Calculating Upper Limits

Gus Sinnis

2 June 1992

1 Introduction

In our daily search paper we calculate 90% **CL** upper limits to the flux from a given source. We adopt the so called 'Bayesian' approach, as discussed in Helene 1983, Kraft 1991, and Protheroe 1984. While Helene and Protheroe discuss the case when the backgound is not known with absolute certainty, in neither paper is the solution given explicitly.

In the case of an uncertain background there is a double integral to be solved, one over all source hypotheses and the second over all possible background scenarios. This integral can be solved exactly, resulting in a double sum over the number of observed events.

I begin with a short aside on the supposed difference between the classical and Bayesian approaches. In fact if one begins with the same assumptions, one arrives at the same answer, so there is no ambiguity in the calculation of an upper limit. I then give the correct equation for calculating an upper limit (restricting ourselves to the 'physical' region) in the presence of an uncertain background. And end with a proposal for what should be included in the daily paper.

2 Classical vs. Bayesian

There has been much arguement over whether one should use the so called 'classical' or 'Bayesian' approach when calculating an upper limit. In the

Bayesian approach one uses Bayes theorem to convert a conditional probability of a given source model being true dependent upon a given observation, to a conditional probability of a given observation dependent upon a source model. One can parameterize the possible source models by a function $g(s, B)$. For a given source strength s and background B, g is taken to be a Poisson distribution. However s is a random variable and one must choose a distribution for s. It is at this point that the classicists part from the Bayesians. The classical claim is that since one knows nothing about the source, one can not input a distribution for s. However, one can insert a distribution that corresponds to total ignorance, namely $P(s) = N$, a flat distribution. The distribution chosen for s is commonly referred to as a **prior** function.

To restrict s to the physical region, one merely chooses $P(s) = 0$ if $s < 0$, equivalent to the statement that there are only sources of cosmic rays, no sinks. Zech 1989 shows that under this choice of prior the Bayesian and classical approaches yield the same answer. In fact this is just what Bayes theorem tells us. The confusion arises because when one naively generalizes the 'classical' definition of an upper limit to the case of non-zero background, one makes use of a totally unbiased prior: $P(s) = N$ for all s, even $s < 0$.

With this choice, S is now unrestricted, if on a given observation $N_{Obs} < B$, no problem - just take S negative. But then $S + B$ can also be negative, and the Poisson probability formula must be modified for negative values of μ. This modification is never performed by the classicists. So they have implicitly restricted themselves to the physical region (chosen a prior) and not properly normalized the probabilities over the allowed range. *The often seen classical formula for upper limits is wrong.*

Both formalisms begin with:

$$P(N|S+B) = \frac{e^{-(S+B)}(S+B)^N}{N!} \qquad (1)$$

With no a priori restrictions on B or S. If one restricts $S > 0$, then B must necessarily be restricted to $B \leq N_{Obs}$. But equation 1 is not normalized within this restricted range of backgrounds. The correct normalization is just:

$$\sum_{i=0}^{N_{Obs}} P(i|B) = \sum_{i=0}^{N_{Obs}} \frac{e^{-B}B^i}{i!} \tag{2}$$

The Bayesian's integrate over source models S, while the classicists sum over observations. Zech shows that the two are mathematically identical, when one properly normalizes equation 1 as shown above. As Steve says, "If you ask the same question you get the same answer", "But only if you do the calculation correctly", Gus.

While the a priori choice of a prior which is zero for negative values of the flux seems like a 'safe' assumption, James 1991, argues that to combine different experiments in an unbiased manner one should report upper limits without excluding the 'unphysical' region, i.e. even report negative flux limits. Given our observations, 1 *possible* source and 2 **definite** sinks, perhaps we should not take our choice of prior lightly (it's a joke!).

3 Calculating an Upper Limit

We assume that the source flux is greater than or equal to zero, and that all such values are equally probable. Then the source probability density function $g(s, B)$ is given by:

$$g(s,B) = N\int_0^\infty \frac{e^{-(s+B)}(s+B)^{N_{Obs}}}{N_{Obs}!}P(B,B_0)dB \tag{3}$$

$$P(B,B_0) = \frac{e^{-\alpha B}(\alpha B)^{\alpha B_0}}{(\alpha B_0)!} \tag{4}$$

Where B_0 is our estimate of the true background, B is the true background, and α is the number of bins used to estimate the background (one over the normal Li Ma α). $P(B, B_0)$ is just the Poisson probability of obtaining a background estimate of B_0 given that the true background is B. In the case of a perfectly determined background $P(B, B_0) = \delta(B - B_0)$.

Then our **CL** upper limit on the flux (one-sided) is given by the value of S_{lim} which satisfies the following equation:

$$\int_0^\infty g(s,B)ds = (1.-\mathbf{CL})\int_S^\infty g(s,B)ds \tag{5}$$

We are finding the value of source flux S such that a fraction $(1.-\mathbf{CL})$ of the source probability density function lies above S, conditioned upon the number of events we observed, and the expected background (and our uncertainty in its determination). This is our **CL** upper limit on the source flux.

By a suitable change of variables and repeated use of the following integral (obtained by repeated integration by parts):

$$\int_A^\infty e^{-x}x^m dx = e^{-A}m!\sum_{i=0}^{m}\frac{A^i}{i!} \tag{6}$$

One obtains:

$$1.-\mathbf{CL} = \frac{e^{-S}\sum_{i=0}^{N_{Obs}}\sum_{r=0}^{i}\mathbf{C}_r^i S^{i-r}(\frac{1}{\alpha+1})^r[\frac{(\alpha B_0+r)!}{i!}]}{\sum_{i=0}^{N_{Obs}}(\frac{1}{\alpha+1})^i[\frac{(\alpha B_0+i)!}{i!}]} \tag{7}$$

where (8)

$$\mathbf{C}_r^i = \frac{i!}{(i-r)!r!} \tag{9}$$

Using an efficient root finding algorithm from Numerical Recipes (ZBRENT) I solve for S. The computation time needed goes like N_{Obs}^2 (because of the double sum over N_{Obs}). To obtain an accuracy of .01% in the confidence level requires roughly seven evaluations of the above equation. For $N_{Obs}=10$ the routine takes about 1 CPU second, for $N_{Obs}=100$ about 30 CPU seconds.

In Figure 1 I show how a flux limit changes with decreasing background uncertainty. For 24 different values of N_{Obs} (7-30), I take the case of $N_{Obs}=B_0$ and plot the fractional limit versus α. One can see that while there is a significant change from $\alpha=1$ to $\alpha=10$, there is little change beyond that. In the current daily analysis we have $\alpha=10$.

4 The Daily Paper

There is still the question of what we wish to report in the paper. One possibility is give the results for a 'typical' day. I interpret this to mean that we find two days, one from each running period, with complete coverage (no down time except for run changes) and give the upper limits as calculated from the number of observed events and the number of expected background events. The other approach is to give 'typical' flux limits. Where a typical flux limit would be calculated using $N_{Obs} = B_0$, i.e. no excess. While the former was the original suggestion, the latter better represents our average limits. I would like to suggest that we report both numbers.

1 The number of observed events N_{Obs}.

2 The number of expected events B_0.

3 The 90% **CL** upper limit to the fraction of cosmic rays FOR THIS DAY.

4 The 90% **CL** upper limit if there had been NO excess.

5 The absolute flux limit (γ's$cm^{-2}sec^{-1}$) from 3 or 4 above.

On the following pages are four tables (two for each day) of the results for two days, Febuary 1 1989 and April 1 1992. Since I will be leaving the country for three weeks any comments about the calculation of our upper limits, or what information should be included in the tables should be sent to Cy.

5 References

Helene, O. 1983, NIM, **212**, 319
James, F. and Roos, M. 1991, Phys. Rev D, **44**, 299
Kraft, R., Burrows, D., Nousek, J. 1991, Ap. J., **374**, 344
Protheroe, R. J. 1984, Astron. Express, **1**, 33
Zech, G. 1989, N.I.M., **A277**, 608

Table 1: 90% confidence level upper limits on the fractional excess in a 2.0° bin for Febuary 1 1989

Source	N Observed	N Expected	90% CL	Typical 90% CL
Cyg X-3	28	24.8	0.500	0.374
Her X-1	31	21.3	0.861	0.423
Crab	22	20.4	0.505	0.430
2CG095+04	17	19.6	0.366	0.432
Geminga	17	16.4	0.532	0.486
2CG078+01	14	25.1	0.183	0.391
2CG075+00	23	23.0	0.415	0.415
2CG065+00	23	24.6	0.354	0.382
2CG135+01	11	13.1	0.464	0.569
2CG121+04	8	9.7	0.563	0.634
PSR1953+29	19	23.5	0.292	0.394
PSR1937+21	16	20.4	0.311	0.430
PSR1929+10	10	11.5	0.528	0.589
PSR0950+08	4	10.5	0.319	0.621
PSR0355+54	15	22.3	0.242	0.412
PSR1951+32	24	25.9	0.338	0.363
PSR1957+20	19	19.8	0.423	0.423
4U0115+63	9	12.4	0.416	0.570
4U1907+09	8	8.4	0.715	0.715
4U0042+32	24	18.4	0.741	0.456
4U0316+41	19	18.8	0.473	0.435
4U0352+30	25	23.7	0.449	0.386
4U0614+09	5	10.3	0.364	0.642
4U1837+04	8	8.1	0.760	0.760
4U1901+03	6	6.5	0.822	0.822
4U1918+15	10	13.2	0.414	0.561
4U1954+31	18	25.2	0.235	0.388
4U1956+35	27	24.6	0.475	0.382

Table 2: 90% confidence level upper limits on the fractional excess in a 2.0° bin for Febuary 1 1989

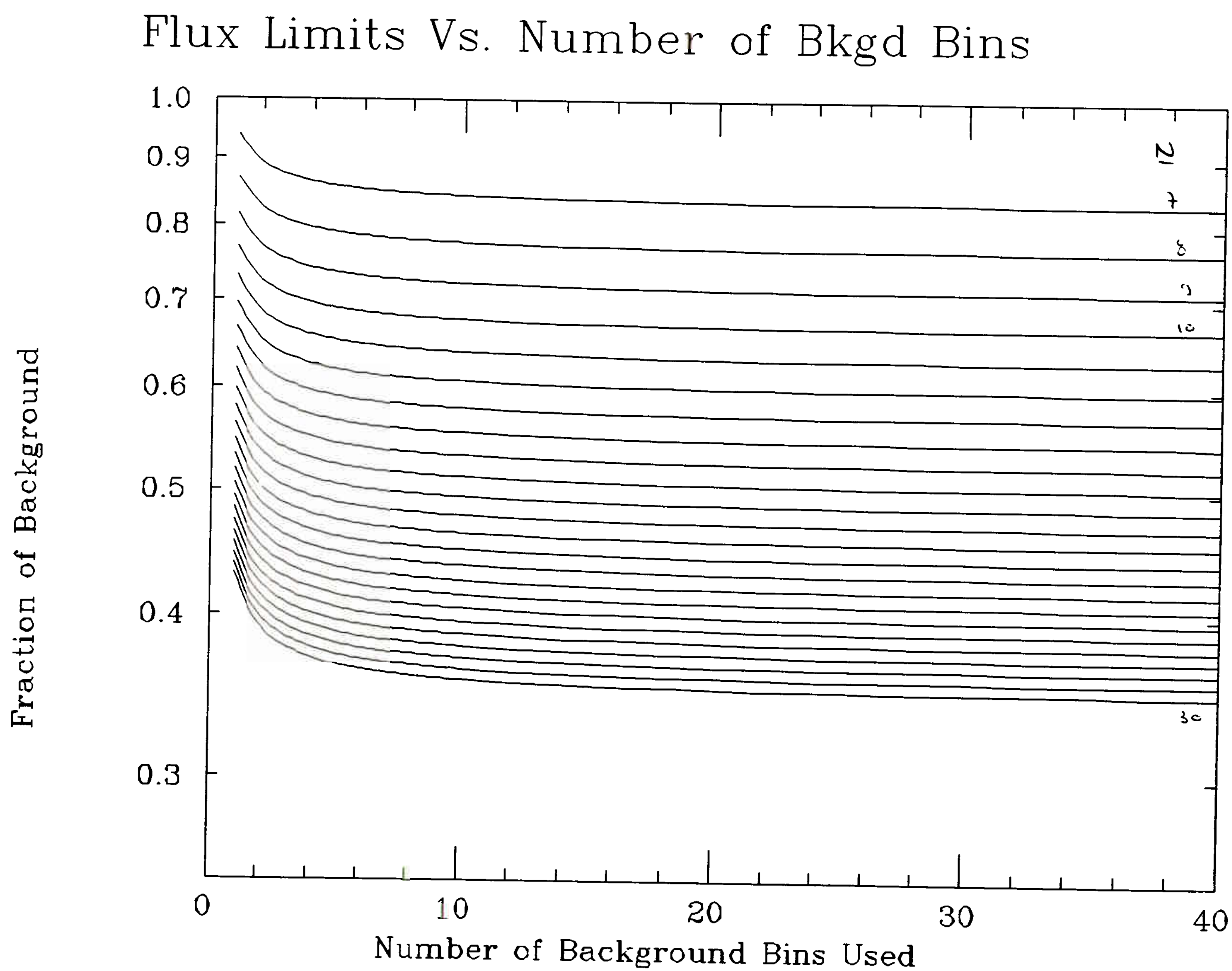
Source	N Observed	N Expected	90% CL	Typical 90% CL
4U2142+38	18	23.3	0.276	0.402
4U2321+58	18	12.2	1.04	0.588
4U1257+28	24	25.3	0.357	0.384
4U1651+39	26	24.0	0.469	0.405
4U1957+40	33	24.9	0.688	0.371
4U2358+21	17	12.8	0.877	0.537
GK Per	26	21.1	0.634	0.432
U Gem	20	19.9	0.454	0.418
AM Herc	22	23.9	0.352	0.379
SS Cygni	23	25.2	0.335	0.388
HZ 43	22	25.7	0.298	0.370
DQ Herc	23	24.1	0.372	0.401
1E2259+58	22	13.6	1.16	0.530
SS 433	11	6.0	1.77	0.929
V404 Cygni	28	24.6	0.510	0.382
Virgo A	7	13.1	0.313	0.569
Andromeda	20	20.4	0.430	0.430
3C279	1	2.9	0.990	1.23
K1	19	19.1	0.457	0.457
K3	24	26.0	0.335	0.387
K4	11	12.7	0.491	0.545
K5	4	7.4	0.512	0.771
K6	22	16.8	0.772	0.462

Table 3: 90% confidence level upper limits on the fractional excess in a 2.0° bin for April 1 1992

Source	N Observed	N Expected	90% CL	Typical 90% CL
Cyg X-3	58	68.1	0.1473	0.2261
Her X-1	71	71.8	0.2133	0.2133
Crab	50	53.1	0.2228	0.2588
2CG095+04	54	52.0	0.2909	0.2630
Geminga	38	41.5	0.2444	0.2896
2CG078+01	66	66.6	0.2238	0.2238
2CG075+00	80	68.9	0.3594	0.2170
2CG065+00	71	66.3	0.2837	0.2274
2CG135+01	31	33.9	0.2779	0.3150
2CG121+04	22	25.4	0.3064	0.3809
PSR1953+29	67	68.2	0.2153	0.2249
PSR1937+21	42	47.8	0.2036	0.2641
PSR1929+10	23	27.7	0.2698	0.3555
PSR0950+08	17	22.3	0.2811	0.4126
PSR0355+54	41	50.1	0.1701	0.2671
PSR1951+32	70	66.3	0.2715	0.2274
PSR1957+20	45	46.6	0.2565	0.2706
4U0115+63	32	31.4	0.3618	0.3389
4U1907+09	26	26.9	0.3562	0.3562
4U0042+32	51	65.5	0.1251	0.2268
4U0316+41	70	65.6	0.2819	0.2256
4U0352+30	66	61.8	0.2902	0.2307
4U0614+09	24	24.9	0.3711	0.3711
4U1837+04	19	17.9	0.5271	0.4433
4U1901+03	17	14.9	0.6492	0.4896
4U1918+15	44	33.2	0.6308	0.3329
4U1954+31	74	63.8	0.3675	0.2269
4U1956+35	83	68.7	0.4059	0.2192

Table 4: 90% confidence level upper limits on the fractional excess in a 2.0° bin for April 1 1992

Source	N Observed	N Expected	90% CL	Typical 90% CL
4U2142+38	76	60.7	0.4651	0.2340
4U2321+58	44	43.9	0.2903	0.2748
4U1257+28	50	60.1	0.1533	0.2419
4U1651+39	71	72.2	0.2090	0.2181
4U1957+40	66	69.5	0.1929	0.2198
4U2358+21	44	45.7	0.2577	0.2719
GK Per	68	59.4	0.3624	0.2400
U Gem	66	52.6	0.4863	0.2536
AM Herc	58	65.2	0.1689	0.2305
SS Cygni	74	75.3	0.2037	0.2124
HZ 43	44	59.1	0.1252	0.2441
DQ Herc	74	65.1	0.3433	0.2317
1E2259+58	54	46.7	0.4069	0.2688
SS 433	28	17.7	1.0463	0.4539
V404 Cygni	73	65.8	0.3174	0.2232
Virgo A	35	32.8	0.3902	0.3226
Andromeda	60	65.5	0.1816	0.2268
3C279	4	3.1	1.7138	1.405
K1	56	63.8	0.1659	0.2269
K3	77	67.8	0.3374	0.2198
K4	30	33.6	0.2671	0.3225
K5	33	27.2	0.5576	0.3719
K6	53	52.9	0.2619	0.2491


Flux Limits Vs. Number of Bkgd Bins
Fraction of Background
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0
10
20
30
40
Number of Background Bins Used

$N_{exp} = N_{obs} = N$