Dangers of Unphysical Regions

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Abstract

We discuss the appearance of negative numbers of events in radiochemical experiments and negative squared antineutrino mass $m_{\bar{\nu}_e}^2$ in tritium beta decay. Going beyond the standard discussion about how to extract upper limits in those cases, we show that the problem is much more profound. We explain the circumstances which are the likely cause of the persistently negative values of $m_{\bar{\nu}_e}^2$ in all modern tritium beta decay experiments.

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Introduction.

A problem in data analysis which turns up occasionally in some experiments and notoriously in others is that of a parameter estimate occurring outside the theoretically allowed physical range of the parameter. The common attitude to this is that one may use the unphysical result to set a limit inside the physical range. If one assumes that a known, e.g. Gaussian, probability density function can be centered on the measured value found in the unphysical range, there exists a standard prescription for translating a confidence interval for the measured value into a confidence interval for the true value 1, 2. The discussion then generally turns around whether one should use the full Gaussian for the confidence interval, or only the part of the Gaussian tail which is inside the physical range, properly renormalized 2, 3, 4.

For this discussion we shall use two well known examples where the problem with unphysical regions appear. The first example is the distinction of a positive signal over background, where both signal and background consist of countable events. Our second example is the case of neutrino mass determination from the shape of the electron energy spectrum in tritium $\beta$-decay. The neutrino mass example was also used in refs. 2, 3, where it was assumed that a Gaussian could meaningfully be centered on the estimated value in the unphysical range. In this paper we shall argue that the problem is more profound, and that the data analysis should be done differently.

Radiochemical experiments.

Consider the detection of radiatively decaying atoms in a radiochemical experiment, such as the solar neutrino experiments 3, 4, 5. The radioactive atoms have been produced by exposure to the neutrino radiation from the sun, and the total number of atoms collected gives information about the solar neutrino flux. The atoms are counted when the radioactive decay takes place in a detector with well known sensitivity, and the signature of these events is that they occur with a well known time constant $\lambda$. There are no other characteristics permitting the distinction of signal events from background events occurring randomly in time. The estimator of the sum of neutrino flux and background is thus a Poisson-distributed discrete random variable. It is essential to note that the number of counts is very small during a period of observation, a ”run”, sometimes zero. The general procedure for how to analyze such data has been well described by Cleveland 6.

The signal events are defined to occur with a time distribution $\exp(-\lambda t)$, and the background is assumed constant in time. Thus the occurrence probability per unit time is given by

$$f(t; a, b) = ae^{-\lambda t} + b,$$

(1)
where $a$ and $b$ are the signal and background intensities, respectively. Since both
the signal and the background are Poisson-distributed non-negative numbers the
physical region is defined by $a$ and $b$ both being non-negative.

The estimators $\hat{a}$ and $\hat{b}$ are found by maximizing the likelihood function (or
minimizing the negative of the log-likelihood function) for $N$ observations of one
event, each at a time $t_i$, $i = 1...N$,

$$L(t_1, ..., t_N|a, b) = e^{-\Delta/\lambda - b T} \prod_{i=1}^{N} (ae^{-\lambda t_i} + b) ,$$
(2)

where $T$ is the total observation time, and $\Delta$ is the sum of the $N$ time intervals
weighted by $\lambda$,

$$\Delta = \sum_{i=1}^{N} e^{-t_i \lambda} - e^{-t_{i-1} \lambda} .$$
(3)

Usually $\hat{a}$ and $\hat{b}$ are not required to be separately non-negative. If $\hat{a}$ and $\hat{b}$ are signif-
ically positive (as in the total fits to a large number of independent experimental
"runs") this causes no problem.

Consider, however, the situation in an individual run when the number of signal
events is zero or nearly zero. If $\hat{a}$ is not required to be non-negative in the fit, the
maximum likelihood may occur for a value of $\hat{a}$ which is negative as a result of a
pure statistical fluctuation.

Or else, there may be an unknown process contributing to the background so
that the data happens to exhibit a component increasing in time, for instance a late
accumulation of events which simulates an intensity increasing with time. Since this
is not taken care of by the $b$ assumed constant, this is misinterpreted as a signal
having the form $f(t; -a, b)$. In other words, the background hypothesis is wrong.

Since there is no physical theory in an unphysical region, $f(t; -a, b)$ is arbitrary,
and could often be replaced by some other arbitrary continuation. Thus if the
likelihood function has a deeper extremum for some negative $a$, this fact cannot
be used to make confidence statements about $\hat{a}$ in the physical region, because the
choice of another continuation might yield a negative $\hat{a}$ corresponding to a different
extremum. In any case one should bear in mind that the information obtained using
$f(t; -a, b)$ is an information on the background, not on $a$.

A further problem is that $f(t; -a, b)$ is not a normalizable probability distribu-
tion. It therefore does not make sense to describe the data by a Gaussian centered
on $-\hat{a}$, and to make inferences from its tail in the physical region.

The only inference one can make about a negative signal is that the hypothesis
(1) is wrong, notably that the background is not well described by a constant. To
prove that the hypothesis (1) is wrong one has to make a goodness-of-fit test in the
physical region, for instance at $a = 0$, not a test which makes use of the arbitrary and ill-defined likelihood in the unphysical region. Unfortunately the widely used chisquare test is not reliable for very small numbers of events.

If the extremum is on the edge of the allowed parameter range there may be a problem with the convergence of numerical search algorithms such as those used in MINUIT [9]. Note that the hypothesis used in an unphysical region may influence the value of $\hat{a}$ in the nearby physical region, because the search algorithms make finite steps around the extremum.

The distribution of a consistent estimator converges in the (weak) limit of infinite volume of the sample to the delta function for the true value. An unbiased estimator, repeatedly measured, returns values on both sides of the true value while converging towards it. However, when the true value is exactly zero (an academic case) and the estimator is a Poisson-distributed random variable restricted to integer non-negative values, the measurement process can only converge from the positive side, thus it appears biased. But this is unavoidable, because mathematical statistics does not admit any estimator for negative values of a Poisson variable. If instead one does use an ad hoc estimator, not prescribed by the physical theory, which can take values on both sides of zero, the gain in apparent unbiasedness is obtained at the price of arbitrariness.

Let us return to the case when a large number of independent experimental runs are done. The discussion has generally concerned the question whether $\hat{a}$ should be constrained to be non-negative in the individual runs before averaging. The answer to this is clear: if the results are non-negative on average, one should not constrain the individual runs because that would bias the final result towards higher values of $\hat{a}$. Although this is not wrong, it implies the loss of real experimental information. The advisable procedure is to fit all the runs simultaneously with one common parameter $\hat{a}$ and with (if necessary) different background parameters $b_j$ for each run $j$. When the ensuing average $\hat{a}$ is in the physical region, no error in procedure would have occurred, because also the runs which individually yielded negative signals would be contributing their share to the total likelihood at the common best value of $\hat{a}$ in the physical region. This is the procedure used for instance by GALLEX [6].

The neutrino mass problem.

Consider now the case of the electron antineutrino mass determination from the shape of the electron energy spectrum in tritium $\beta$-decay. The spectrum given by Fermi theory is

$$f(E|A, m^2, E_0, b) = A p E \ F(E, E_0) \ (E_0 - E) \ {[(E_0 - E) - m^2]^{1/2} + b}. \tag{4}$$

$F(E, E_0)$ is called the Fermi function (see e.g. ref. [2]), $p$ is the electron momentum, and the root is taken to be real and positive. Note that the $e$-antineutrino mass $m$
enters only in the form $m^2$. The other parameters to be determined by the fit are the total decay energy $E_0$, a positive normalization constant $A$, and the background $b$ assumed constant. (Sometimes the background is described by an empirical function, e.g. $b + cE$ \[12\], but this does not affect our general argumentation.)

The physical region is defined by conditions on $m^2$ and $E_0$. Clearly $m^2$ must be non-negative. From the factor $(E_0 - E)$ we see that the theoretical electron spectrum would be negative for energies $E > E_0$, and the square root becomes imaginary for $E > E_0 - m$. Oddly enough, the square root term in Eq. (4) is positive and real for all energies $E < E_0$ if $m^2$ were allowed to be negative. This curious fact is the cause of problems encountered in all fits, as has been pointed out before \[13\], and as we shall discuss below.

The theory of beta decay does prescribe the electron energy spectrum to have the form (4), but the atomic physics or molecular physics of the tritium compound might cause modifications. The Fermi function depends on approximations which we shall not discuss here. The experimental resolution function has to be folded into the final spectrum, and all possible instrumental distortions might not be well understood. In any case, the assumption \[10, 11\] that the response (resolution) function of the $\beta$-spectrometer is Gaussian can not be rigorously proved for the tail of the response function.

Thus the form of the signal is not well known and the hypothesis (4) as well as the assumption for the background may be wrong. An accumulation of events at energies near or beyond $E_0$ have been reported \[10, 11\] indicating problems with Eq. (4). The experimental background is not due to tritium $\beta$-decay, and thus its distribution does not respect the kinematical limit $E < E_0 - m$.

The estimators $\hat{m}^2$ and $\hat{E}_0$ are random variables which depend on the data and the method, e.g. in all recent experimental works (see \[14\] and references therein, and refs. \[10, 11\]) the method is least squares minimization, the ”chisquare” method \[1\].

The comments we made on the unphysical region in the radiochemical case are mostly the same here, but there are important differences due to the more complicated mathematical form of the ”signal”. From the expression (4) we obtain for $E = E_0 - m$ if $m \neq 0$

$$df((E_0 - m)|A, m^2, E_0, b)/dm^2 = \infty \text{ .} \quad (5)$$

Moreover, taking into account that the Fermi function $F(E, E_0)$ has no singularity at $E = E_0 - m$ we obtain, if $m \neq 0$, from the expression (4) for $E = E_0 - m$ and any $n = 1, 2, ...$

$$|d^n f((E_0 - m)|A, m^2, E_0, b)/dE^n| = \infty \text{ .} \quad (6)$$

Thus there is no analytic continuation of the theoretical ”signal” (4) from the physical region into the unphysical region. It follows that it does not make sense to
describe the data by a Gaussian centered at $-\hat{m}^2$, and make inferences from its tail in the physical region.

And even if it did make sense (putting in an empirical analytic continuation "by hand" \[10, 11\] and thereby changing the given problem of estimating the physical nonnegative $m^2$), one cannot derive a confidence limit on $m$ from $-\hat{m}^2$ \[3\].

There are two possible reasons for obtaining a negative $\hat{m}^2$ in a numerical search for minimum chisquare. The first reason is trivial, and not of statistical nature: there is a real accumulation of events near the end point $E = E_0 - m$ caused by instrumental problems or unknown physics or a wrong background hypothesis. Since Eq. \(4\) does not account for this, it must be modified.

The conclusion is then the same as in the radiochemical case. A goodness-of-fit test of the hypothesis \(4\) should be made in the physical region, not at $-\hat{m}^2$. There is again the caveat about the chisquare method not being a suitable test in a region with very low statistics.

The second reason is quite non-trivial \[13\]. No tritium decay electron can have an energy $E > E_0 - m$, so data obtained in that range must be background. Yet it is impossible to restrict the fit of Eq. \(4\) to the physical range $E \leq E_0 - m$ and replacing it in the $E > E_0 - m$ range by a pure background term, because $E_0$ is an unknown and itself a parameter to be determined in the fit. And even if we knew from theory the approximate value of $E_0$ (as was assumed in \[11\]), the problem is the same, because we do not know the antineutrino mass.

This problem was already understood by the writers of MINUIT, who built an explicit check into the program, prohibiting the user from supplying different functions in different parameter ranges if the ranges depend on one of the parameters to be estimated \[3\].

Therefore, it is almost unavoidable that the fit covers data in some part of the unphysical range $E > E_0 - m$, where the numerical search must make steps into the region of negative $\hat{m}^2$ in order to keep the root in \(4\) real. And, as already mentioned in the radiochemical case, search algorithms like those used in MINUIT \[3\] only converge if they can make finite steps around the extremum, thus stepping $E_0$ occasionally into the range $E_0 < E + m$. The convolution of the energy resolution function into the spectrum may also be a cause for excursions into this unphysical range.

Of course, this situation is avoidable if one has sufficiently good estimates for $E_0$ and $m$ to be able to restrict the fit to experimental data in the range $E \ll (E_0 - m)$ far from the unphysical region, as were done in the past (see \[14\] and references therein). Although one then obtains non-negative estimates for $m^2$, the resulting statistical errors (dispersion) are big since the $\beta$-spectrum for $E$ far from $E = E_0 - m$ is very insensitive to the unknown antineutrino mass.
We believe that the described circumstances are the main reason why all modern experiments \[1, 10, 11\] have obtained results in the unphysical range \( \hat{m}^2 < 0 \). We are currently carrying out simulations to demonstrate this quantitatively \[13\], but it would still be preferrable if the experimental groups would confirm this on real data.

**Conclusions.**

For both cases studied, the determination of the solar neutrino flux by radiochemical methods and the determination of the electron antineutrino mass from the end point of the electron spectrum in tritium \( \beta \)-decay, the conclusions are the same. An analysis which yields a signal estimate which is zero or negative obviously tells that there is no signal, only background. Thus the information obtained from the unphysical region with a negative signal is not an information on the signal parameter, but on the background.

In the radiochemical case the functional form of the signal in the unphysical region is an increasing function which approaches a constant. If the background happens to have this form, for physical reasons or because of statistical fluctuations, a negative signal is the apparent result. The same is true in the electron antineutrino mass case but more importantly, the squared antineutrino mass is forced to be negative by attempts to fit the electron spectrum and the background in the energy region beyond the physical end point of the spectrum.

In both cases, a fit which is better in the unphysical region than in the physical region is an accident, because the function which is correct in the physical region is arbitrary in the unphysical region, and could often be replaced by some other arbitrary continuation. Thus an extremum of the likelihood function in the unphysical region cannot be used to make confidence statements about the parameter in the physical region, because the choice of another arbitrary function would yield a different result.

In particular it is impossible to obtain the confidence statement about the real antineutrino mass from a negative unphysical estimator, \( \hat{m}^2 < 0 \). All one can conclude (barring mistakes on the functional form of the background) is that \( m \neq 0 \), because if it were zero, there would not be any square root in Eq. \[1\], and nothing would force the fit into the region of negative \( \hat{m}^2 \).

To decide whether the function composed of signal plus background is an adequate description of the data, one has to make a goodness-of-fit test in the physical region. It is misleading to make a likelihood ratio test comparing the likelihood in an unphysical region with the likelihood in the physical region, because the former is meaningless and the functions are not the same. It is doubtful whether the chisquare method is a suitable goodness-of-fit test near the edge of a physical region, because chisquare is not reliable for small samples. The resolution of this problem is to find
other statistical tests which are adapted to the situation.

We have shown that there are circumstances which cause a fit to the electron spectrum in tritium $\beta$-decay to yield a negative $m^2$ value. Since these circumstances are present in all modern analyses [4, 10, 11], we believe we have found the reason for the anomalous results.

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