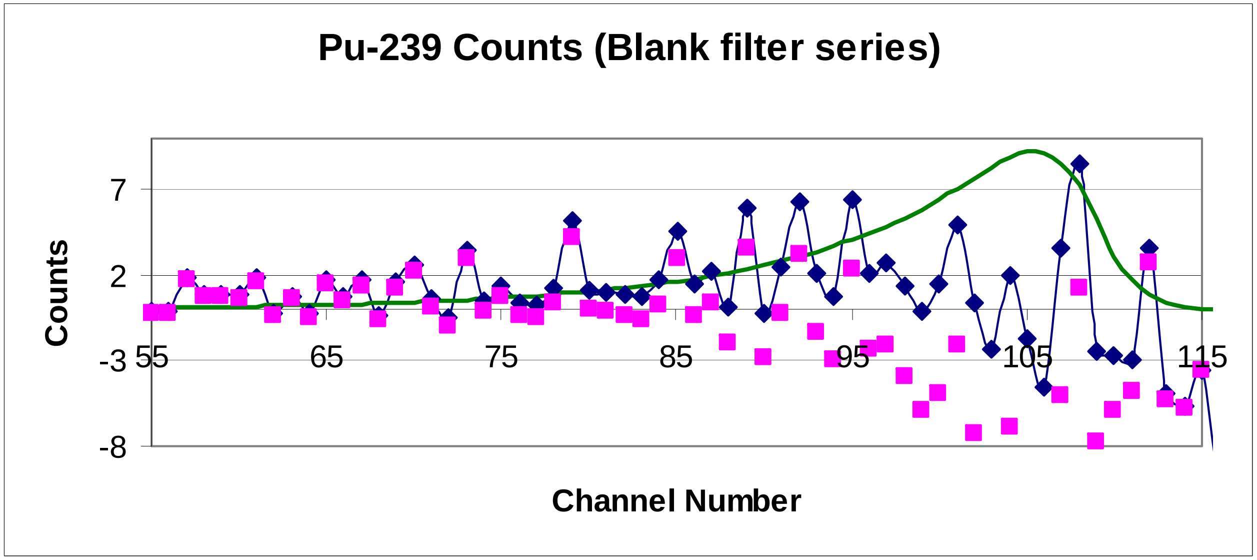
Calculating σ(0) for alpha spectroscopy …



Higher energy peak tails overlap to influence background

$$\sigma_0 = \sqrt{2(T_{8.78} + T_{7.68} + T_{6.0} + ...}$$

Inaccurate tail subtraction can leave residuals that can lead to spurious peak fitting … a blank effect tricky to quantify …



Count data April 17 21:16:02

Some questions …. (?)

Which is more important – accurate count of the target radionuclide, or assuring blank statistics are determined accurately ?

What should you (your instrument) report if a net count is less than the DL ?

Minimum detectable activity (MDA) is an activity large enough that it is unlikely not to set off the alarm … level with acceptably low 'false negatives' …?

The Decision Level is an amount of activity large enough to claim "detected" …that it is unlikely to be a "false alarm"…

… is one more important than the other?

Some references …

J. Donn and R. Wolke, "The Statistical Interpretation of data from measurements of low-level radioactivity", HP, Jan. 1977.

D. Strom, "False alarms, true alarms, and statistics…", Continuing Ed. Lecture, HPS July 15, 1998 (see PNNL website)

L. Currie, "Limits for qualitative detection and quantitative determination", Anal.Chem. 1968; also NUREG/CR-4007

ISO 11929-(1 – 8), "Determinationn of the detection limit and decision threshold for ionizing radiation", 2005. (says values are compared to DT; DL compared to "guideline values"..)

G.Miller, H.Martz, T.Little, and R.Guilmette, "Using exact Poisson liklihood functions in Bayesian interpretation of counting measurements", LA-UR-01-2443, 2001. (say the use of DL itself seems problematical …may lead to loss of information)