Effect of Correlations Between Model Parameters and Nuisance Parameters When Model Parameters are Fit to Data

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The effect of correlations between model parameters and nuisance parameters is discussed, in the context of fitting model parameters to data. Modifications to the usual $\chi^2$ method are required. Fake data studies, as used at present, will not be optimum. Problems will occur for applications of the Maltoni-Schwetz theorem. Neutrino oscillations are used as examples, but the problems discussed here are general ones, which are often not addressed.

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I. INTRODUCTION

Correlation between background parameters and model parameters occurs if there are off-diagonal elements in the overall covariance matrix for background plus signal or if there is a direct dependence between a model parameter and a background. For example, in neutrino oscillation experiments, an initially $\nu_e$ beam oscillates producing some $\nu_x$ events. The $\nu_x$ beam becomes smaller as some of the $\nu_e$ have oscillated. In some models this disappearance is considerably larger than the $\nu_e$ appearance. If there is disappearance of the $\nu_x$, then $\pi^0$ production by $\nu_x$, a principle $\nu_e$ background, also decreases. The correlation coefficient for this example is negative. Fits often include estimates for this kind of correlation by using the full covariance matrix and/or modifying the background estimates after each iteration.

However, correlation of background and signal can also occur simply because the shape of the background spectrum matches the shape of the signal. They are correlations only in the sense that the spectrum over bins of the signal is similar to that of the background and the correlation is found by a regression analysis. These correlations should, perhaps, be distinguished by being called “regression correlations”. The present report emphasizes this kind of correlation which is often not considered at all. Modifications to $\chi^2$ fitting are required for these regression correlations. If the correction for these regression correlations is not included, then the experimental $\chi^2$ will not have a $\chi^2$ distribution. The best fit point then will be incorrect and confidence regions will be too large. Even fake data studies will not give correct results if these corrections are not included and the “effective number” of degrees of freedom obtained from fake data studies will be affected. Correction for this new correlation makes the experimental $\chi^2$ distribution be more like the $\chi^2$ distribution with number of degrees of freedom equal to the number of bins minus the number of parameters fit.

II. NOTATION

Suppose data have been obtained for a histogram with $N_{\text{bins}}$. The $i$th bin has $N_{\text{data}}(i)$ events.

The model used for fitting the data has two kinds of parameters. The first kind are nuisance parameters which are called “systematic errors”. There are $N_{\text{bkd}}$ of these parameters. They constitute backgrounds, $B_j(i)$ where $i = 1, \ldots, N_{\text{bins}}$, and $j = 1, \ldots, N_{\text{bkd}}$. The backgrounds have been evaluated in independent experiments previously giving estimates for the mean value of each $(B_m)_j(i)$ and the covariance matrix of the error in the mean value $\text{cov}_{B_j}$. There are correlations from bin to bin, so that the covariance matrix is not, in general, diagonal. The total background is

$$B_m^{\text{tot}}(i) = \sum_{j=1}^{N_{\text{bkd}}} [(B_m)_j(i)].$$

Define the “signal” as

$$N_{\text{sig}}(i) = N_{\text{data}}(i) - B_m^{\text{tot}}(i).$$

The covariance matrix of the signal in bins $i, j$ is given as

$$\text{cov}_{\text{sig}}(i, j) = \text{cov}_{\text{data}}(i, j) + \text{cov}_{\text{Btot}}.$$
III. A TOY MODEL

Suppose one is fitting a parameter to a signal model of the form $T(i) = tf(i)$, where $t$ is a constant to be fit and $f(i)$ is a known function of the bin number $i$. Suppose, further, that there is a single background $B(i)$, which is uncorrelated with the model parameter. The fit is done by using the method of Equation 3. For a $\chi^2$ fit, the numerator in each bin is $[N_{\text{data}}(i) - (B_m(i) - N_{\text{th}}(i))]^2 = [N_{\text{data}}(i) - B_m(i) - tf(i)]^2$. The denominator is the covariance for the numerator. The statistical covariance of the data is the uncertainty expected for the current values of $T(i)$ and $B_m(i)$ which is just $T(i) + B_m(i)$. In addition there is a term for the uncertainty in $B_m$, $\text{cov}_{B(i)}$. The denominator is $T(i) + B_m(i) + \text{cov}_{B(i)}$. Let $t_0$ be the result of that fit. The error is assigned to the $t$ parameter by the usual $\Delta\chi^2$ method.

Now suppose that the background has the form $bf(i)$, where $b$ is a constant and $f(i)$ is the same function that appeared for the model parameter. The model and background are now completely correlated. Since $f(i)$ is a common factor for model and background, the numerator for the $\chi^2$ fit can be written as $[N_{\text{data}} - (t + b)f(i)]^2 = [N_{\text{data}} - zf(i)]^2$, where $z = t + b$. The background experiment has previously obtained a mean and error for the parameter $b$. The fit here obtains a mean and error for the parameter $z = t + b$.

Assume, incorrectly, that the $\chi^2$ denominator remains the same as for the uncorrelated fit. Then, if $b$ is estimated by $(b_m)$, the new fit for $t$ is the same as the old one, $t_{\text{fit}} = t_0$.

However, the variance matrix is not the same as it was for the previous fit. For this new fit, the background is part of the parameter $z$ being fitted. There is no mention of $b$; only $z$ appears in the fit. The term $\text{cov}_{B(i)}$ is not included in the denominator of the $\chi^2$ term. In terms of likelihood,

$$\mathcal{L}(\text{data}|t, b) \mathcal{L}(b) = \mathcal{L}(\text{data}|t + b) \mathcal{L}(b) = \mathcal{L}(\text{data}|z) \mathcal{L}(b),$$

$$\int \mathcal{L}(\text{data}|z) \mathcal{L}(b) db = \mathcal{L}(\text{data}|z).$$

The probabilities for $z$ and $b$ are independent. When the fit is obtained, the estimate of the error in $z$ is determined in the usual $\Delta\chi^2$ manner. The estimate of $t$ is taken as the difference between $z$ and the mean value for the background, $(b_m)$. If the fit has gone to the same place, the result again will be $t_0$. The error in the estimate of $t$ is obtained in the usual way by adding the errors in $z$ and in $(b_m)$ in quadrature. This means that the uncertainty in $t$ will also be the same as it would be if the correlation were ignored.

Since the $\chi^2$ in this fit does not have $\text{cov}_{B(i)}$ as part of the denominator of the $\chi^2$ fit, then, if the fit goes to the same place, the $\chi^2$ is larger than the $\chi^2$ would have been if the correlation were not taken into account and the probability of the fit is lower. The probability of the fit is systematically underestimated if the correlation is ignored. The subtlety here is that this is a fit. If a fixed value of $t$ is used and there is no fit, the $\chi^2$ distribution would be correct if the $\text{cov}_{B(i)}$ is included. However, the fitted value of $t$ is not affected by the $\text{cov}_{B(i)}$, and the $\chi^2$ for the fitted value is too low.

Note that, in practice, some uncertainties affect both the signal and background in the same way. For the MiniBooNE experiment, errors in scintillation fraction and errors on pion production cross sections are of this form. These errors should be included in the covariance used in the fit.

For the MiniBooNE experiment, does the $\pi^0$ background resemble the signal? $\pi^0$ background numbers for the neutrino exposure are obtained from Table 6.5 of the MiniBooNE Technical Note 194 [2]. The neutrino spectrum and the neutrino quasi-elastic cross sections were read from Figures 2 and 5 from a MiniBooNE neutrino elastic scattering Physical Review article [3]. Results are shown in Figure 1. For $\Delta m^2 = 2$ or 1 eV$^2$, the mean and $\sigma$ of the $\pi^0$ background and the signal are quite close and the correlations are large.

Another method to treat this problem would be to make a combined fit for the background and signal using the histograms for both signal and background. However, if there are many backgrounds, the “curse of dimensionality” makes this impractical. In addition the many backgrounds may have been obtained by many different methods.

In the next two sections, the problem of partial regression correlations of signal with one or more backgrounds at a given model point will be treated. Complications due to dependence on model parameters of these quantities and other problems will be discussed in sections VI-VIII.

IV. PARTIAL CORRELATIONS

In practice, regression correlations are almost never complete; it is necessary to consider partial correlations between signal and background. The model for the theory is taken as $tf(i)$, where $t$ is a constant and $f(i)$ is a known function of bin number. Assume that the only significant regression correlation is the one between the model and $B_k(i)$. The model for the background is taken as $B_k(i) = b_kg(i)$, where $b_k$ is constant and $g(i)$ is a known function of bin number. Let $s$ denote the predicted signal given $t$. Let $M_f$ and $\sigma_f$ be the mean and standard deviation of $f(i)$ and let $M_g$ and $\sigma_g$ be the mean and standard deviation of the background, $g(i)$. The variation here is the variation over the bins of the histogram. Let $x_s^*(i)$ be the part of the background correlated to the signal. Consider a plot of background versus theory, where the points are the values for each bin. A straight line regression fit of background on signal yields

$$\frac{x_s^*(i) - M_g}{\sigma_g} = \rho \frac{f(i) - M_f}{\sigma_f}. \quad (5)$$
FIG. 1: The top figure shows the energy spectrum expected for the π^{0} background. The mean is 0.940 GeV and the standard deviation is 0.341 GeV. The middle figure shows the energy spectrum expected for the neutrino oscillation signal if Δm^2 = 2 eV^2. The mean is 0.910 GeV, the standard deviation is 0.305 GeV and the correlation with the π^{0} spectrum is 0.718. The bottom figure shows the energy spectrum expected for the neutrino oscillation signal if Δm^2 = 1 eV^2. The mean is 0.739 GeV, the standard deviation is 0.305 GeV and the correlation with the π^{0} spectrum is 0.771.

The regression correlation coefficient is given by

\[ \rho = \frac{E \{ (g - M_g)(f - M_f) \}}{\sigma_g \sigma_f}, \]  

where \( E \) means the expectation value over bins.

Since this was a straight line fit \( x^*_s(i) \) has the same bin dependence as the signal. Note that Equations 5 and 6 are normalization independent because of the divisions by \( \sigma \).

\[ x^*_s(i) = M_g + \frac{\rho \sigma_g}{\sigma_f} (f(i) - M_f). \]  

Define an “effective” correlation \( \rho_{e,f} = \rho \sigma_g/\sigma_f \). Let \( \Delta_{sk}(i) \) be the uncorrelated part of the background

\[ \Delta_{sk}(i) = b_k [g(i) - x^*_s(i)] = b_k [g(i) - M_g - \rho_{e,f}(f(i) - M_f)]. \]  

The covariance matrix due to the uncertainty in the experimental values obtained for background from the experiments determining the background is given by:

\[ \text{cov}_{\Delta_{sk}}(i, j) = [g_k(i) - M_g - \rho_{e,f}(f(i) - M_f)] [g_k(j) - M_g - \rho_{e,f}(f(j) - M_f)] \sigma_{b_k}^2. \]  

(9)

The new covariance matrix for the fit uses only this uncorrelated part of \( B_k \):

\[ \text{cov}_{\text{new}} = \text{cov}_{\text{data}} + \text{cov}_{\Delta_{sk} + \sum_{k \neq k} B_j}. \]  

(10)

The fit is then made to

\[ N_{\text{fit}}(i) = (t + b_k \rho_{e,f} b_k) f(i). \]  

(11)

\( N_{\text{sig}} \) had subtracted the estimates of all background. \( N_{\text{fit}} \) adds to \( N_{\text{sig}} \) the estimate of the correlated part of \( B_k \). The fitting parameter is taken as

\[ z f(i) = (t + \rho_{e,f} b_k) f(i). \]  

(12)

After the fit the estimate for \( t \) is found from

\[ t_{\text{fit}} = z_{\text{fit}} - \rho_{e,f} b_k. \]  

(13)

The covariance of \( t \) is given by

\[ \text{cov}_{t} = \text{cov}_{z_{\text{fit}}} + \text{cov}_{\rho_{e,f} b_k}. \]  

(14)

V. CORRELATIONS OF SEVERAL BACKGROUND PARAMETERS WITH THE SIGNAL

It may be that several nuisance parameters have significant regression correlation with the signal. One needs to find the regression correlation of the signal with the totality of the nuisance parameters. This correlation can be calculated by standard methods [4]. Let \( \Lambda \equiv (\lambda_{ik}) \) be the moment matrix over bins for the nuisance parameters with \( t \) added as an extra parameter. \( \Lambda^{ik} = (t, k) \) cofactor of \( \Lambda \), that is \((-1)^{i+k} \) the determinant of \( \Lambda \) with row \( i \) and column \( k \) removed.

Define the correlation matrix:

\[ P \equiv (\rho_{ik}) = (\lambda_{ik} / \sigma_i \sigma_k). \]  

(15)

Note that, as was the case for Equation 6, \( P \) is independent of the normalization. For a variable \( y \) use \( y' = y - M_y \). Let

\[ (B'_{s})^*_s(i) \equiv \sum_{k \neq s} \beta_{sk} B'_k(i). \]  

(16)

where \( \beta_{sk} \) are constants chosen to minimize the expectation value over the bins

\[ \frac{1}{N_{\text{bins}}} \sum_i [(B'_s)^*_s(i) - (S')^2(i)]]^2, \]
where \( S(i) \) is the predicted number of data minus background events, given \( t \). It can be shown that

\[
\beta_{sk} = -\Lambda^{sk}/\Lambda^{ss} = -\sigma_s P^{sk}/(\sigma_k P^{ss}).
\]  

(17)

\( \beta_{sk} \) is not independent of the normalization of the backgrounds. The method finds the appropriate linear sum of backgrounds which has the highest correlation with the signal. Problems can arise if non-linear effects are important, as will be noted in section VIII. Go back from primed coordinates to unprimed coordinates. The mean of \( B_s^* \) is \( M_{B_s^*} = \sum_{k=1}^{N_{bkrd}} \beta_{sk} M_{B_k} \), where \( M_{B_k} \) is the mean over the histogram bins of the backgrounds \( B_k \). \( B_s^* \) can now be taken as an effective single background for determining the correlation with signal. \( B_s^* \) will not, in general, have the same dependence on bins as the signal. As was the case for the one background case, a linear regression correlation \( x_s^*(i) \) between the signal and the \( B_s^* \) for fixed values of the model parameters is needed. Suppose the model depends on one parameter and the dependence is given as before by \( tf(i) \) where \( f(i) \) is known. The regression line of \( B_s^* \) on signal yields

\[
\rho^* = \frac{\lambda f B_s^*}{\sigma_f \sigma_{B_s^*}},
\]  

(18)

\[
\lambda f B_s^* = \frac{1}{N_{bins}} \sum_{i=1}^{N_{bins}} \left( \sum_{k=1}^{N_{bkrd}} \beta_{sk} [B_k(i) - M_k] [f(i) - M_f] \right).
\]  

(19)

\[
\frac{x_s^*(i) - M_{B_s^*}}{\sigma_{B_s^*}} = \rho^* \frac{f(i) - M_f}{\sigma_f},
\]  

(20)

or

\[
x_s^*(i) = M_{B_s^*} + D(i) \lambda f B_s^*; \quad D(i) = \frac{f(i) - M_f}{\sigma_f}.
\]  

(21)

The uncorrelated part of the background is

\[
\Delta^*(i) = \sum_{k=1}^{N_{bkrd}} B_k(i) - x_s^*(i) = \sum_{k=1}^{N_{bkrd}} B_k(i) - M_{B_s^*} - D(i) \lambda f B_s^*
\]  

(22)

\[
\Delta^*(i) = \sum_{k=1}^{N_{bkrd}} \sum_{j=1}^{N_{bins}} \beta_{sk} B_k(j) (1 + D(i)[f(j) - M_f])
\]  

\[
+ \sum_{k,j,m} \beta_{sk} B_k(m) D(i)[f(j) - M_f].
\]  

(23)

Next the covariance of \( \Delta^*(i) \) with respect to uncertainties in the \( B_k(i) \) as determined in preliminary background experiments is calculated.

\[
cov_{\Delta^*(i)} = T1 + T2 + T3,
\]  

(24)

\[
T1 = \sum_{k,l} \cov[B_k(i)B_l(i)],
\]  

\[
- \frac{2}{N_{bins}^2} \sum_{k,l,j} \beta_{sl} (1 + D(i)[f(j) - M_f]) \cov[B_k(i)B_j(j)],
\]  

\[
+ \frac{2}{N_{bins}^2} \sum_{k,l,j,m} D(i)[f(j) - M_f] \beta_{sl} \cov[B_k(i)B_l(m)],
\]  

(25)

\[
T2 = \frac{1}{N_{bins}^2} \sum_{k,l,j,m} \beta_{sk} \beta_{sl} (1 + D(i)[f(j) - M_f]) (f(m) - M_f) \cov[B_k(j)B_l(m)],
\]  

\[
- \frac{2}{N_{bins}^2} \sum_{k,l,j,m,n} \beta_{sk} \beta_{sl} (1 + D(i)D(i)) [f(j) - M_f] [f(m) - M_f] \cov[B_k(j)B_l(n)].
\]  

(26)

\[
T3 = \frac{1}{N_{bins}^2} \sum_{k,l,j,m,n,p} \beta_{sk} \beta_{sl} (1 + D(i)) [f(j) - M_f] [f(m) - M_f] \cov[B_k(n)B_l(p)].
\]  

(27)

\[
cov_{new} = cov_{data} + cov_{\Delta^*B^*},
\]  

(28)

Since, by construction, \( x_s^*(i) \) has the bin dependence of \( f(i) \), define \( b^* \) by

\[
x_s^*(i) = b^* \rho_{eff}^* f(i), \quad \rho_{eff}^* = \frac{\rho^* \sigma_{B_s^*}}{\sigma_f}.
\]  

(29)

The calculation then proceeds in analogy with that given in the previous section, Equations 11-14, with the obvious substitutions.

**VI. MULTIPLE MODEL PARAMETER CALCULATIONS**

For multiple model parameters, it is necessary to apportion the correlated part of the background among the fitting parameters \( z_k \). For one parameter we had:

\[
z f(i) = (t + \rho_{eff}^* b^*) f(i).
\]  

Here \( f(i) \) is the spectral shape of the model parameter as a function of bins in the histogram. Now there are several model parameters \( t_k f_k(i) \) and corresponding fit parameters \( z_k \).
Note that the apportionment is only necessary after the fit since each parameter \( z_k f_k(i) \) will have the spectral shape \( f_k(i) \) of the model parameter. The overall \( \chi^2 \) can be obtained without knowing the apportionment. This has the important advantage that the apportionment procedure need be done only once, not at each stage of the fit.

If the model spectrum is a simple sum of the terms for the various parameters, a method similar to that used for several backgrounds is followed. Let \( \Lambda_{\text{model}} \equiv \{ (\Lambda_{\text{model}})_{ik} \} \) be the moment matrix for the model parameters determined from the spectrum over the histogram bins with the background distribution \( (x_i^b) \) added as an extra parameter. Here the previous \( x_i^b \) has been retitled \( x_i^s \) for clarity in the present section.

Let \( \Lambda_{\text{model}} \) be the moment matrix for the model parameters, that is \( (-1)^{i+k} \times \) the determinant of \( \Lambda_{\text{model}} \) with row \( i \) and column \( k \) removed.

Define the correlation matrix:

\[
P_{\text{model}} \equiv \left( (\rho_{\text{model}})_{ik} \right) = \left( (\Lambda_{\text{model}})_{ik} / [(\sigma_{\text{model}})_i (\sigma_{\text{model}})_k] \right).
\]

Let

\[
\alpha_{ik} = -\Lambda_{ik}^{bb} / \Lambda_{model}^{bb} = -[\sigma_{model}]_{b} P_{model}^{bb} / [(\sigma_{model})_k P_{model}^{bb}).
\]

(31)

The \( \alpha_{ik} \) are the apportionment parameters. These parameters may need an overall renormalization so that

\[
(x'_i(i) = \sum_{k \neq b} \alpha_{ik} t_k f'_k(i),
\]

(32)

where the primed variables have been defined to have zero mean, \( y' = y - M_y \); \( M_y \) is the mean of \( y \).

\[
z_k(i) = (1 + \alpha_{ik}) t_k f_k(i).
\]

(33)

However, often the model parameters are not just simple sums. Consider the simple neutrino oscillation fit, used in MiniBooNE. The two parameters \( \Delta m^2 \) and \( \sin^2 2\theta \) occur as a product, not a sum. The latter parameter is just a scale parameter determining the size of the effect. All of the spectral shape information is contained in \( \Delta m^2 \). In terms of the notation \( t f(i), t \) is determined by \( \sin^2 2\theta \) and \( f(i) \) by \( \Delta m^2 \). The two parameters work together to produce a single spectrum. For a background which matches the shape for a given \( \Delta m^2 \), any mis-estimate of the background will appear in the fitted value of \( \sin^2 2\theta \) and the entire correlated part of the background should be associated with that parameter.

\[
z_{\sin^2 2\theta} f_{\sin^2 2\theta}(i) = (1 + \alpha_{b} \sin^2 2\theta) t_{\sin^2 2\theta} f_{\sin^2 2\theta}(i)
\]

(34)

The individual terms in the sum of model terms will sometimes be these composite terms. This occurs, for example in fits of neutrino data for sterile neutrino hypotheses. There will sometimes also be more complicated dependences than the simple ones here and it is necessary to examine the situation for each particular experiment. These same considerations apply to the backgrounds treated in the previous section.

### VII. SOME FURTHER COMPLICATIONS

For simplicity use the conditions for Section IV, one background parameter, one model parameter for this discussion. Generalization to more general situations is straightforward.

Suppose that there is a systematic uncertainty which is correlated between background and data. The fit for \( z \) includes the data uncertainty (perhaps a normalization uncertainty), but is otherwise unchanged. However, when one is finding the uncertainty in \( t = z - \rho_{eff} b \), there is a correlation between the uncertainty in \( z \) and in \( b \) which must be taken into account.

The background is \( B(i) = b(i) \). Until now it has been assumed that the spectrum function \( g(i) \) is fixed. Suppose there is an uncertainty in \( g(i) \). This causes an uncertainty in \( \rho \) which can be calculated using standard error propagation techniques. The uncertainty in \( \rho \) will introduce an uncertainty in the fraction of background subtracted from data for the fit to \( z \). This uncertainty must be included in the covariances used to fit \( z \). This does change the \( \chi^2 \) of the fit for \( z \). The uncertainty in \( \rho \) must also be included in the uncertainty for \( t = z - \rho_{eff} b \).

### VIII. INCORPORATING THESE CORRELATIONS IN PRACTICE

In practical situations it often occurs that the backgrounds and correlations vary with the model parameters. An appropriate fitting procedure for \( \chi^2 \) fits needs to include these point-to-point changes in correlations.

For the best fit, the regression correlation should be evaluated at each step just as the effects of changes in systematic errors are often evaluated at each step. The \( \chi^2 \) for the best fit is then the lowest \( \chi^2 \) obtained and has the regression correlation correction appropriate to that best fit set of parameters.

For determining confidence regions, consider a parameter point \( A \). If the absolute \( \chi^2 \) is to be used and \( A \) is a fixed point, not the result of a fit, then the regression correlations should not be included in the calculation of \( \chi^2 \). However, if the \( \Delta \chi^2 \) method is used, this is a comparison of two values obtained in a fit. The \( \chi^2 \) at \( A \) using the regression correlations at \( A \) minus the best fit \( \chi^2 \) using the regression correlations at the best fit should then be used.

If a fake data study is used, the procedure is similar. There is no change in the choice to the usual procedure for choosing Monte Carlo events. The regression correlations do not enter and only the usual backgrounds are randomly varied.

What happens next depends upon the question asked. Suppose there is no fit and the question asked is, “What is the distribution of \( \chi^2 \) if the model parameters are fixed?” For this question, the regression correlations do not enter.

However, if there is a fit, then for each fake data MC example, the calculations are done as indicated above for
point A and for the best fit using the regression correlations. Then, the procedure for the fake data study is done as before, just counting the fraction of MC samples having a higher $\chi^2$.

If the model and background correlations vary with the model point and the regression correlations are ignored, the best fit point will be different. Furthermore, confidence regions will be too large even for the fake data studies, since the width of the experimental $\chi^2$ confidence regions will be too large even for the fake data. The model point and the regression correlations are ignored, the best fit point will be different. Furthermore, confidence regions will be too large even for the fake data studies, since the width of the experimental $\chi^2$ distribution will include the variances from the full backgrounds, rather than just those from the uncorrelated parts of the background. At present, the use of an "effective number of degrees of freedom" is frequently employed to give corrections for the direct calculations, but not for the fake data studies. That correction is far less precise than the procedure studied here. With this new procedure the effective number should be closer to the real number (although it may still useful to include the new effective number as a residual correction).

IX. THE MALTONI-SCHWETZ THEOREM

Suppose one is examining the compatibility of two sets of data for a given hypothesis, data set 1 and data set 2. Suppose one finds the best fits for the model parameters for data set 1, data set 2, and for the combined data sets 1 plus 2. Let the number of parameters fit for the three fits be $N_1$, $N_2$ and $N_{1+2}$. The Maltoni-Schwetz theorem [4] then states that

$$\chi^2_{MS} = \chi^2_{1+2} - \chi^2_1 - \chi^2_2,$$

(35)

is a measure of the compatibility of the data sets. If they are compatible, $\chi^2_{MS}$ has a $\chi^2$ distribution with $N_{MS} = N_1 + N_2 - N_{1+2}$ degrees of freedom.

Consider, as an example, the question of explaining some possible neutrino experiment anomalies as being due to the presence of two sterile neutrinos. The model for this hypothesis assumes several $\sin^2 2\theta$-like variables, several $\Delta m^2$-like variables and a $CP$ phase. The first data set corresponds to the appearance of $\nu_e$ events from an originally $\nu_\mu$ beam and the second data set is for the disappearance of $\nu_\mu$ events from an originally $\nu_\mu$ beam.

Fits have been made using both $\nu_e$ appearance and $\nu_\mu$ disappearance experiments [5] [6]. Both kinds of experiments are fit reasonably well with this model, but, using the Maltoni-Schwetz formalism, tension is found between the appearance and the disappearance experiments.

For the J. M. Conrad et al. fits [5], the number of fitted variables for each of the three data sets was $N_{app} = 5$; $N_{dis} = 6$; and $N_{comb} = 7$. This leads to $N_{MS} = 5 + 6 - 7 = 4$. For the disappearance experiments there is no $\pi^0$ background. There is a $\pi^0$ background for some of the appearance experiments including the MiniBooNE experiment which has a large weight within the appearance experiment sample. In previous sections it was found that, if the correlations with backgrounds were not taken into account, the $\chi^2$ for the appearance experiment was lower than it should be.

In addition, because of the sensitivity of the appearance experiment to the $\pi^0$ background, an error in the estimate of that background can have a disproportionate effect [7]. For the combined data fit, if the $\pi^0$ background is larger than the value estimated, some $\sin^2 2\theta$ type parameters will want to be bigger than they should be for the appearance bins, but not for the disappearance bins, giving some tension within the combined data set, i.e., increasing the $\chi^2$. Furthermore the number of degrees of freedom for MS is only four, which makes the discrepancy turn into an extremely low probability. The MS method is especially sensitive to these errors. Even without the correlations considered here, much of the tension between the appearance and disappearance results goes away if it is assumed that the MiniBooNE estimate of the $\pi^0$ background is low by 1.4 $\sigma$.

X. SUMMARY

Methods are given for using the $\chi^2$ method when correlations between nuisance parameters and parameters being fitted occur. These methods are appropriate whenever these correlations exist.

1. If nuisance parameter-signal shape correlations are not taken into account, $\chi^2$ fits will systematically overestimate the probability of the fit. The experimental $\chi^2$ will not have a $\chi^2$ distribution.

2. Fake data studies without including these correlations will not be optimum. The use of “effective number of degrees of freedom” will help the situation, but will not be as precise as the methodology introduced here.

3. One must use caution in applying the Maltoni-Schwetz theorem to find the compatibility of two sets of data to a model hypothesis. The theorem may indicate incompatibility if there are correlations between the nuisance parameters and the signal and/or if there are problems with the estimations of nuisance variables.

XI. ACKNOWLEDGEMENTS

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