BLIMIT - Yet Another Program To Compute Upper Limits

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Abstract

This note describes the program `blimit`, developed within the DØ Run II Single Top Group, to compute upper limits on cross-sections given an observed count n, an estimate of the effective integrated luminosity $\hat{a} \equiv \hat{\epsilon}\hat{\mathcal{L}} \pm \delta a$ and an estimate of the background $\hat{b} \pm \delta b$. The program is intended to replace the DØ Web-based limit calculator with one that can handle large relative uncertainties, sensibly.

I. INTRODUCTION

In the absence of sufficient data to measure a cross-section the accepted practice is to set an *upper limit*, at some specified *confidence level* (CL), on the cross section for the process under investigation; that is, the convention is to make an assertion of the form

$$\sigma < \sigma^{\mathrm{u}}(\mathbf{x}) \;\text{ at 95 \% CL,} \tag{1.1}$$

where $\mathbf{x}$ represents the *observed* data and $\sigma^{\mathrm{u}}(\mathbf{x})$ the upper limit on the cross-section σ. There are two well-established interpretations of the above statement:

- **frequentist** — In an ensemble of infinitely many experiments — in each of which an upper limit has been calculated using the *same* frequentist procedure, but not necessarily for the same quantity, 95 % of assertions of the form $q < q_U(\mathbf{x})$ would be true. We note that, with respect to the ensemble of experiments, each quantity q is presumed to be a *fixed* number while, in general, $q_U(\mathbf{x})$ varies from one experiment to another. Note also that a confidence level is a property not of the single statement $q < q_U(\mathbf{x})$ but rather of the ensemble of such statements of which the statement we actually make in our *single* experiment is presumed to be a member [1]. Consequently, without an explicit specification of the (infinite) ensemble into which our experiment is considered to be embedded the confidence level is undefined.

  comments — We note that a real, but *finite*, ensemble exists, namely, the ensemble of all published 95% upper limits. However, since we do not know the true answers for *every one* of the published limits, we have no operational way to ascertain their *coverage*; that is, we cannot ascertain if the fraction of upper limits that exceed their associated true values q is in fact, at least, 95 %. It is therefore unclear what objective utility can be ascribed to such an ensemble, albeit a *real* one.

  On the other hand, on a computer we can always simulate a virtual ensemble — a virtual DØ, and calculate its coverage properties since we know the true values of q. But since these ensembles are *not real*, again it is unclear what is their operational utility, other than to verify that some procedure works, on average, as one would wish it to, within the virtual ensemble.

- **Bayesian** — The *degree of belief* in the statement $\sigma < \sigma^{\mathrm{u}}(\mathbf{x})$ is 95 %. Note that the confidence level, being a degree of belief, pertains to the statement actually made and not to any embedding of that statement in an ensemble of such. This of course does not prevent us from studying, if we believe it useful, the coverage properties of the Bayesian limits with respect to any virtual ensemble we wish. This is done, typically, to check that the coverage is roughly the same as the assigned degree of belief.

If pressed hard most particle physicists would claim to adhere to the frequentist interpretation of limits. In practice, most find it very hard *not* to think about them in a Bayesian way. Given this psychological reality, together with a host of cogent conceptual and technical arguments [2], the DØ Collaboration [3], and later CDF, agreed to use Bayesian methods to compute upper limits. The DØ Web-based limit calculator was a simple outcome of this agreement. Recently, this recommendation has been re-affirmed [4]. (The DØ Limits Committee, however, leaves as an option the use of the CL_S method [5]. (HBP: My own view is that CL_S does not represent a conceptual advance.)

The `blimit` program was developed to overcome a limitation in the Web-based limit calculator. `blimit` computes Bayesian upper limits also, but, unlike the Web-based calculator, `blimit` is designed to handle, sensibly, large relative errors as well as small ones.

II. MATHEMATICAL BACKGROUND

Many different lines of reasoning [2] lead to the conclusion that Bayes' theorem

$$p(\theta, \lambda|\mathbf{x}) = \frac{p(\mathbf{x}|\theta, \lambda)\, \pi(\theta, \lambda)}{\int_{\mathbf{\Theta}} \int_{\mathbf{\Lambda}} p(\mathbf{x}|\theta, \lambda)\, \pi(\theta, \lambda) d\lambda\, d\theta}, \tag{2.1}$$

is the appropriate mathematical framework to perform coherent inferences about a set of parameters (θ, λ), where θ represents one or more *parameters of interest*, for example a cross-section, and λ represents all other parameters such as acceptances and backgrounds, referred to collectively as *nuisance parameters*. The functions $\pi(\theta, \lambda)$, $p(\mathbf{x}|\theta, \lambda)$ and $p(\theta, \lambda|\mathbf{x})$ are the *prior*, *model* and *posterior* densities, respectively. Sometimes (and loosely) $p(\mathbf{x}|\theta, \lambda)$ is referred to as the *likelihood*. The prior encodes, probabilistically, what is known (or assumed) about the parameters independently of the data $\mathbf{x}$, but in light of full knowledge of the model density, while the posterior density encodes, probabilistically, a synthesis of the knowledge gained from the data and the prior knowledge. The model density encodes what is known about the set of possible observations.

A. Model

The `blimit` program uses the model

$$p(n|\sigma, a, b) = \text{Poisson}(n, a\sigma + b), \tag{2.2}$$

where n is the observed count, $a = \epsilon\mathcal{L}$ is the acceptance times efficiency, ϵ, times the integrated luminosity $\mathcal{L}$ and b is the background. We assume that we have estimates $\hat{a} \pm \delta a$ and $\hat{b} \pm \delta b$ for the effective luminosity and background, respectively.

B. Prior

We first factorize the prior density $\pi(\sigma, a, b)$ as follows

$$\begin{aligned} \pi(\sigma, a, b) &= \pi(a, b|\sigma)\, \pi(\sigma), \\ &= \pi(a|b, \sigma)\, \pi(b|\sigma)\, \pi(\sigma), \end{aligned} \tag{2.3}$$

into a prior $\pi(\sigma)$ for the cross-section and two that depend on the nuisance parameters a and b, conditional on the value of the cross-section. We assume that our *a priori* knowledge of any one of the parameters a, b and σ is independent of our *a priori* knowledge of the other two. We can then write $\pi(a|b, \sigma) = \pi(a)$ and $\pi(b|\sigma) = \pi(b)$. Given $\pi(a)$ and $\pi(b)$, it is convenient first to compute the *marginal model density* (or marginal likelihood, if one prefers)

$$p(n|\sigma) = \int \int p(n|\sigma, a, b)\, \pi(a)\, \pi(b)\, da\, db, \tag{2.4}$$

and re-write Eq. (2.1) as

$$p(\sigma|n) = \frac{p(n|\sigma)\, \pi(\sigma)}{\int p(n|\sigma)\, \pi(\sigma)\, d\sigma}. \tag{2.5}$$

To complete the inference about the cross-section we need functional forms for the priors $\pi(a), \pi(b)$ and $\pi(\sigma)$ that reflect, in some way, what we know about these parameters—or wish to *assume* about them, independently of the data at hand. We assume the following

$$\pi(a) = \text{Gamma}(a\alpha, A + 1), \tag{2.6}$$

$$\pi(b) = \text{Gamma}(b\beta, B + 1), \tag{2.7}$$

$$\pi(\sigma) = 1/\sigma^{\max}, \tag{2.8}$$

where $A = (\hat{a}/\delta a)^2$, $B = (\hat{b}/\delta b)^2$, $\alpha = A/\hat{a}$, $\beta = B/\hat{b}$ and $\sigma^{\max}$ is some reasonably large upper bound on the cross-section. The choice for $\pi(\sigma)$ is merely a convenient convention [3]. The choices for the other priors can be motivated as follows. Consider how, typically, we estimate a background. We construct a sample of background events, apply cuts, and find that B events pass the cuts. That number is then scaled to the observed integrated luminosity to yield the estimate $\hat{b} = B/\beta \pm \delta b \,(= \sqrt{B}/\beta)$. If the background efficiency is small, we can assume that the probability to observe B events is given by Poisson$(B, b\beta)$ where b is the mean count for which $\hat{b}$ is an estimate. The information we now have about the unknown parameter b is captured in its posterior density $p(b|B) \propto \text{Poisson}(B, b\beta)\, \pi_B(b)$, where $\pi_B(b)$ is the prior associated with this background "experiment". If we take $\pi_B(b)$ to be flat in b, then $p(b|B) = \text{Gamma}(b\beta, B+1) \propto \text{Poisson}(B, b\beta)$. The posterior density $p(b|B)$ can now serve as the prior density $\pi(b)$ for the next level of inference. An identical argument applies to the prior $\pi(a)$.

With this simple model and prior, the marginal density, Eq. (2.4), can be computed exactly by expanding the term $(a\sigma + b)^n$, in the Poisson distribution, using the binomial theorem, thereby transforming the double integral into a sum of products of two 1-dimensional integrals, each of which can be expressed as a gamma function. The result is

$$p(n|\sigma) = \alpha^{A+1}\beta^{B+1}\sum_{r=0}^{n} C_r \frac{\sigma^r}{(\sigma+\alpha)^{A+r+1}}, \tag{2.9}$$

where

$$C_r = \frac{\Gamma(A+r+1)}{\Gamma(A+1)\Gamma(r+1)} \frac{\Gamma(B+n-r+1)}{\Gamma(B+1)\Gamma(n-r+1)!}. \tag{2.10}$$

C. Limits

Given the posterior density $p(\sigma|n)$, computed as in Eq. (2.1), the upper limit σ^{u} is obtained by solving

$$CL = \int_0^{\sigma^{\mathrm{u}}} p(\sigma|n)\, d\sigma \tag{2.11}$$

for σ^{u}, where CL is the desired confidence level. See the README file in the `blimit` release for practical details.

Acknowledgments

The `blimit` program grew out of the work of the Run II DØ Single Top Group.

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[2] R. T. Cox, "Probability, Frequency, and Reasonable Expectation," Am. J. Phys. **14**, 1-13 (1946); H. Jeffreys, *Theory of Probability*, 3rd edition, Oxford University Press, (1961); E.T.Jaynes and L. Bretthorst, *Probability Theory, the Logic of Science*, Oxford, 2003.

[3] I. Bertram *et al.*, DØNote 3476, "A Recipe for the Construction of Confidence Limits" (1998).

[4] DØ Limits Committee, G. Landsberg *et al.*, 2004.

[5] See, for example, "Calculating CL_S Limits," H. B. Prosper, DØNote 4492, June 8, 2004.