Is Anything There?
Evaluation of Statistical Decision Rules for Radioactivity Counting Experiments

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Applied Modeling and Computations in Nuclear Science
American Chemical Society
Washington, DC 30 August 2005

Work supported by the U.S. Department of Energy under Contract No. DE-AC06-76RLO 1830

Outline

- The Measurands and the Observables
- The *two* “counting problems”
- Individual sample decision levels and the “Great Leap of Inference”
- Compare measurements with decision threshold, not detection level
- Decision strategies (Bayesian and classical)
- Probabilistic blank and environmental background subtraction

The Measurands and the Observables

Battelle

Notation 1: The Measurands - [Unknown] Population Parameters

- By convention, Greek letters denote population parameters
- These reflect the *measurand*, the “true state of Nature” that we are trying to infer
- ρ_b: long-term blank count rate (s^{-1})
- ρ_n: long-term net count rate (s^{-1}) (due to analyte in unknown)
- ρ_g: long-term gross count rate (s^{-1})

Notation 2: The Measurands - [Unknown] Population Parameters

- Parameters are needed for sampling from population distributions
- μ_b: number of blank counts expected during t_b
- μ_g: number of gross counts expected t_g
- $\sigma(\rho_n)$: standard deviation of long-term net count rate (s^{-1})

Relationships Among Population Parameters

$$\text{number of counts} = \text{rate} \times \text{time}$$

$$\mu_{\mathrm{b}} = \rho_{\mathrm{b}} t_{\mathrm{b}}$$

$$\mu_{\mathrm{g}} = (\rho_{\mathrm{b}} + \rho_{\mathrm{n}}) t_{\mathrm{g}}$$

$$\sigma(\rho_{\mathrm{n}}) = \sqrt{\frac{\rho_{\mathrm{b}}}{t_{\mathrm{b}}} + \frac{\rho_{\mathrm{b}} + \rho_{\mathrm{n}}}{t_{\mathrm{g}}}}$$

The Observables

- Same apparatus for blank and sample
- Assume count times known (time preselection)
- Assume no non-Poisson variance

Notation - 3: Observed Quantities

- Convention: Roman letters denote observed quantities
- N_b: number of blank counts observed
- N_g: number of gross counts observed
- t_b: blank count time (s)
- t_g: gross count time (s)
- R_b: blank count rate (s^{-1})
- R_g: gross count rate (s^{-1})
- R_n: net count rate (s^{-1})
- $s(R_n)$: standard deviation of net count rate (s^{-1})

Classical Statistics: Traditional Relationships Among Observed Quantities

$$R_b = \frac{N_b}{t_b}; R_g = \frac{N_g}{t_g}$$

$$R_n = R_g - R_b = \frac{N_g}{t_g} - \frac{N_b}{t_b}$$

$$s(R_n) = \sqrt{\frac{\mathrm{Var}(N_g)}{t_g^2} + \frac{\mathrm{Var}(N_b)}{t_b^2}} \approx \sqrt{\frac{N_g}{t_g^2} + \frac{N_b}{t_b^2}}$$

The Two Aspects of the Counting Problem

The Two Counting Problems

- Radioactive decay is a Bernoulli process described by a binomial or Poisson distribution
- The "forward problem"
  - from properties of the process, we predict the distribution of counting results (mean, standard deviation (SD))
  - measurand $\rightarrow$ distribution of possible observations
- The "reverse problem"
  - measure a counting result
  - from the counting result, we infer the parameters of the underlying binomial or Poisson distribution (mean, SD)

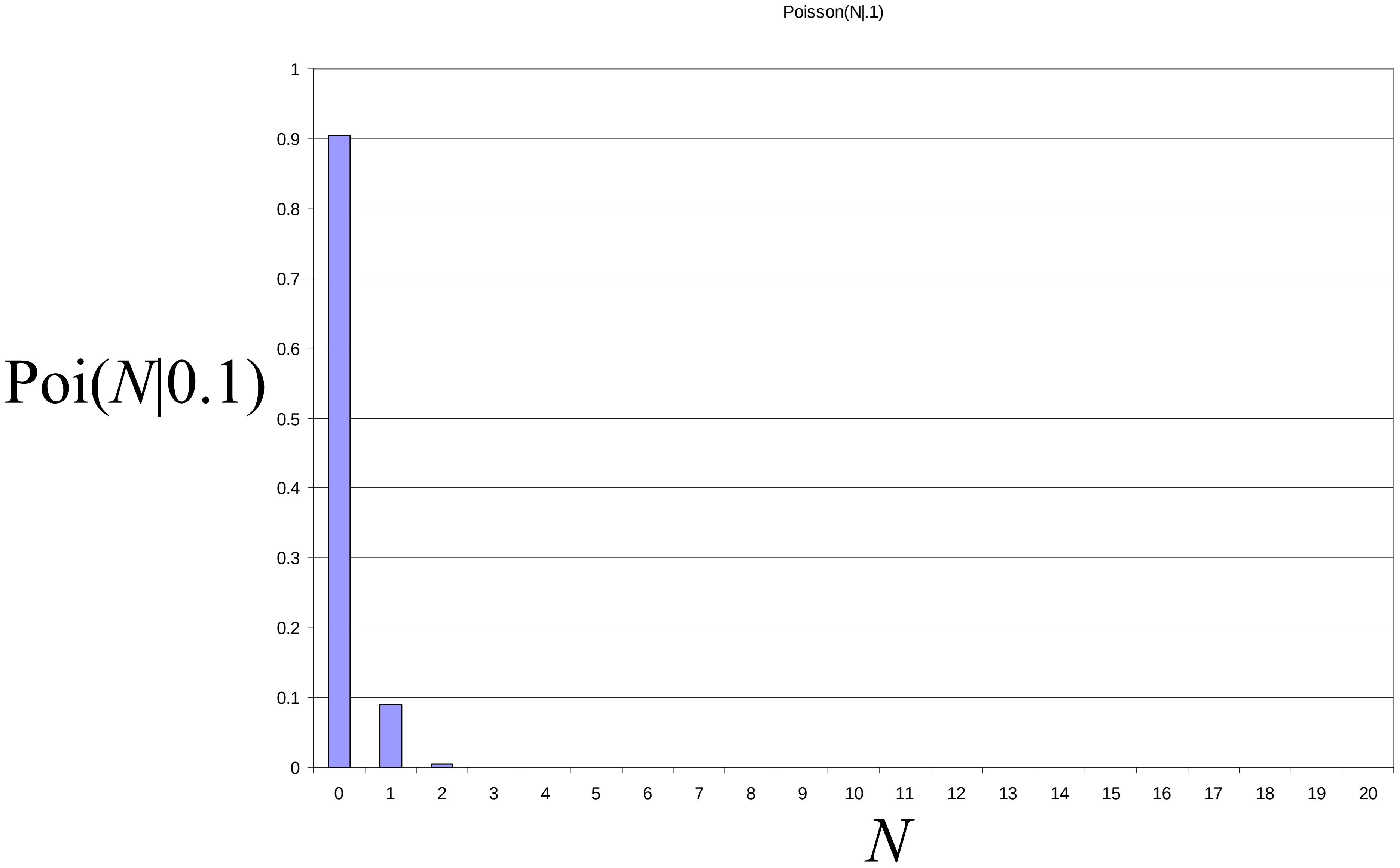
    see, e.g., Rainwater and Wu (1947)
  - this is the problem we're really interested in!

The Forward Problem

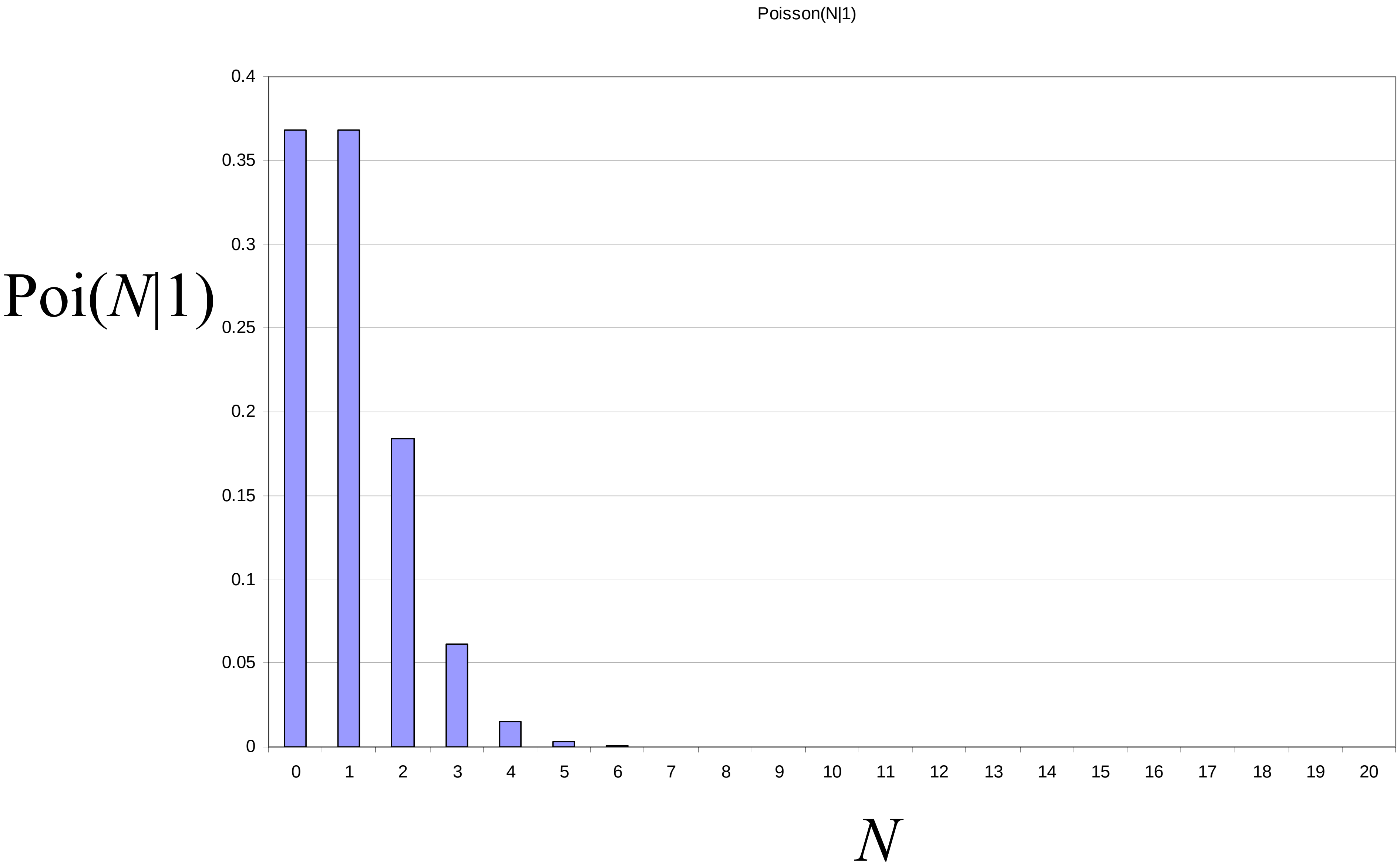
The Forward Problem

- Use Poisson statistics to predict the distribution of observations from a given value of the measurand
- The measurand is best thought of as a count rate ρ
  - otherwise it is difficult to deal with different counting times
- The observable is a number of counts sampled from a Poisson distribution with mean ρt
- $\mathrm{Var}(\mathrm{Poi}(N \mid \rho t)) = \rho t$

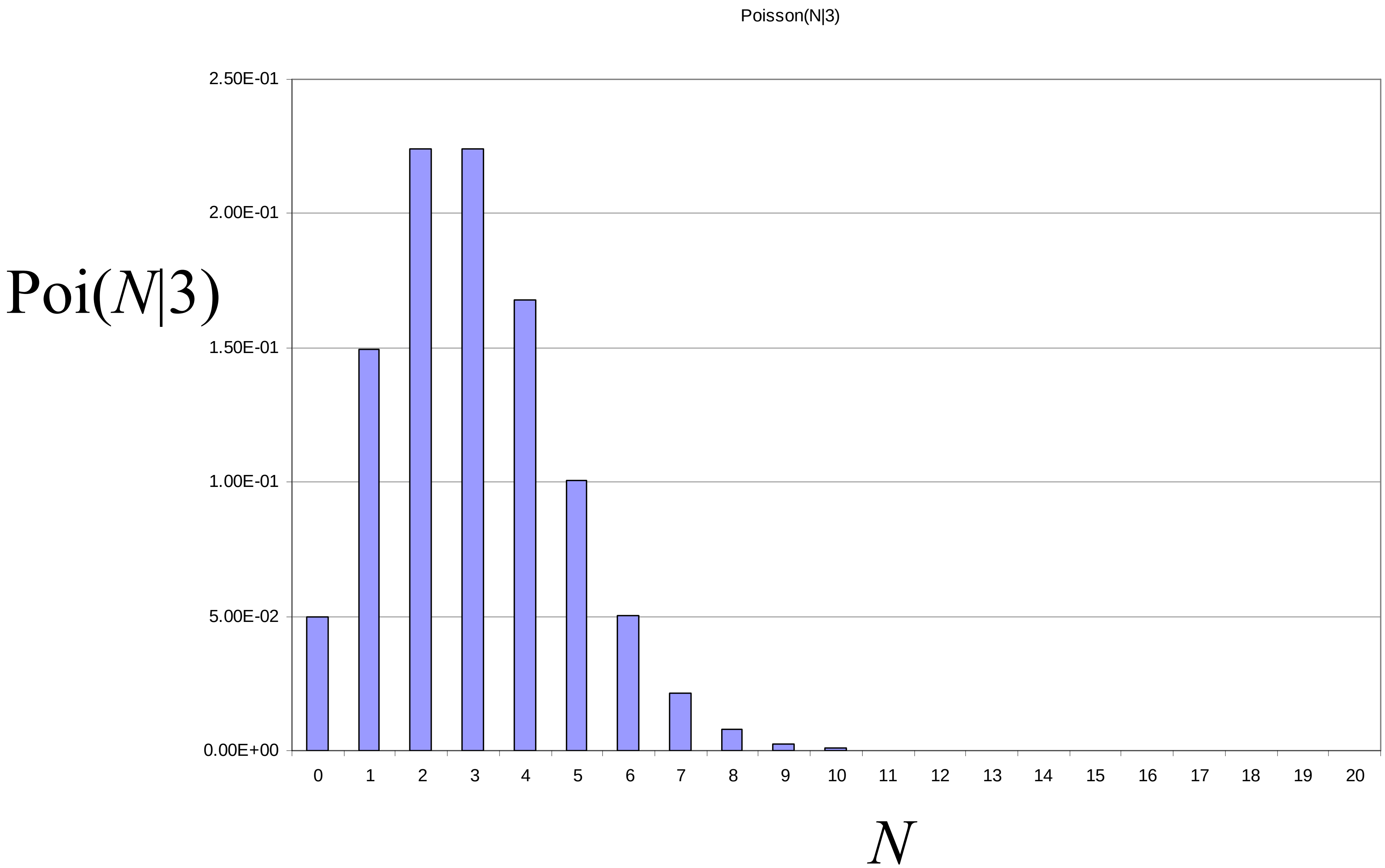
Poisson Distribution, $\mu = \rho t = 0.1$



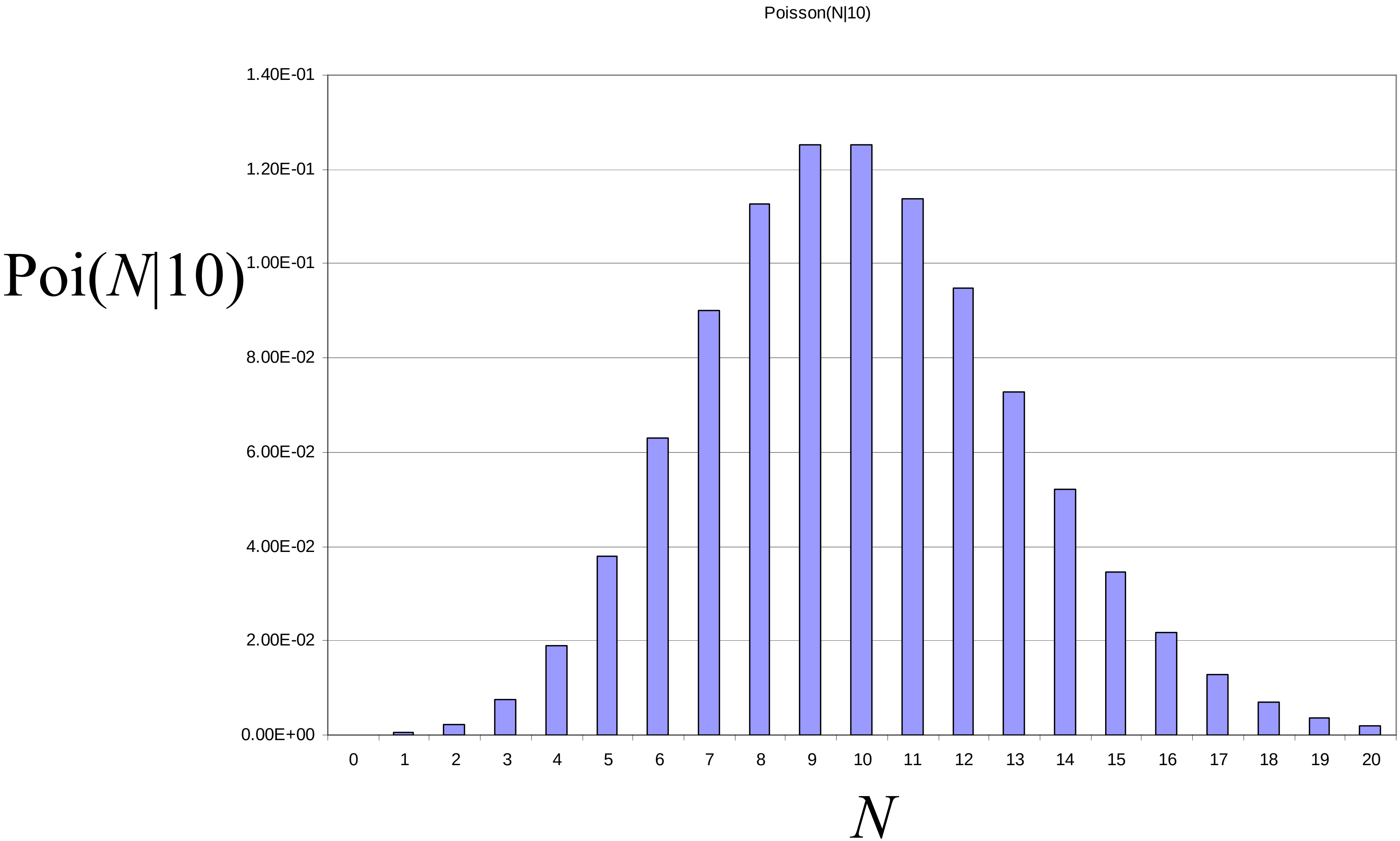
Poisson Distribution, $\mu = \rho t = 1$



Poisson Distribution, $\mu = \rho t = 3$



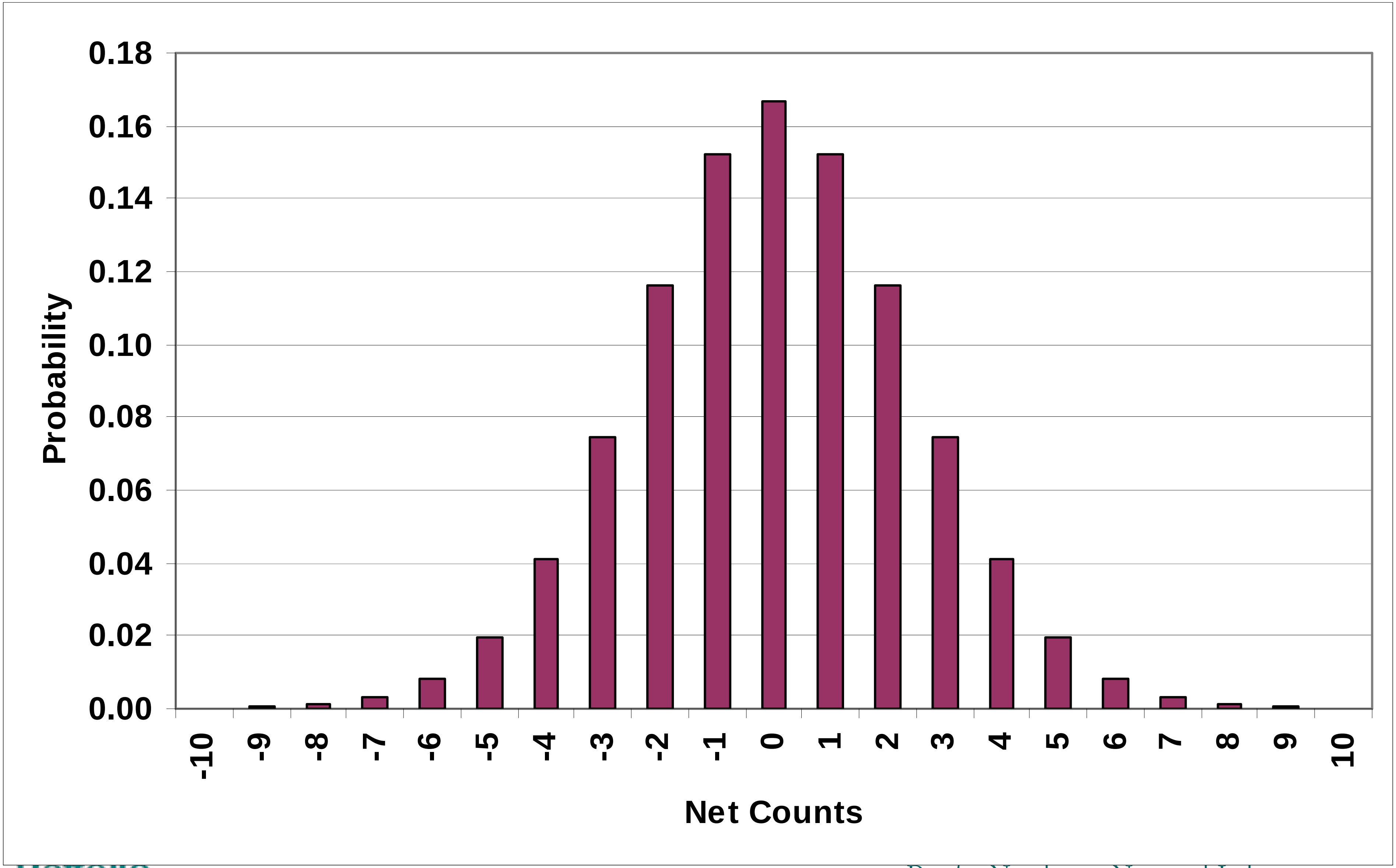
Poisson Distribution, $\mu = \rho t = 10$



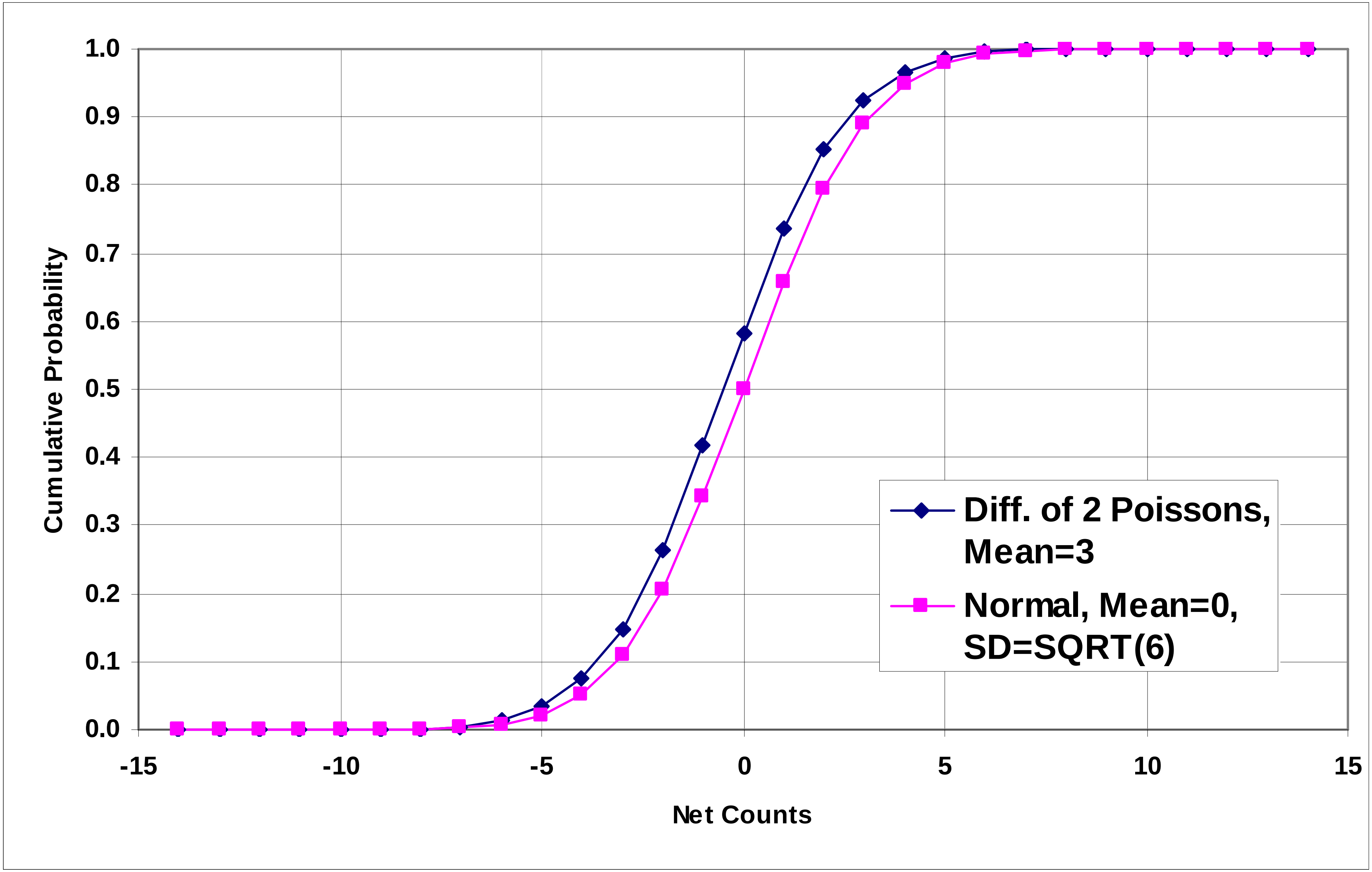
The Critical Task

- Estimating N_b', the contribution of background to N_g
- We use N_b to estimate $\rho_b t_b$

Difference of 2 Poissons with $\mu = \rho t = 3$



Difference of 2 Poissons with $\mu = \rho t = 3$



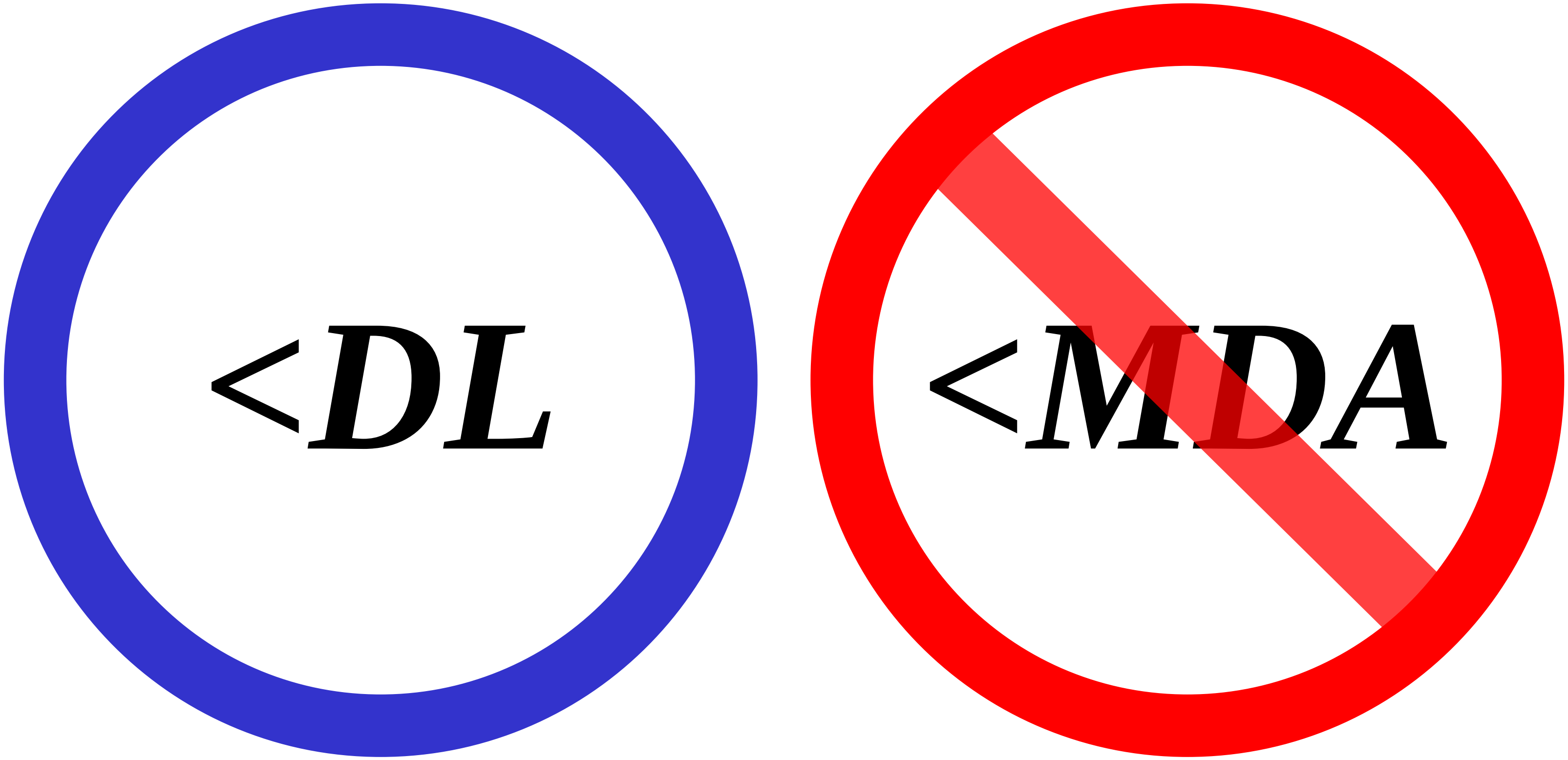
The Reverse Problem

The Reverse Problem: Using Observed Quantities to Estimate Population Parameters (Measurands)

- Classical statisticians
  - use R_n to *estimate* ρ_n
  - use $s(R_\mathrm{n})$ to *estimate* $\sigma(\rho_\mathrm{n})$
    - *ofter a poor assumption for low numbers of counts*
- Bayesian approach shown later

Decision Rules

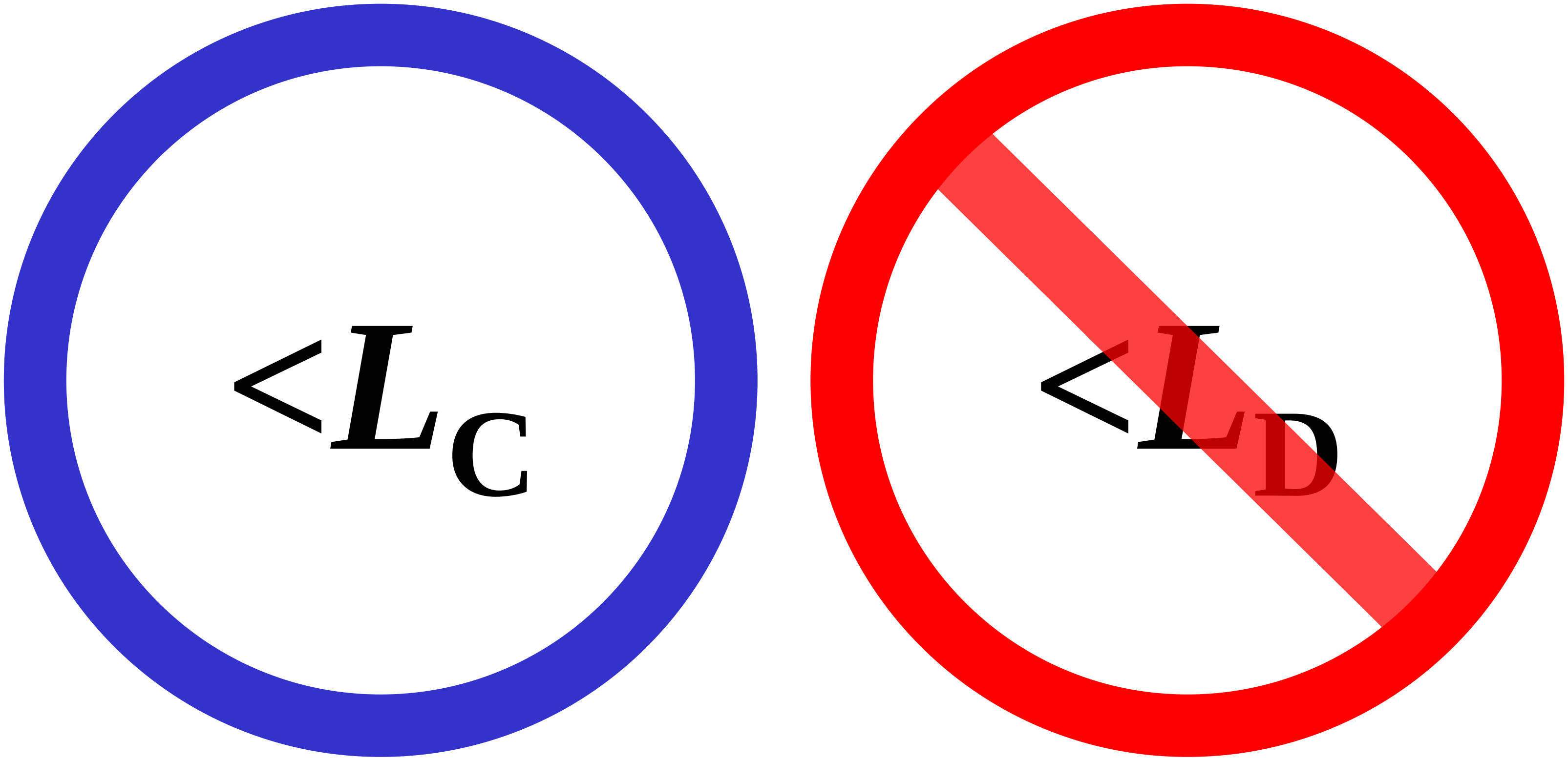
Battelle



Always compare a result with *DL*

Never compare a result with MDA!

Translation:



Always compare a result with L_C

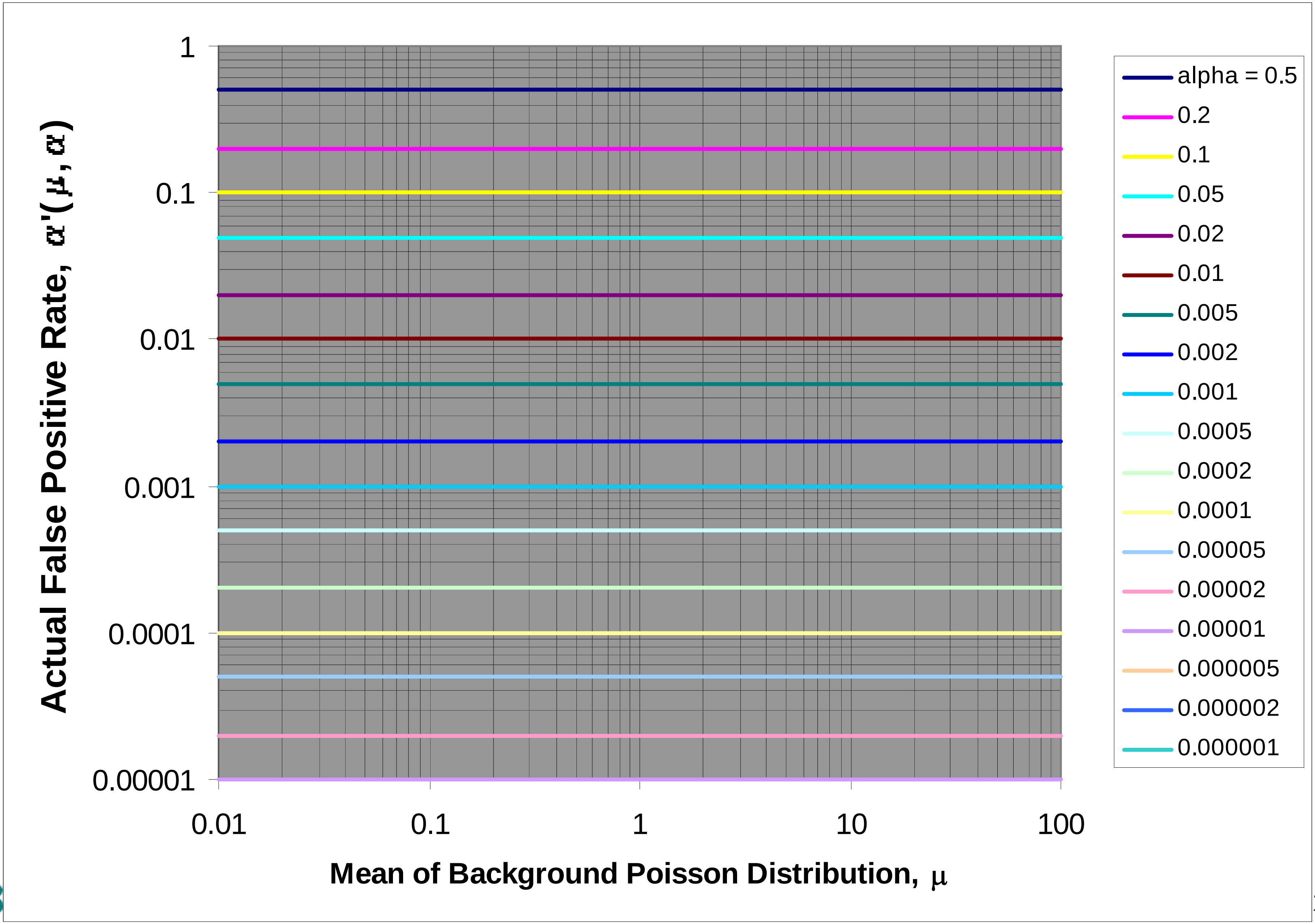
Never compare a result with L_D!

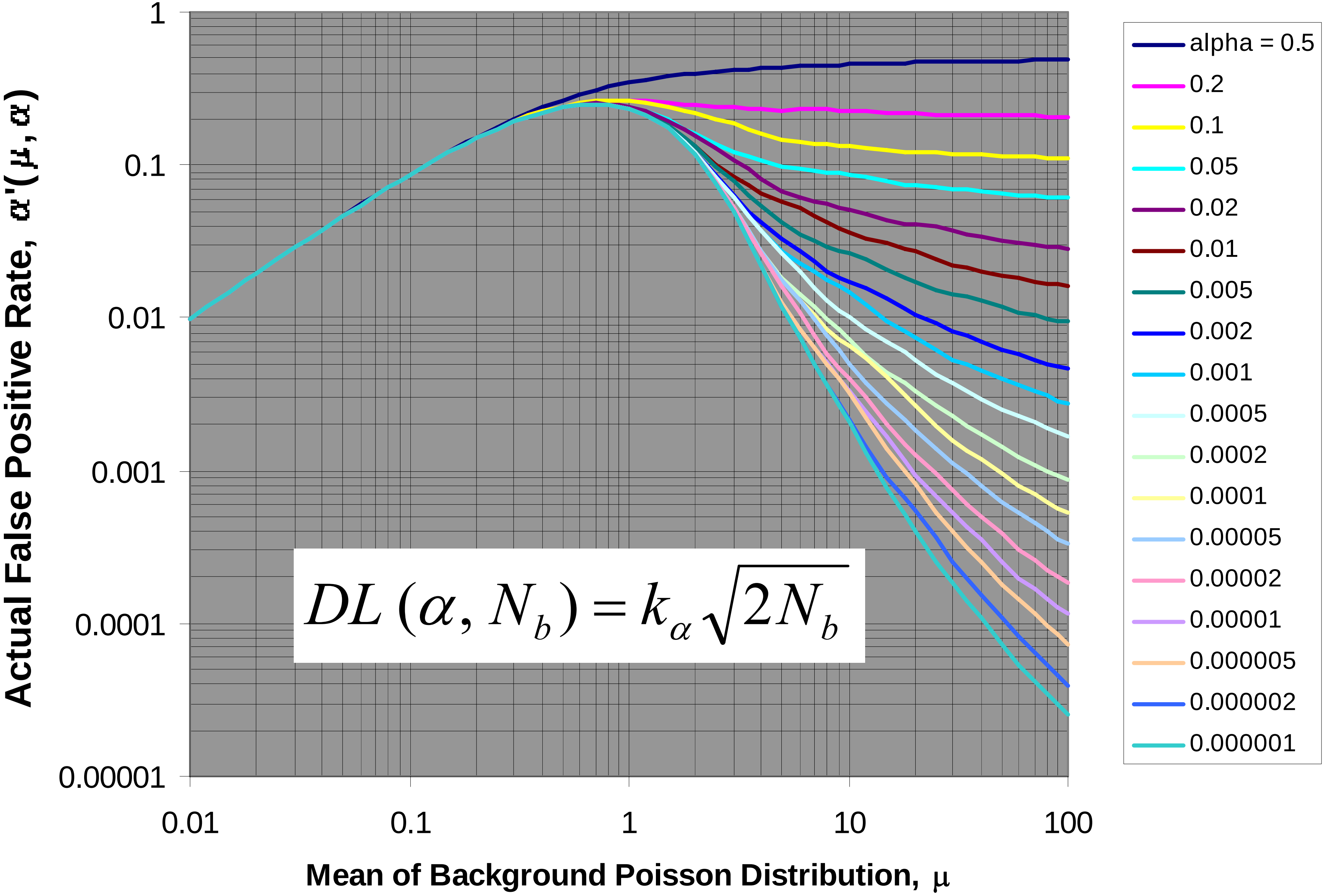
The Common Decision Rule

- Nicholson's (1963) D_2 rule; Currie's (1968) rule; ANSI/HPS N13.30-1996; MARSSIM; Equation 15a, Table 1 of ISO 11929-1:2000
- For $\alpha = 0.05$, expressed as a rate, for non-paired blank:

$$DL_{\mathrm{N13.30}}(R_{\mathrm{n}},\alpha) = k_{\alpha}\sqrt{\frac{N_{\mathrm{b}}}{t_{\mathrm{b}}}\left(\frac{1}{t_{\mathrm{b}}}+\frac{1}{t_{\mathrm{g}}}\right)}$$

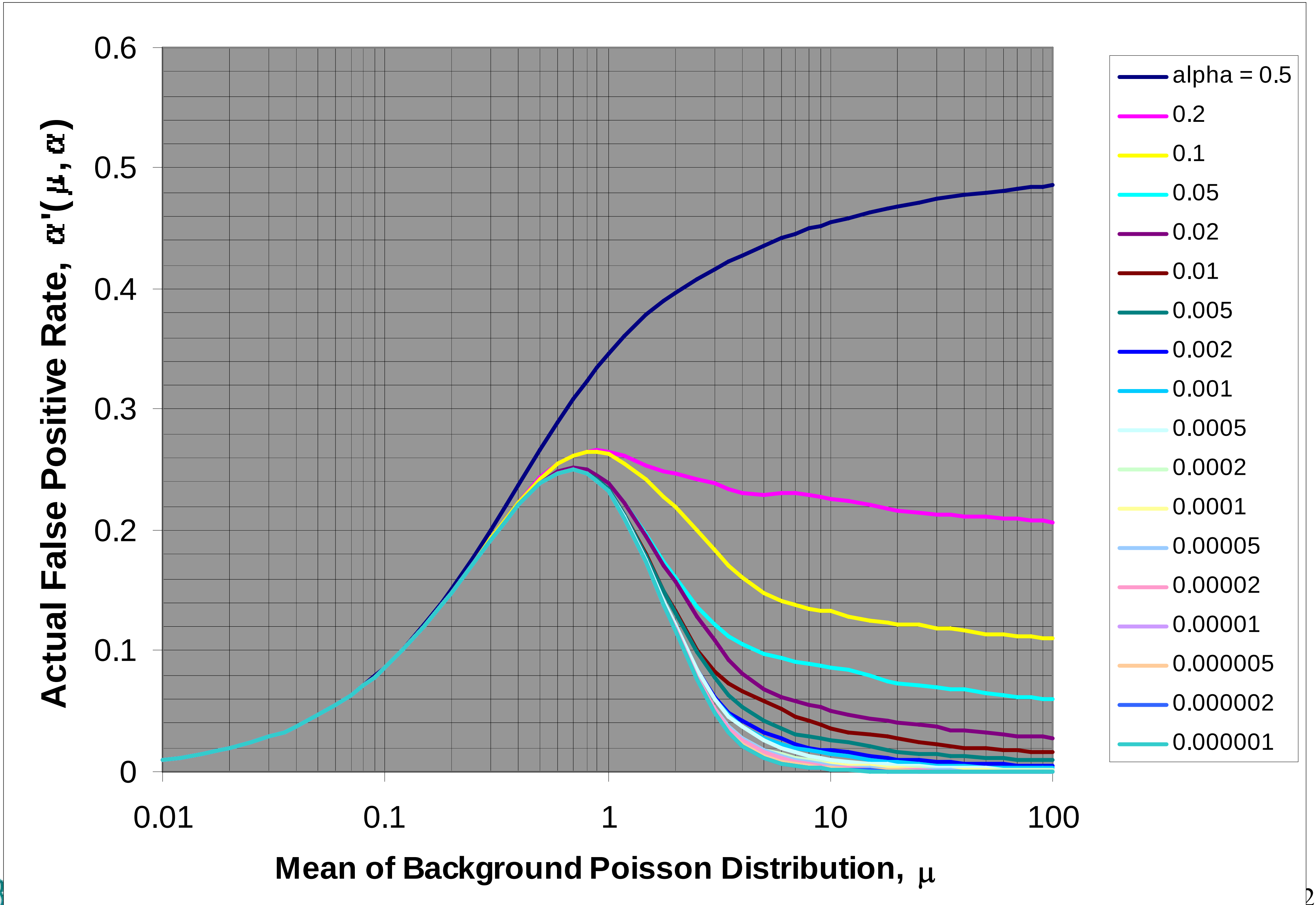
Ideal (Impossible) *DL*





Actual False Positive Rate, α'(μ, α)
1
0.1
0.01
0.001
0.0001
0.00001
0.01
0.1
1
10
100
Mean of Background Poisson Distribution, μ
$DL(\alpha, N_b) = k_\alpha \sqrt{2N_b}$
alpha = 0.5
0.2
0.1
0.05
0.02
0.01
0.005
0.002
0.001
0.0005
0.0002
0.0001
0.00005
0.00002
0.00001
0.000005
0.000002
0.000001

$$DL(\alpha, N_b) = k_\alpha \sqrt{2N_b} \text{ (on a linear vertical scale)}$$



Why the N13.30 Decision Rule Fails at Very Low Background Rates

- false assumption that observed values N_b and $N_b^{1/2}$ are good estimates of the mean and standard deviation of background

The Bayesian Approach to the Reverse Problem

The Reverend Thomas Bayes 1702-1761

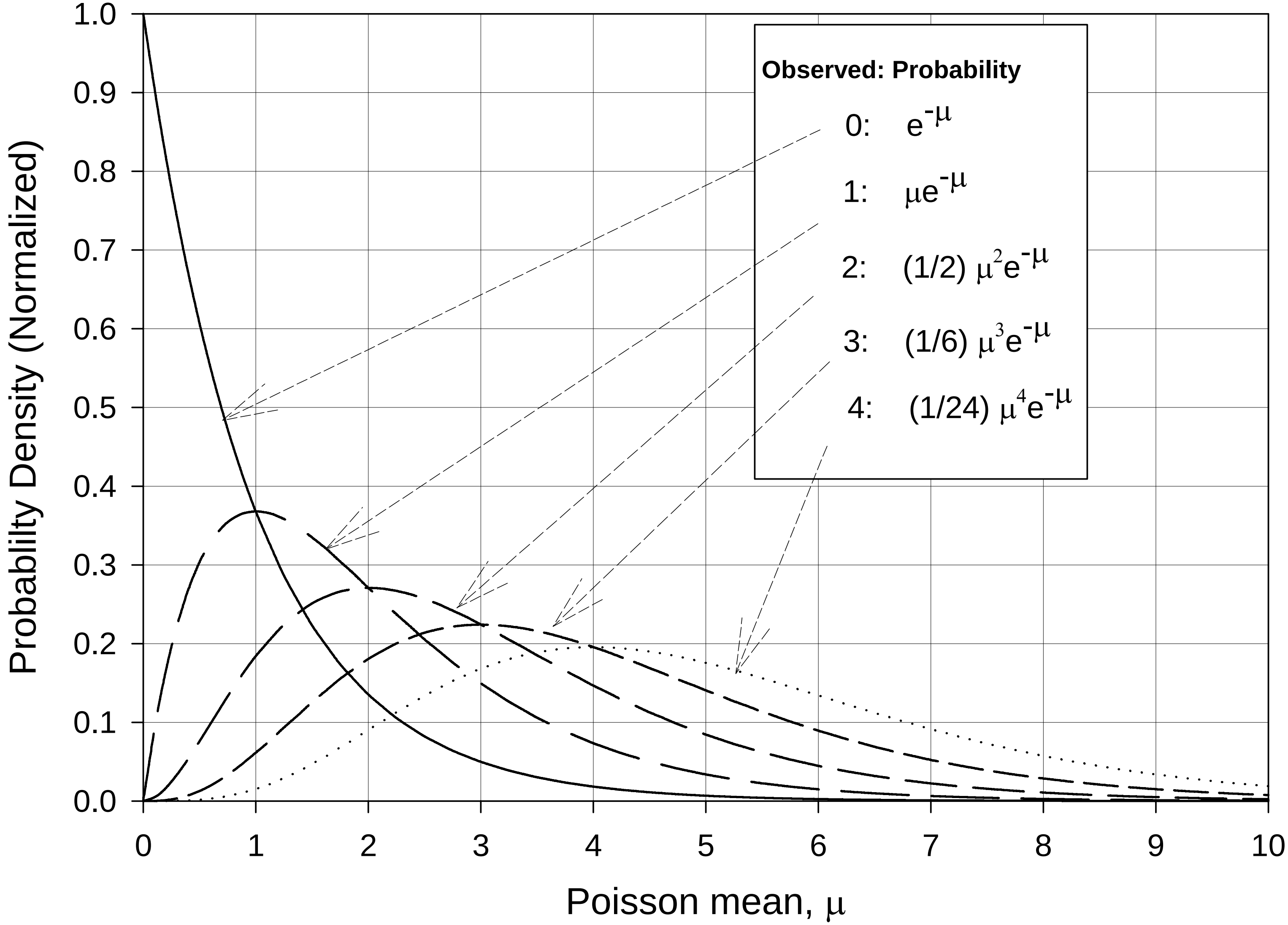
- *Probability is that degree of confidence dictated by the evidence through Bayes's theorem. -- E.T. Jaynes*

Philosophical Statement of Bayes's Rule

$$P(\text{measurand} \mid \text{evidence}) = \frac{L(\text{evidence} \mid \text{measurand})P(\text{measurand})}{\text{normalizing factor}}$$

- The measurand or "state of nature" (e.g., count rate from analyte) is what we want to know
- The "evidence" is what we have observed
- The likelihood of the "evidence" given the measurand is what we know about the way nature works
- The probability of the state of nature is what we believed before we obtained the evidence

Posterior Probability Densities for μ
Uniform Prior



Bayesian Approach

- Assuming uniform "flat" *prior* probability distribution: any value of N is equally likely
- If N counts observed
  - N is maximum likelihood, but $N + 1$ is expectation value:

$$< N_b > = N_b + 1$$

  - variance and standard deviation are simple

$$\mathrm{Var}(< N_b >) = N_b + 1$$

$$s(< N_b >) = \sqrt{N_b + 1}$$

- *Correct on the average!*

Quasi-Bayesian Statistics:
Relationships Among Observed Quantities

- R_n is the same for the paired blank case, slightly different if $t_b \neq t_g$
- $s(R_n)$ is larger because of $N+1$

$$R_b = \frac{N_b + 1}{t_b};\ R_g = \frac{N_g + 1}{t_g}$$

$$R_n = R_g - R_b = \frac{N_g + 1}{t_g} - \frac{N_b + 1}{t_b}$$

$$s(R_n) = \sqrt{\frac{N_g + 1}{t_g^2} + \frac{N_b + 1}{t_b^2}}$$

What Are Alternative Decision Rules?

- "N_b + 1" Decision Rule
- Altshuler & Pasternak (A&P; 1963) / Turner (1995) Eq. 11.68
- Keith McCroan's generalization of A&P
  - (= ISO 11929-1:2000)
- James H. Stapleton's rule
- Nicholson (1963) D_1 rule
- Nicholson (1963) D_3 rule
- Nicholson (1963) D_e "exact" / Sumerling & Darby (1981) rule
- Bayesian approach
- Rigaud's (2003) rule

“N_b + 1” Decision Rule

- Question: If one observes N_b counts, what is the ***expectation value*** of the background distribution that gave rise to this observation (see figure)?
- Bayesian Answer (uniform prior): $\mu_b = N_b + 1$

$$DL_{N+1}(R_n, \alpha) = k_\alpha \sqrt{\frac{(N_b + 1)}{t_b}\left(\frac{1}{t_b} + \frac{1}{t_g}\right)}$$

Altshuler & Pasternak's 1963 Decision Rule

$$DL_{\text{A\&P/Turner}}(R_{\text{n}},\alpha) = \frac{k_{\alpha}^{2}}{2t_{\text{g}}} + \frac{k_{\alpha}}{2}\sqrt{\frac{k_{\alpha}^{2}}{t_{\text{g}}^{2}} + 4R_{\text{b}}\left(\frac{t_{\text{g}} + t_{\text{b}}}{t_{\text{g}}t_{\text{b}}}\right)}$$

McCroan/MARLAP/ISO Decision Rule

- Generalization of Altshuler & Pasternak

$$DL_{\mathrm{McCroan}}(R_{\mathrm{n}},\alpha) = \frac{k_\alpha^2}{2t_{\mathrm{b}}} + \frac{k_\alpha}{2}\sqrt{\frac{k_\alpha^2}{t_{\mathrm{b}}^2} + 4R_{\mathrm{b}}\left(\frac{1}{t_{\mathrm{g}}} + \frac{1}{t_{\mathrm{b}}}\right)}$$

- MARLAP; same as ISO (*ISO notation*):

$$DL_{\mathrm{ISO}}(R_{\mathrm{n}},\alpha) = R_{\mathrm{n}}^{*} = \frac{k_{1-\alpha}^2}{2t_0}\left(1 + \sqrt{1 + \frac{4R_0 t_0}{k_{1-\alpha}^2}\left(1 + \frac{t_0}{t_{\mathrm{S}}}\right)}\right)$$

- Only differs from A&P when count times differ
- notation problem: Strom uses k_α where ISO uses $k_{1-\alpha}$

An Obvious Argument?

- using *both* the background and gross sample measurements to estimate the background increases the power of the test

Stapleton's Decision Rule

$$z_{\text{Stapleton}}(N_{\text{g}}, t_{\text{g}}, N_{\text{b}}, t_{\text{b}}, d) = \frac{2\sqrt{\dfrac{N_{\text{g}}+d}{t_{\text{g}}}} - \sqrt{\dfrac{N_{\text{b}}+d}{t_{\text{b}}}}}{\sqrt{\dfrac{1}{t_{\text{g}}} + \dfrac{1}{t_{\text{b}}}}}$$

- d is an arbitrary number, $0 < d < 1$; 0.4 is good
- z is standard normal deviate for this combination of N_{b}, N_{g}, t_{b}, t_{g}, and d
- Compare z to k_{α} to determine whether you've detected activity at your chosen α

Rigaud's (2003) Decision Rule

$$L_{\mathrm{C}} = 0.5\left(\frac{1}{t_{\mathrm{g}}} + \frac{1}{t_{\mathrm{b}}}\right) + k_{\alpha}\sqrt{R_{\mathrm{b}}\left(\frac{1}{t_{\mathrm{s}}} + \frac{1}{t_{\mathrm{b}}}\right)}$$

Nicholson (1963) D_1 Decision Rule

$$DL_{\text{Nicholson } D_1}(R_n, \alpha) = k_\alpha \sqrt{\frac{N_b}{t_b^2} + \frac{N_g}{t_g^2}}$$

Nicholson (1963) D_3 Decision Rule

$$DL_{\text{Nicholson } D_3}(R_n, \alpha) = k_\alpha \sqrt{\frac{N_b + N_g}{t_b t_g}}$$

Nicholson (1963) D_e "Exact" / Sumerling & Darby (1981) Decision Rule

- difference of 2 Poissons is distributed as a binomial
- Number of trials, $N_{\text{total}} = N_\text{b} + N_\text{g}$
- probability of success = $t_\text{g}/(t_\text{g}+t_\text{b})$
- the null hypothesis that the sample is blank is rejected if a blank sample would have produced a gross count as large or larger than the observed 100α% of the time or less, that is, if

$$\sum_{i=N_\text{g}}^{N_{\text{total}}} \binom{N_{\text{total}}}{N_\text{g}} Q_0^i (1-Q_0)^{N_{\text{total}}-i} \le \alpha$$

where

$$Q_o = \frac{\rho_\mathrm{b} t_\mathrm{g}}{\rho_\mathrm{b} t_\mathrm{g} + \rho_\mathrm{b} t_\mathrm{b}} = \frac{t_\mathrm{g}}{t_\mathrm{g} + t_\mathrm{b}}$$

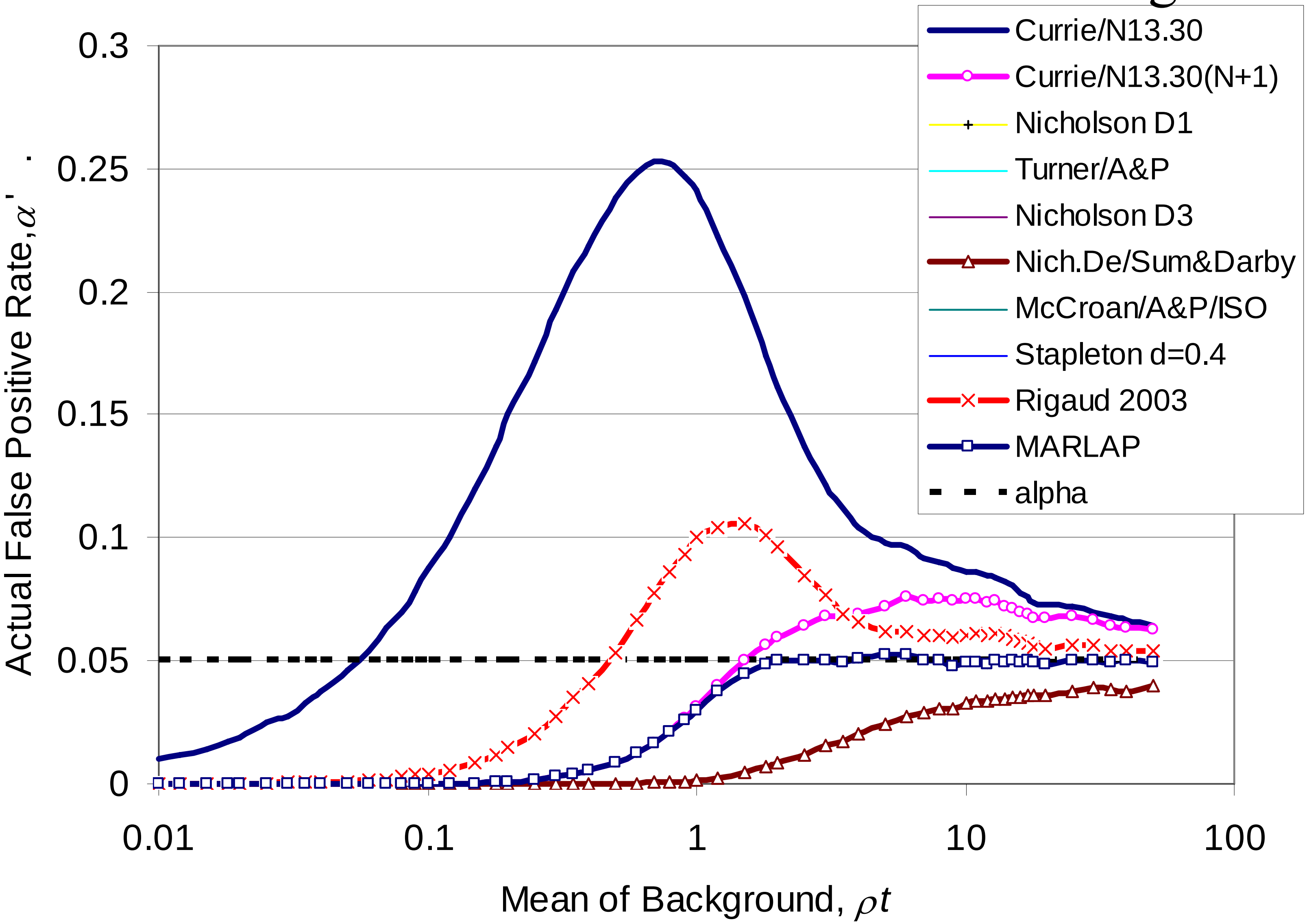
and

$\binom{N_\mathrm{total}}{N_\mathrm{g}}$ is a binomial coefficient.

Test of Decision Rules

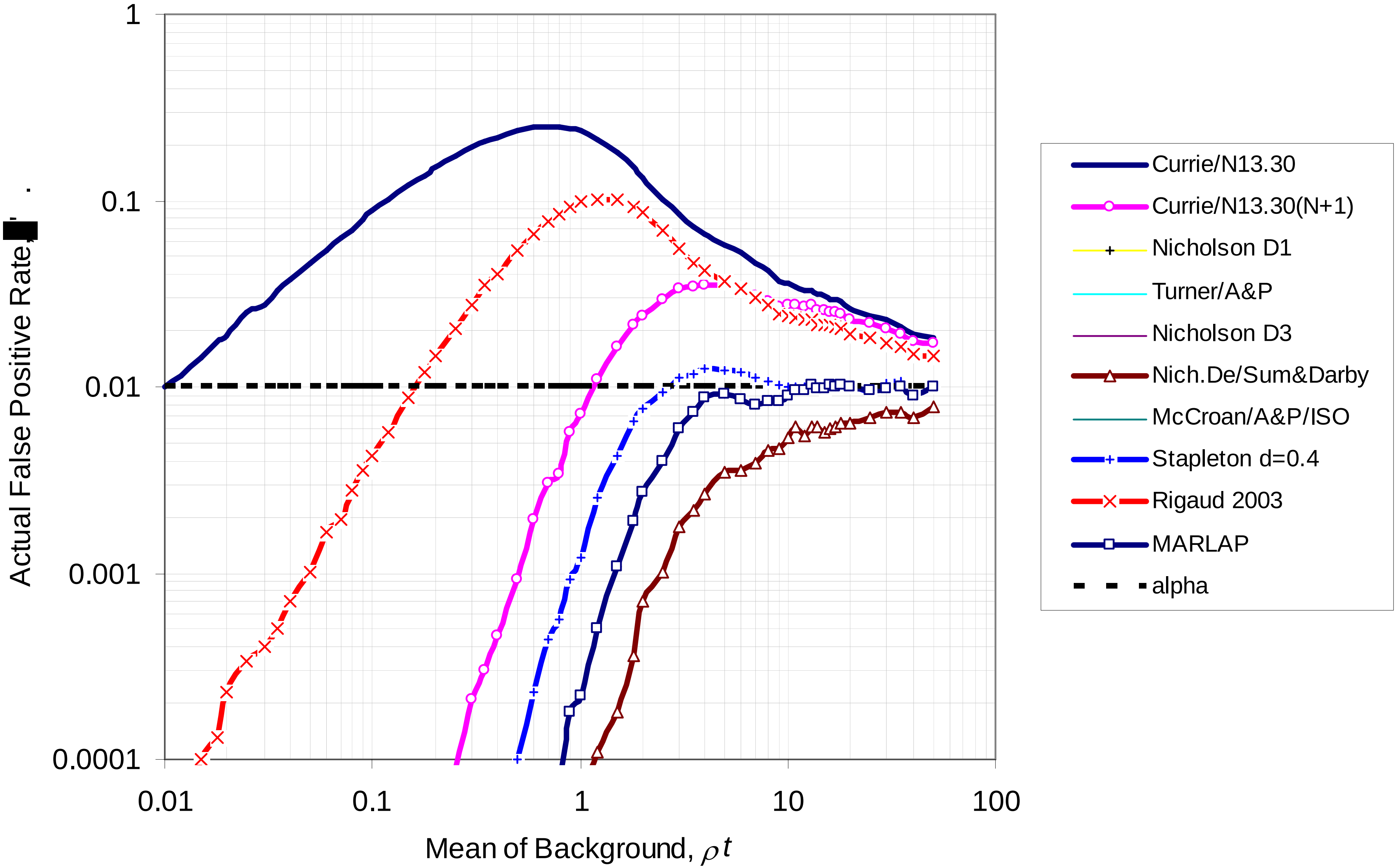
- Monte Carlo simulation (Strom and MacLellan 2001)
- 3,141,593 trials at each of
  - 6 values of α, 0.001 to 0.05
  - 57 values of $\mu_b = \rho_b t_b$ (0.01 to 50)
- MacLellan's exact calculation (MacLellan and Strom 1999) not possible for exact (binomial) or Stapleton's tests or Nicholson's D_1 and D_3 rules, because they use both N_b and N_g.
- Monte Carlo agrees exactly where comparison is possible

$\alpha = 0.05$, Paired Blank $t_b = t_g$



Nicholson D1, D3, Turner/A&P, McCroan/A&P/ISO, Stapleton d = 0.4 all coincide for $\alpha = 0.05$

$\alpha = 0.01$, Paired Blank $t_b = t_g$



Results when $t_b = t_g$, $N_b < 10$

- Nicholson D_1, Turner/A&P, Nicholson D_3, and McCroan/ISO/MARLAP all coincide when $t_b = t_g$ at $\alpha = 0.05$
- Nicholson D_2/Currie/N13.30/MARSSIM is poorest
- "$N + 1$" rule is much better, but not adequate
- Rigaud (2003) not good despite claims
- Stapleton's rule is best, followed by the quartet, followed by D_e/S&D
- No rule is good below $N_b = 3$; smaller α is worse
- Need further work for different count times, $t_b \neq t_g$
- ANSI/HPS N13.30 under revision

Conclusions

- Estimating background's contribution to gross counts remains a problem for low numbers of counts
- If you have observed 2 or fewer background counts, your decision rule may fail
- Stapleton's *d* value rule is the best for paired blank problem
- MARLAP
- The well-known blank is a great leap of inference

Software Utility

PNNL Counting Statistics Utility