Comments on the 'Matrix' and 'Ratio' Methods for the Oscillation Analysis

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Summary

We are comparing two of the methods proposed for the neutrino oscillation analysis: one using smearing and unsmearing matrices and the one involving ratios of the relevant distributions.

We argue that the 'matrix' method provides the simplest and logically consistent framework of the analysis of the MINOS data and it minimizes the dependence (a.k.a. systematic error) due to poorly known input models.

Various 'ratio' methods methods which can be derived from the matrix method do not use any additional information, hence they do not reduce the systematic errors. On the other hand they introduce additional dependence on the poorly known models hence they are systematically inferior to the 'matrix' method. Some of the formulations of the 'ratio' method introduce considerable logical complications into the analysis logic, like multiple smearing/unsmearing of data in the far detector.

1 Introduction

It is usual case that the detectors used to measure physical quantities introduce smearing and distortions which modify the distributions of the quantities of interest and this experimental effects must be taken into account in the analysis process. There are two related, but different, modes of the corrections for the experimental resolution functions, which are often termed as 'smearing' or 'unsmearing'.

1.1 Smearing Correction

When a detector is used to measure a distribution $T(E)$ of a physical quantity E the resulting measurement is

$$O(E^{'}) = \int T(E)S(E,E^{'})dE \tag{1}$$

where $T(E)$ is the true distribution of the quantity E, $O(E^{'})$ is the observed (result of the experiment) distribution as a function of the measured value $E^{'}$ of the quantity in question and the function $S(E,E^{'})$ is the response function (or the resolution function) of the detector. The value of the function $S(E,E^{'})$ gives the probability of the obtaining the measurement result of $E^{'}$ when the true value of the measured quantity is $E^{'}$. The response function is a property of the measuring apparatus alone and it must be determined in a calibration process.

This function is independent the distribution of the measured quantity. In general the domains of the arguments E and E' are different, as the measurement may produce an unphysical value.

Smearing correction is applied in the situations when the true distribution of the measured quantity is known and we want to reproduce or predict the experimentally measured distribution.

In practical applications the experimental results are expressed in terms of binned distributions dN/dE' rather than analytic functions and the predicted distribution can be expressed as

$$\left[\frac{dN}{dE'}\right]_i = \sum_j \hat{S}_{ij} \left[\frac{dN}{dE}\right]_j \tag{2}$$

where $\left[\frac{dN}{dE'}\right]_i$ and $\left[\frac{dN}{dE}\right]_j$are the numbers or the events in bin $i(j)$ of the observed (true) distributions. As a consequence of the experimental smearing the vectors of the observed and true distributions have different dimensions, hence the transformation matrix $\hat{S}_{ij}$ is rectangular and the inverse transformation does not exist. The matrix $\hat{S}_{ij}$ can be evaluated numerically with the help of Monte Carlo simulation program. This matrix is obtained from a two-dimensional histogram of a smeared *vs* true value of the quantity E, with its columns (corresponding to the same bin of the true value of E) normalized to unity. With such a normalization a matrix element S_{ij} has an interpretation of a probability that an event with true value of E falling into bin j will have be measured value of E' falling into bin i. If the bin sizes are small compared to the feature size of the distributions measured the matrix $\hat{S}_{ij}$ is a property of the experimental apparatus only and it does not depend on the shape of the measured distributions. The matrix $\hat{S}_{ij}$ can be determined once and subsequently used to evaluate smeared distributions corresponding to various assumed true distributions.

1.1.1 Approximated Smearing

In some situations the full treatment of the smearing may be unnecessary or impossible (memory limitations in the very early days of computers provide a rare example of the latter). In such a situation the smeared distribution $\left[\frac{dN}{dE'}\right]_i$ corresponding to an assumed true distribution $\left[\frac{dN}{dE}\right]$ can be evaluated by applying a 'smearing correction'

$$\left[\frac{dN}{dE'}\right]_i = [AS]_i \left[\frac{dN}{dE}\right]_i \tag{3}$$

where the approximate smearing correction $[AS]_i$ for a bin i of the distribution is evaluated by assuming some true distribution $T(E)$, smearing it and taking a bin-by-bin ratio of the smeared and true distributions:

$$[AS]_i = \frac{\left[\frac{dN}{dE'}\right]_i}{\left[\frac{dN}{dE}\right]_i}, \; for\ some\ assumed\, T(E) \tag{4}$$

It is important to stress that the smearing correction factor $[AS]_i$ is, in general, different from the diagonal element of the smearing matrix $\hat{S}_{ij}$, $[AS]_i \neq \hat{S}_{ii}$.

If the distribution used to determine the approximate smearing correction is identical to the actual true distribution then both smearing methods produce identical results inside the 'physical domain'. In general, though, the approximate smearing procedure is inferior for several reasons:

- it requires an assumption about the plausible shape of the distribution which is being measured
- correctness of its results depend on the proximity of the assumed distribution to the one being measured. As an example a smearing correction for a flat distribution tend to be very small (at least at some distance from the edges of the domain) whereas the correction to a steeply falling spectrum tend to be very substantial (depending on the slope of the spectrum and the detector resolution)
- it is limited, by construction, to the domain of the true values of the quantity E and it cannot be used to determine the content of an underflow or overflow bin.

1.2 Unsmearing Correction

The most typical experimental problem is that of 'unsmearing', i.e. determination of the form of the true distribution from the shape of the observed distribution and the knowledge of the detector resolution function. Equation 1. is the Fredholm equation of the first kind and it can be solved if the kernel $S(E, E')$ is known in an analytical form, but this approach is rarely used in practice. In an usual case of binned distributions it is often very tempting to try to solve the Eq. 2 by inverting the smearing matrix $\hat{S}_{ij}$:

$$\left[\frac{dN}{dE}\right]_i = \sum_j \hat{S}_{ij}^{-1} \left[\frac{dN}{dE'}\right]_j \tag{5}$$

This is not possible, unfortunately, as the matrix $\hat{S}_{ij}$ is in general rectangular reflecting the fact that the domain of the observed quantities is larger than that of the true ones. During the smearing process some of the information is

lost and the original distribution cannot be retrieved without some additional assumptions.

If the true distribution was known, then one could define an 'unsmearing' matrix $\hat{U}_{ij}$ defined as

$$\left[\frac{dN}{dE}\right]_i = \sum_j \hat{U}_{ij} \left[\frac{dN}{dE'}\right]_j \tag{6}$$

The matrix $\hat{U}_{ij}$can be determined from the same two-dimensional histogram of the observed *vs* true quantities as the smearing matrix described above with the following differences:

- histogram is transposed
- columns of the transposed histogram (now corresponding to a bin of the true values of E) are normalized to unity

With such a construction the matrix element $\hat{U}_{ij}$ denotes a probability that the event with the actual value of measured quantity of E' falling into the bin j corresponds to a true value of E falling into the bin i. In contrast to the smearing matrix $\hat{S}_{ij}$ which can be determined independent of the shape of the measured distribution, the unsmearing matrix requires an a priori assumption. Fortunately, the adequacy of this assumption for a specific experiment can be easily verified by comparing the result of the unsmearing (Eq.(6)) with the assumed distribution. An iterative procedure can be applied if the initial guess is judged inadequate.

1.2.1 Approximate Unsmearing

In a manner similar to the approximate smearing case, one can apply an approximate unsmearing procedure

$$\left[\frac{dN}{dE}\right]_i = [AU]_i \left[\frac{dN}{dE'}\right]_i \tag{7}$$

where the unsmearing correction $[AU]_i$ is determined in an analogous fashion

$$[AU]_i = \frac{\left[\frac{dN}{dE}\right]_i}{\left[\frac{dN}{dE'}\right]_i}, \; for\ some\ assumed\ T(E) \tag{8}$$

As in the smearing case, the approximate procedure in inferior to the complete unsmearing one:

- correctness of its result depends on the proximity of the assumed distribution the one being determined. This is true for both methods, but the sensitivity of the method using full unsmearing matrix is smaller. In the specific case of the beam transfer matrix the sensitivity of the approximate unsmearing method is about four times bigger that that of the full matrix.

- it is limited, by construction, to the domain of the true values of the quantity E and it ignores any information contained in the content of an underflow or overflow bin.

2 Oscillation Analysis of the MINOS Data

Neutrino oscillation parameters are determined from the observed neutrino energy spectrum in the far detector: the oscillation probability $P(E)$ is determined as a ratio of the actual to the expected energy distributions as a function of true neutrino energy. There are at least two possible approaches to the determination of the oscillation parameters:

- one can try to determine the best estimate of the expected (i.e. with no oscillation) neutrino event spectrum at the far detector as a function of true neutrino energy and correct the measured distribution in the far detector for the acceptance and smearing to obtain the actual distribution of the neutrinos. The ratio of these two distributions is a direct determination of the disappearance probability as a function of neutrino energy at the distance of 735 km and can be used to fit the oscillation parameters, or other physics hypothesis

- one can construct the best estimate of the observed spectrum at the far detector as a function of the oscillation parameters and determine which set of parameters provides the best fit to the measured spectrum

We use the latter method to analyze our data. Application of this method requires the knowledge, or the best estimate, of the un-oscillated neutrino spectrum as a function of true neutrino energy at the far detector. Modification of this spectrum by the oscillation probability and subsequent modeling of the acceptance and smearing effects produces the oscillated spectrum which can be compared with the measured one.

In the absence of the sufficiently precise data on the hadron production and interactions, relatively poor knowledge of the neutrino cross sections at low energies and possible imperfections of our modeling of the neutrino beam line the primary source of information on the expected neutrino event spectrum in the far detector comes from the neutrino event spectrum measured at the near detector. Several steps are necessary to derive the desired un-oscillated event spectrum at the far detector from the near detector data. For (hoped for) clarity we ignore here small correction for the neutral current background in

the near and far detectors and for the contribution of ν_τ interactions. For the same reason we also ignore some other subtle corrections, like averaging over the fiducial volume of the near detector. All these effects must be properly included in the analysis.

- the observed energy distribution needs to be converted (unsmeared) to the true energy distribution
- the true energy distribution of the observed sample must be corrected for the energy-dependent acceptance to produce a true energy distribution of a 'complete' sample of events
- events energy distribution must be converted to the neutrino flux using some guess of the neutrino total cross section
- neutrino flux at the near detector must be projected to the far detector
- predicted neutrino flux at the far detector must be converted to the predicted event spectrum using neutrino total cross section

3 'Matrix' Analysis Method

Predicted spectrum of events in the far detector for some oscillation hypothesis can be expressed as:

$$F_i^{pred,M} = \sum_j S_{ij}^F \, \frac{MC_j^{F,R}}{MC_j^{F,G}} \, P_k^{osc} \, \sigma_k \, \sum_l B_{kl} \, \frac{1}{\sigma_l} \, \frac{MC_l^{N,G}}{MC_l^{N,R}} \, \sum_m US_{lm}^N \, D_m \qquad (9)$$

where:

- D_m is the number of the events reconstructed in the near detector in the bin m
- US_{mn}^N is the near detector unsmearing matrix element. It expresses the probability that the event reconstructed in bin m belongs in fact to bin l
- $\frac{MC_l^{N,G}}{MC_l^{N,R}}$ is the inverse of average acceptance (trigger, event classification, analysis) in the $l-th$ energy bin, of the near detector, where $MC_l^{N,G(R)}$ denotes the number of near Monte Carlo events generated (accepted) in the bin l of the true neutrino energy
- σ_l is the average value of the neutrino total cross section in the energy bin l

- B_{kl} is the near-to-far beam transfer matrix. It is conceptually identical to the unsmearing matrix with the value of B_{kl} reflecting the probability that the hadron decay which produced the neutrino in the near detector with energy in the bin l will produce a neutrino in the far detector with energy in the bin k

- P_k^{osc} is the average oscillation probability for the energies in the $k-th$ bin

- $\frac{MC_j^{F,R}}{MC_j^{F,G}}$ is the average acceptance of the far detector (including the analysis) in the neutrino energy bin j

- S_{ij}^F is the far detector smearing matrix. It expresses the probability that the event with true energy in bin j will be reconstructed with the observed energy in bin i

There are three principal sources of the corrections described above. GMINOS Near simulation is used to determine the unsmearing and acceptance corrections, GNUMI beam simulation is used to determine the beam transfer matrix and GMINOS Far simulation is used to determine the acceptance and smearing correction for the far detector. Their dependence on the poorly known models is the main source of the 'beam-related' systematic error of the oscillation analysis. Possible sources of these systematic errors are:

- near detector neutrino spectrum. It affects mildly the unsmearing correction US_{mn}^N. This error is presumably rather small and can be eliminated completely by iterative procedure

- uncertainties in hadron production cross sections, beam line geometry, modeling of hadron interactions etc.. lead to a systematic error on the beam transfer matrix B_{kl} . This matrix is determined primarily by the geometry of the beam line and it is quite insensitive to the hadron production modeling and beam elements alignment.

  The beam transfer matrix is nearly diagonal and it has very small systematic error in the 'peak' energy region corresponding to the parent mesons focused by the horns. In the tail region, corresponding to the relatively divergent beam, the beam matrix has significant off-diagonal terms describing the contribution of large angle mesons to the neutrino beam.

- knowledge of the neutrino cross section. It enters in the phase of conversion of the event spectrum to neutrino flux and back into the event spectrum. To a large extent the errors in the total cross section cancel in the expression Eq.(9). The cancellation is nearly complete in the peak area, where the matrix is nearly diagonal.

- modeling of exclusive cross sections (primarily the y-distribution) enters through the acceptance correction. Owing to a very similar construction of far and near detectors the potential errors in the modeling of the exclusive

cross sections tend to cancel in the analysis, as they enter with different signs in far and near detectors.

This analysis method exploits the similarity of the detectors and the related cancellation (or reduction) of the systematic errors to the fullest possible extent. The residual systematic errors must be evaluated, naturally.

The apparent complexity of Eq. (9) is intentional, it is meant to expose the logical steps of the analysis and to identify the instances where the analysis depends on external inputs and assumptions. In practice a much more compact form can be used by a suitable redefinition of matrices involved:

$$F_i^{pred,M} = \sum_j FD_{ij}\ P_j^{osc}\ \sum_k E_{jk}\ \sum_l ND_{kl}\ D_l \tag{10}$$

where:

- $ND_{kl} = US_{lm}^N \times \frac{MC_l^{N,G}}{MC_l^{N,R}}$ is a Near detector correction matrix, including unsmearing and acceptance
- $E_{jk} = \sigma_j\ B_{jk}\ \frac{1}{\sigma_k}$ is Near-to-Far event transfer matrix
- $FD_{ij} = S_{ij}^F \times \frac{MC_j^{F,R}}{MC_j^{F,G}}$ is a Far detector correction matrix, including acceptance and smearing

4 The F/N Ratio Method

This analysis method replaces (or at least it pretends to replace) the Eq.(9) with a much simpler expression:

$$F_i^{pred,R1} = \frac{MC_i^{F,S}}{MC_i^{N,S}} \times D_i \tag{11}$$

where $MC_i^{N,S}$ ($MC_i^{F,S}$) is a number of near (far) detector Monte Carlo events reconstructed with energy falling into the bin i

It is an attractive simplification, hence it is worthwhile to explore this method in depth. We will do it in several steps.

4.1 Is the Equation(11) True?

Intuitively the equation (11) looks correct. But in general, it is not true. A simple example of the failure of this equation is the situation where far detector is off-axis and the energy spectra of these two detectors do not overlap. Whereas this is of academic rather than practical interest and it does not imply that the Eq. (11) is not 'good enough' the for MINOS analysis it illustrates the fact that the validity of the Eq. (11) cannot be taken for granted and its suitability for our analysis must be demonstrated. This is in contrast to the 'matrix' method which is valid in any circumstances.

4.2 Approximations Behind the F/N Ratio Method

Apparent simplicity of the Eq. (11) is related to several hidden assumptions and/or approximations. The Eq. (11) is an approximate form of the Eq. (9) and the validity or the systematic error of this analysis method depend on the validity of these approximations. These approximations are:

- replace unsmearing matrix of the near detector US^N_{lm} by an approximate smearing $\frac{MC^{N,R}_m}{MC^{N,S}_m}\,\delta_{lm}$
- replace the beam transfer matrix B_{kl} by an approximate transfer ratio $\frac{MC^{F,G}_k}{MC^{N,G}_k}\delta_{kl}$
- replace the smearing matrix for the far detector S^F_{ij} by the approximate smearing $\frac{MC^{F,S}_i}{MC^{F,R}_i}\delta_{ij}$

With the diagonal beam transfer 'matrix' the cross section terms cancel completely and for $P^{osc}_k = 1$ one recovers the Eq.(11). For a prediction of the far detector reconstructed spectrum without oscillations the F/N ratio method is just an approximation of the 'Matrix' method. It offers no specific advantages (other than avoiding matrix multiplication) but suffers increased sensitivity to possible inadequacies of the models used in the Monte Carlo generation. An additional drawback of the ratio method is the dependence of the approximate smearing of the far detector $\frac{MC^{F,S}_i}{MC^{F,R}_i}$ on the neutrino spectrum used to generate the distribution involved, whereas the full smearing matrix S^F_{ij} is independent of it.

Most (if not all) tests of the performance of the F/N ratio method consist of the comparison of the far detector reconstructed GMINOS spectrum with the one obtained from the near detector event sample via Eq. (11). Unfortunately, this is not quite relevant comparison as the spectrum $F^{pred,R1}_i$ is not logically equivalent to that determined from the Eq. (9).

4.3 Determination of Oscillation Parameters in the F/N Ratio Method

Far detector spectrum $F^{pred,R1}_i$ as obtained from the Eq. (11) can be used to determine significance of the neutrino disappearance observed at the far detector, but it is not suitable for the determination of the oscillation parameters. For the oscillation fit we need to obtain the shape of the observed for some set of oscillation parameters and this must be done as a function of true, rather than observed energy. The true spectrum is obtained from the $F^{pred,R1}_i$ by using the unsmearing matrix for the far detector US^F_{lm}. After the application of the oscillation formula the final prediction for the far detector spectrum is

$$F_i^{pred,R2} = \sum_j S_{ij}^F \, P_j^{osc} \, \sum_k US_{jk}^F \, F_k^{pred,R1} \tag{12}$$

A true un-oscillated far detector spectrum used in the analysis corresponds to the $F_i^{pred,R2}$ with $P_j^{osc} = 1$, rather than $F_k^{pred,R1}$. The claims have been advanced that the F/N ratio method has an advantage over the 'matrix' method due to its ability to reproduce unexpected sharp features in the measured spectrum, should they occur at the far and near detectors at the same values of measured energies. This is not true, as the unsmearing and smearing of the far detector spectra necessary to obtain a true prediction $F_i^{pred,R2}$ washes any sharp features out.

A complication due to the necessity of smearing and unsmearing of the far detector spectra is a serious drawback for the F/N ratio method:

- the far detector spectrum is not treated in a consistent and logical way. It is first smeared (albeit implicitly) using an approximate method, depended on an assumption about the true form of the spectrum, then it is unsmeared with a complete unsmearing matrix (dependent on the assumed true form of a distribution) and finally smeared again, this time in a complete, assumption free way

- Unsmearing matrix US_{jk}^F depends on the assumed shape of the spectrum. During the fitting procedure, as the oscillation parameters change so does the change of the spectrum. Consistency would require that the unsmearing matrix is determined at every step of the iteration. This is prohibitively complicated, hence yet another approximated treatment needs to be applied.

It is important to point out that more formulations of the 'ratio' methods can be used by choosing any of the subsets of the approximations listed above. In particular, but using only first two approximations one may obtain, as an intermediate stage, the predicted true spectrum of neutrinos in the far detector. Such a method would avoid the complications described above and it would simplify the analysis considerably.

5 Determination of the Systematic Errors via Mock Data Challenge: the Issue of Statistics

We determine the systematic errors due to various unknowns or possible imperfections by evaluating the variation of the fitted parameters with various 'tweaks'. To make sure that statistical fluctuation do not obscure the systematic effects these studies are performed with a nominally very high statistics, corresponding to $POT = 10^{22}$. Unfortunately our sample of GNUMI fluxes is quite limited, corresponding to some $POT = 10^7$ or so. Meaningful beam

predictions are obtained by weighing neutrinos with their relative probabilities of entering the MINOS detectors. These weights vary substantially, by factors up a 100, with occasional excursions by factors above 1000. The primary consequence of the weighted event scheme are fluctuations much larger than 'apparently statistical' if they are measured by the square root of the expected number of events. The true statistical errors can be probably evaluated if the dispersion of weights is used as a measure of the observed fluctuations. [This argument is frequently brought forward by Jim Hylen.]

Generation of GMINOS events involves the use of GNUMI flux files: neutrinos are further re-weighted for different position inside the detector and many are discarded to model the rising cross section. Lack of sufficient GNUMI statistics necessitates multiple use of the same flux files. Due to differences in detector geometry and the beam spectrum the re-use of the flux files is different in the far and near detectors. Multiple, but different at the far and near detectors, reuse of the same flux files coupled with large fluctuation of neutrino weights may lead larger than expected fluctuations which are not properly taken into account by the fitting procedure, when the statistical errors are expected to be very small. Improper account for the statistics may lead to some errors in the estimate of the systematic errors. It may be a problem for the future analyzes, it is probably not a significant issue at present.

Situation may be different, though, if we try to select the analysis method by the apparent size of the systematic errors. Given the general smallness of the systematic errors a significant differences between methods may arise if they have differences in their sensitivities to the above-mention imperfections in the treatment of statistics. This may be the case of the comparison between the 'matrix' and the 'F/N ratio' method in their approach to the projecting the near spectrum to the far detector. The 'matrix' method is using the full statistics of the GNUMI flux files to determine the beam transfer matrix B_{kl}. The 'F/N ratio' method uses an approximation in the form $\frac{MC_k^{F,G}}{MC_k^{N,G}}\delta_{kl}$. Apart from the usual problems this approximation is in addition prone to the problem with abnormal fluctuations, which, in addition, may be different in the far and near detectors . While this is a potential problem when this method is applied to the real data, it may be an apparent, but illusional, advantage in the Mock Data Challenge setting, as it may reduce some of the abnormal fluctuations.