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IHEP 2000-17

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**STATISTICAL PROPERTIES OF THE ESTIMATOR
USING COVARIANCE MATRIX**

Protvino 2000

Abstract

Alekhin S.I. Statistical properties of the estimator using covariance matrix: IHEP Preprint 2000-17. – Protvino, 2000. – p. 12, figs. 2, refs.: 17.

Statistical properties of the estimator using a covariance matrix for the account of point-to-point correlations due to systematic errors are analyzed. It is shown that the covariance matrix estimator (CME) is consistent for realistic cases (when systematic errors on the fitted parameters are not extremely large comparing with the statistical ones) and its dispersion is always smaller than the dispersion of the simplified χ^2 estimator applied to the correlated data. The CME bias is negligible for the realistic cases if the covariance matrix is calculated during the fit iteratively using the parameter estimator itself. Analytical formula for the covariance matrix inversion help to perform fast and precise calculations even for very large data sets. All this allows for an efficient use of the CME in the global fits.

Аннотация

Алехин С.И. Статистические свойства оценивающей функции построенной на основе ковариационной матрицы: Препринт ИФВЭ 2000-17. – Протвино, 2000. – 12 с., 2 рис., библиогр.: 17.

Рассмотрены статистические свойства оценивающей функции, использующей для учета систематических ошибок ковариационную матрицу. Показано, что эта оценивающая функция дает состоятельную оценку для реалистичных случаев (т.е., если систематические ошибки настраиваемых параметров не превышает во много раз статистическую ошибку). Дисперсия этой оценки всегда меньше, чем дисперсия полученная при помощи упрощенной оценивающей функции не учитывающей корреляции данных, а смещение пренебрежимо мало для реалистичных случаев, если ковариационная матрица вычисляется при подгонке итеративно с использованием текущей оценки фитируемого параметра. Аналитические формулы для обращения ковариационной матрицы позволяют проводить быстрые и точные вычисления даже для больших наборов данных. Все это делает оценивающую функцию на основе ковариационной матрицы эффективным инструментом для глобального анализа данных.

INTRODUCTION

Modern particle physics development becomes more and more based on the analysis of precise experimental data. This demands the refining of all stages of the data inference including the account of correlations due to systematic uncertainties which are often comparable or even larger than the statistical ones. In particular, this problem is important for the precise tests of Standard Model and determination of the parton distributions (see Refs. [1,2]). Many authors for the sake of simplicity very often use approaches which ignore point-to-point correlations due to systematic errors, i.e. sum up all the errors in quadrature or drop systematic errors at all. It is evident that if the systematic errors are an important source of the data uncertainty, such approaches can lead to the distortion of the estimated errors on the fitted parameters. At the same time the construction of estimators accounting for the correlations is not straightforward since the competitive probabilistic model of data can be used in the analysis. Essentially two generic models are possible: One based on the frequentist treatment of systematic shifts and another one based on the Bayesian approach. This paper is concentrated on the analysis of statistical properties of the estimators within the Bayesian treatment of systematic errors. Introduction into this scope given in Ref. [3] contains argumentation in favor of this approach. The only point that we would like to underline in particular here is that the Bayesian approach provides convenient handling many sources of systematic errors, when classical treatment, which implies the introduction of an additional parameter for each source of systematic errors, can cause a great problem with the interpretation/representation of the function of a large number of arguments.

A natural way to account for point-to-point correlations due to systematic errors within the Bayesian approach is to use the covariance matrix associated with systematic errors (see e.g. Refs. [4,5]). Meanwhile, there are concerns that the covariance matrix estimator (CME) can result in biased values of the parameters values and their dispersions (see Refs. [6,7,8,9]). In this connection it is worth recalling that the estimators accounting for the data correlations often exhibit poor statistical properties regardless they use covariance matrix or not. For example, as it has been shown in Ref. [10], the sample dispersion estimated from the correlated Monte Carlo data sets can acquire the bias equal to the dispersion value itself¹. At the same time the

¹This effect is connected with well known fact that the sample dispersion gives a biased estimation of the

estimators would be unbiased if the covariance matrix is not evaluated from the measurements. Indeed, for example, the unbiased estimator for the correlated Monte Carlo data was constructed in Ref. [11] using the modeled covariance matrix.

Running this way, one can hope to construct the unbiased estimators accounting for systematic errors through covariance matrix, but to be aware of its unbiasedness the study of their properties is needed. In view of the lack of the comprehensive information in literature, this paper is devoted to the analysis of the statistical properties of such estimators with a particular attention to the bias control. Through the paper the CME properties are compared with the properties of the simplest χ^2 estimator (SCE) as well as it has been made earlier in Ref. [12].

1. THE SIMPLEST χ^2 ESTIMATOR

To illustrate our method of the statistical properties analysis, we start from the analysis of uncorrelated measurements. In this case, if the data sample $\{y_i\}$ is supposed to be explicitly described by a theoretical model $t_i = f_i(\theta^0)$,

$$y_i = t_i + \mu_i \sigma_i, \quad (1)$$

where μ_i are independent random variables, σ_i are statistical errors, $i = 1 \dots N$, N is the total number of points in the sample. We adopt that a theoretical model parameter θ^0 is scalar, the generalization of the formula on the case of vector parameter is evident. If y_i are obtained in the counting experiment with a large number of events, μ_i are Gaussian distributed, although it is not crucial for our consideration. As a rule, the values of σ_i given in the experimental publications, are the estimators of the y_i standard deviations, i.e. are random variables, but we neglect their fluctuations. The SCE is based on the minimization of functional

$$\chi^2(\theta) = \sum_{i=1}^N \frac{(f_i(\theta) - y_i)^2}{\sigma_i^2} \quad (2)$$

or, equivalently, the solution of the equation

$$\xi(\theta) \equiv \frac{1}{2} \frac{\partial \chi^2}{\partial \theta} = 0. \quad (3)$$

The solution $\hat{\theta}$ of Eq. (3) is the estimator of parameter θ , which is the random variable depending on $\{y_i\}$. To investigate statistical properties of $\hat{\theta}$, we expand the function $\xi(\theta)$ around θ^0 and then apply the Legendre inversion to obtain the series for $\hat{\theta}$ (see Ref. [13] for the details of method). Introducing

$$\begin{aligned} X &= \xi(\theta^0), & a &= - \left\langle \frac{\partial \xi(\theta^0)}{\partial \theta} \right\rangle, \\ b &= \left\langle \frac{\partial^2 \xi(\theta^0)}{\partial \theta^2} \right\rangle, & Y &= \frac{\partial \xi(\theta^0)}{\partial \theta} - \left\langle \frac{\partial \xi(\theta^0)}{\partial \theta} \right\rangle, \end{aligned}$$

one can obtain

$$\hat{\theta} - \theta^0 = \frac{X}{a} + \frac{XY}{a^2} + \frac{bX^2}{2a^3} + \dots \quad (4)$$

studied distribution dispersion; the correlations merely amplify this bias.

where $\langle \rangle$ means the averaging over the samples and the rejected part of the expansion contains the terms with the higher powers of $1/a$ and/or X and Y . In this approximation the dispersion of $\hat{\theta}$ is

$$D(\hat{\theta}) = \frac{\langle X^2 \rangle}{a^2}$$

and the bias is

$$B(\hat{\theta}) = \frac{\langle X \rangle}{a} + \frac{\langle XY \rangle}{a^2} + \frac{b \langle X^2 \rangle}{2a^3}.$$

For the SCE applied to sample (1), one can easily obtain

$$\begin{aligned} \langle X \rangle &= 0, \\ \langle X^2 \rangle &= -a = \sum_{i=1}^N \frac{[f'_i(\theta_0)]^2}{\sigma_i^2}, \\ \langle XY \rangle &= \frac{b}{3} = \sum_{i=1}^N \frac{f'_i(\theta_0) f''_i(\theta_0)}{\sigma_i^2}, \end{aligned} \quad (5)$$

where $f'_i(\theta)$ denotes derivative on θ . The dispersion and the bias of this estimator are

$$D_0^U(\hat{\theta}) = -\frac{1}{a}, \quad B_0^U(\hat{\theta}) = -\frac{b}{6a^2}. \quad (6)$$

If $f_i(\theta)$ are the linear functions of θ , series (4) is truncated and equation (3) can be solved exactly. One can see that in this case the estimator bias vanishes. For a nonlinear data model expansion (4) contains an infinite number of terms, but the contributions from the highest terms to the estimator dispersion and bias are inversely proportional to the powers of $D(\hat{\theta})$ or proportional to the central moments of y_i higher than the second. In first case these contributions are progressively suppressed in comparison with the main term, if the data statistics grows. In second case for a realistic distribution of y_i its high moments falls and these contributions are also suppressed (remind that such behaviour of a distribution high moments is assumed in deducing the central limit theorem of statistics). All this can justify the application of expansion (4) to the analysis of a nonlinear data model: The above formula can be applied to the data model with a “weak nonlinearity”, i.e. if its nonlinearity is not significant on the scale of the parameter standard deviation.

Now let the sample have a common additive systematic error. In accordance with the Bayesian approach to the treatment of systematic errors, the measured values are given by

$$y_i = t_i + \mu_i \sigma_i + \lambda s_i, \quad (7)$$

where s_i are systematic shifts for each point and λ is the random variable with zero average and unity dispersion². Consider the case of one source of systematic error, generalization on the many sources case is straightforward. For sample (7), we lose statistical independence of measurements and, with account for their correlations, the relevant expression for the dispersion and bias are more complicated

$$\langle X^2 \rangle = \sum_{i,j=1}^N \frac{C_{ij}}{\sigma_i^2 \sigma_j^2} f'_i(\theta_0) f'_j(\theta_0) = -a + \left[\sum_{i=1}^N \frac{s_i}{\sigma_i^2} f'_i(\theta_0) \right]^2,$$

²Emphasize, that λ is not necessary Gaussian distributed.

$$\begin{aligned}\langle XY \rangle &= \sum_{i,j=1}^N \frac{C_{ij}}{\sigma_i^2 \sigma_j^2} f'_i(\theta_0) f'_j(\theta_0) \\ &= \frac{b}{3} + \left[\sum_{i=1}^N \frac{s_i}{\sigma_i^2} f'_i(\theta_0) \right] \left[\sum_{i=1}^N \frac{s_i}{\sigma_i^2} f''_i(\theta_0) \right],\end{aligned}$$

where a and b are given by Eq. (5), C_{ij} is the covariance matrix for $\{y_i\}$

$$C_{ij} = s_i s_j + \delta_{ij} \sigma_i \sigma_j, \quad (8)$$

and δ_{ij} is the Kronecker symbol. In terms of the N -component vectors

$$\rho_i = \frac{s_i}{\sigma_i}, \quad \phi_1^i = \frac{f'_i(\theta_0)}{\sigma_i}, \quad \phi_2^i = \frac{f''_i(\theta_0)}{\sigma_i}$$

the dispersion and the bias in this case can be expressed as

$$D_0^A(\hat{\theta}) = \frac{1}{\phi_1^2} (1 + \rho^2 z_1^2), \quad (9)$$

$$B_0^A(\hat{\theta}) = -\frac{\phi_2}{2\phi_1^3} \left[\left(1 + \frac{3}{2}\rho^2 z_1^2\right) z_{12} - \rho^2 z_1 z_2 \right], \quad (10)$$

where ρ, ϕ_1, ϕ_2 denote the vectors modulus, z_1 is the cosine of angle between $\vec{\rho}$ and $\vec{\phi}_1$, z_2 – between $\vec{\rho}$ and $\vec{\phi}_2$, z_{12} – between $\vec{\phi}_1$ and $\vec{\phi}_2$. The dispersion of $\hat{\theta}$ is larger than for uncorrelated data because now it also accounts for the fluctuations due to systematic errors. As to the bias, it remains zero for the linear data model.

If systematic errors are multiplicative

$$y_i = (t_i + \mu_i \sigma_i)(1 + \lambda \eta_i), \quad (11)$$

where η_i quantify the systematic errors. If both statistical and systematic errors are small comparing with t_i

$$y_i \approx t_i + \mu_i \sigma_i + \lambda \eta_i t_i,$$

the covariance matrix is

$$C_{ij} = \eta_i \eta_j t_i t_j + \delta_{ij} \sigma_i \sigma_j, \quad (12)$$

and the expressions for the bias and dispersion are the same as for the additive systematics case after the substitution $s_i \rightarrow \eta_i t_i$.

Eq. (9) can be split into the parts which correspond to the statistical and systematic fluctuations. One can see that, when vectors $\vec{\rho}$ and $\vec{\phi}_1$ are orthogonal, the systematic error on $\hat{\theta}$ is equal to zero and the total dispersion is suppressed. Such suppression can be illustrated at the example of the asymmetry extraction from the data with a general offset error. Let $f_i(\theta) = \theta x_i$ and both statistical and systematic errors be constant through the sample: $s_i = s$, $\sigma_i = \sigma$. Then $\rho_i = s/\sigma$, $\phi_1^i = x_i/\sigma$ and $z_1 \sim \sum x_i$. If the positive and negative values of x_i compensate each other in the measurements, $z_1 = 0$ and the systematic error vanish. The appropriate data filtration can also be used to suppress dispersion (9). To clarify the mechanism of this suppression, let us trace the effect of a separate data point on the dispersion value. Add to the data set a

point with statistical error σ_0 , systematic error s_0 and the data model $f_0(\theta)$. If the initial data set is large and the systematic error is comparable with statistics, i.e.

$$\begin{aligned} N &\gg 1, & \rho &\gg 1, \\ \phi_1 &\gg \frac{f'_0(\theta_0)}{\sigma_0}, & \rho\phi_1 z_1 &\gg \frac{s_0}{\sigma_0^2} f'_0(\theta_0), \end{aligned} \quad (13)$$

the change of $D_0^A(\hat{\theta})$ after adding a new point is

$$\Delta D_0^A(\hat{\theta}) \approx \frac{2\rho}{\phi_1^3} \frac{1}{\sigma_0^2} \left[z_1 s_0 f'_0(\theta_0) - \frac{\rho z_1^2}{\phi_1} [f'_0(\theta_0)]^2 \right]. \quad (14)$$

The second term in brackets is always negative and describes the decrease of dispersion due to an improved statistical precision. At the same time the first term can be negative or positive, depending on the signs of z_1 and s_0 . Its absolute value can be larger than the absolute value of the second term and then $D_0^A(\hat{\theta})$ can increase or decrease after adding the new point. This is a manifestation of inconsistency of the SCE applied to the correlated data set. The balance between terms of Eq. (14) is defined by the distribution of $f'_i(\theta_0)/s_i$, and cuts of the tails of this distribution can decrease the estimator dispersion.

2. THE COVARIANCE MATRIX ESTIMATOR

If the systematic error is additive and the covariance matrix is known a priori and given by (8), one can use for the parameter estimation the following functional minimization

$$\chi^2(\theta) = \sum_{i,j=1}^N (f_i(\theta) - y_i) E_{ij} (f_j(\theta) - y_j), \quad (15)$$

where E_{ij} is the inverted covariance matrix. This problem can be reduced to the uncorrelated case using the linear transformation of the vector $\{f_i(\theta) - y_i\}$ and the estimator is linear for the linear data model. Besides, if statistical and systematics fluctuations obey the Gaussian distribution, this estimator provides the minimal dispersion due to the Cramer-Rao inequality.

One can easily derive the expressions necessary to calculate the estimator bias and dispersion

$$\begin{aligned} \langle X \rangle &= 0, \\ \langle X^2 \rangle &= -a = \sum_{i,j=1}^N f'_i(\theta_0) E_{ij} f'_j(\theta_0), \\ \langle XY \rangle &= \frac{b}{3} = \sum_{i,j=1}^N f'_i(\theta_0) E_{ij} f''_j(\theta_0). \end{aligned}$$

Substituting in the above relations the explicit expression for E_{ij}

$$E_{ij} = \frac{1}{\sigma_i \sigma_j} \left(\delta_{ij} - \frac{\rho_i \rho_j}{1 + \rho^2} \right)$$

we obtain the estimator dispersion

$$D_M^A(\hat{\theta}) = \frac{1}{\phi_1^2} \left[1 + \frac{\rho^2 z_1^2}{1 + \rho^2 (1 - z_1^2)} \right] = \frac{1}{\phi_1^2} \xi_M, \quad (16)$$

where ξ_M is the ratio of the total dispersion to the pure statistical one. If $\vec{\rho}$ and $\vec{\phi}_1$ are collinear, the dispersion of the estimator is

$$D_M^{A,\parallel}(\hat{\theta}) = \frac{1 + \rho^2}{\phi_1^2},$$

which coincides with the SCE dispersion (9). One can see that if $\vec{\rho}$ and $\vec{\phi}_1$ are not collinear, the SCE dispersion (9) is always larger than the CME dispersion (16). This can be readily explained qualitatively. For the SCE the fitted curve tightly follows the data points and, if these points are shifted due to the systematic errors fluctuations, the parameter gains appropriate systematic errors. At the same time, since for the CME the information on the data correlations is explicitly included in χ^2 , the correlated fluctuation of the data due to systematic shift does not necessary lead to the fitted curve shift and the parameter deviation gets smaller than for the SCE. The exclusion occurs if $z_1 = 0$, when $\vec{\rho}$ and $\vec{\phi}_1$ are collinear and the systematic shift can be perfectly compensated by the change of parameter. If these vectors are orthogonal, the CME dispersion is

$$D_M^{A,\perp}(\hat{\theta}) = \frac{1}{\phi_1^2}$$

i.e. it is just the same as the dispersion of SCE applied to the data set without correlations given by Eq. (6). Qualitatively it corresponds to the measurements scheme, when the systematic shifts for different points compensate each other, e.g. as in the example considered at the end of Sec. 1.

For the modern experiments systematic errors are often of the same order as statistical ones and if $N \gg 1$, then $\rho \gg 1$. In this limit and if $\vec{\rho}$ and $\vec{\phi}_1$ are not collinear,

$$D_M^A(\hat{\theta}) \approx \frac{1}{\phi_1^2(1 - z_1^2)} \quad (17)$$

and

$$D_0^A(\hat{\theta}) \approx \frac{\rho^2 z_1^2}{\phi_1^2}. \quad (18)$$

One can see that in the second case the estimator standard deviation rises linearly with the increase of the systematics, whereas the CME dispersion saturates. This difference can be illustrated at the numerical example inspired by the elastic proton-proton scattering. Let us choose

$$f_i = U \exp(-V x_i), \quad x_i = 0.1i,$$

where $U = 100, V = 10, i = 1 \dots 9$. Generating 100 data sets (7) with these f_i and

$$\sigma_i = 0.01 \sqrt{\frac{U}{f_i}}, \quad s_i = \frac{\kappa}{x_i} \quad (19)$$

we minimized functionals (2) and (15) varying U and V to obtain their estimators \hat{U} and \hat{V} . The values of $(\hat{U} - U)^2$ and $(\hat{V} - V)^2$ for all of the generated data sets were averaged to obtain the estimators dispersions. The results on the standard deviation of \hat{U} for different values of κ are given in Fig. 1 (the picture for \hat{V} is similar). One can see that at large κ the CME and the SCE standard deviations differ by factor of 3.

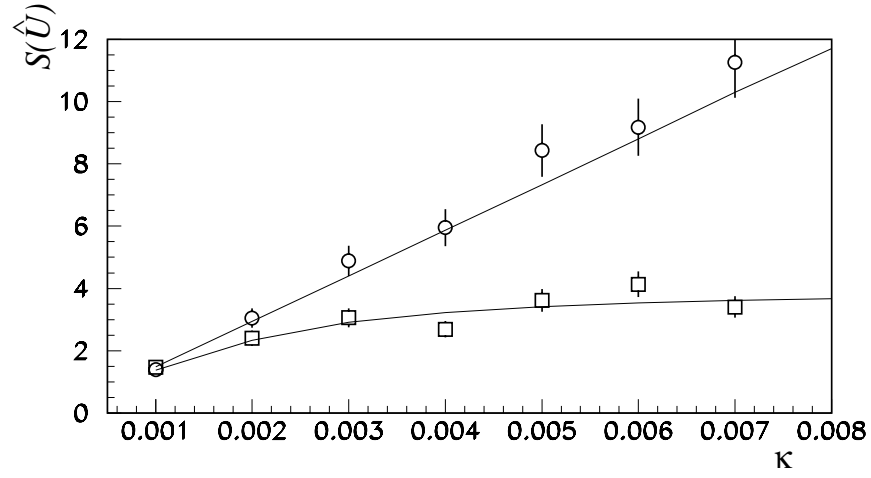


Fig. 1. The standard deviations of SCE (circles) and CME (squares) for \hat{U} at different scales of systematic errors κ . The lines correspond to the calculation performed with the two-dimensional generalization of Eqs. (9,16).

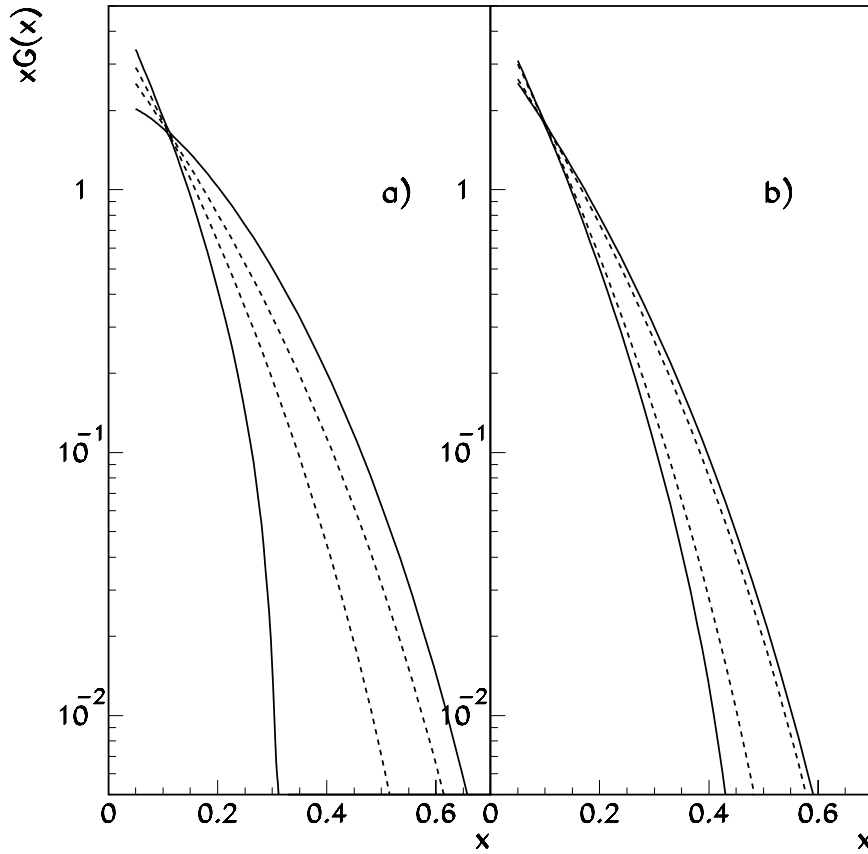


Fig. 2. Bounds of gluon distribution obtained from the LO QCD fit to BCDMS data with different estimators (the SCE: a; the CME: b). Full lines correspond to the total experimental errors, dashed ones – to the statistical only.

The example of dispersion suppression observed in the analysis of real experimental data can be found in Ref. [14]. In this paper we performed the leading order QCD fit to the inclusive deep inelastic scattering data of Refs. [15,16] obtained by the BCDMS collaboration in order to determine the parton distribution functions and the strong coupling constant value α_s . The two different estimators were used and the different estimates were obtained. For the SCE the standard deviation of $\alpha_s(M_Z)$ is 0.015, while for the CME it is 0.007. The difference in the gluon distribution bounds for these estimators is given in Fig. 2. One can see that the standard deviation of the gluon distribution for the CME is also about half of the SCE standard deviation.

If $z_1 \neq 1$, the change of CME dispersion after adding a new point to the large sample as defined by Eq. (13) is

$$\Delta D_M^A(\hat{\theta}) \approx -\frac{1}{\phi_1^4(1-z_1^2)^2} \frac{1}{\sigma_0^2} \left[f'_0(\theta_0) - \frac{\phi_1 z_1}{\rho} s_0 \right]^2.$$

This change is always negative, which proves the CME consistency. Remind, that this is not necessary for the SCE (see Sec. 1). The same conclusion can be drawn from the comparison of Eqs. (17) and (18). Indeed, the CME dispersion falls with increase of statistical significance of the data set (i.e. decrease of σ or rise of N) while the SCE dispersion does not. Note, that due to consistency of the CME, the filtration procedure described in Sec. 1 is not meaningful for it.

The CME bias is

$$B_M^A(\hat{\theta}) = -\frac{\phi_1 \phi_2}{2} \left[D_M^A(\hat{\theta}) \right]^2 \left(z_{12} - \frac{\rho^2}{1+\rho^2} z_1 z_2 \right),$$

which vanishes for the linear data model and saturates in the limit of $\rho \gg 1$ contrary to the SCE. In the numerical example (19) at $\kappa = 0.007$ the CME bias is 0.07, whereas the SCE bias is 0.13.

For the multiplicative systematic errors the covariance matrix is unknown a priori and one is to calculate it using the parameter estimator. Proceeding this way in the minimization of the functional (15), we get

$$a = -\sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f'_j(\theta^0) - \frac{1}{2} \sum_{i,j=1}^N E''_{ij} C_{ij}. \quad (20)$$

The difference with corresponding expression for the case of additive systematic errors is in the second term of Eq. (20). For the linear data model this term is

$$a^{(2)} = \frac{1}{2} \sum_{i,j=1}^N E''_{ij} C_{ij} = \frac{\phi_3^2}{2(1+\rho^2)^2} [\rho^4(z_3^2 - 1) - 3\rho^2 z_3^2 + 1],$$

where

$$\phi_3^i = \rho_i' = \frac{\rho_i}{f_i} f'_i(\theta^0) = \eta_i \phi_1^i,$$

ϕ_3 is the modulus of $\vec{\phi}_3$ and z_3 is the cosine of the angle between $\vec{\phi}_3$ and $\vec{\rho}$. The ratio of the second term of Eq. (20) to the first term $a^{(1)} = \sum f'_i(\theta^0) E_{ij} f'_j(\theta^0)$ is

$$\frac{a^{(2)}}{a^{(1)}} = \frac{\phi_3^2}{\phi_1^2} \cdot \frac{\rho^4(z_3^2 - 1) - 3\rho^2 z_3^2 + 1}{(1+\rho^2)^2} \xi_M. \quad (21)$$

If $\xi_M \sim O(1)$ (that is valid for most real cases), $a^{(2)} \sim O(\eta^2)a^{(1)}$ for all values of ρ , i.e. it is suppressed comparing with the first term for small η . Neglecting as elsewhere the third and fourth central moments of $\{y_i\}$, one can obtain that $\langle X^2 \rangle \approx -a$ and the estimator dispersion for multiplicative systematic errors $D_M^M \approx D_M^A$.

In the case of multiplicative systematics errors Eq. (3) is nonlinear even for the linear data model. As a consequence, the expressions responsible for the bias

$$\begin{aligned} \langle X \rangle &= \frac{1}{2} \sum_{i,j=1}^N E'_{ij} C_{ij}, \\ b &= 3 \sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f''_j(\theta^0) + 3 \sum_{i,j=1}^N f'_i(\theta^0) E'_{ij} f'_j(\theta^0) + \frac{1}{2} \sum_{i,j=1}^N E'''_{ij} C_{ij}, \\ \langle XY \rangle &= \sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f''_j(\theta^0) + 2 \sum_{i,j=1}^N f'_i(\theta^0) E'_{ij} f'_j(\theta^0) - \frac{1}{4} \sum_{i,j=1}^N E''_{ij} C_{ij} \sum_{i,j=1}^N E'_{ij} C_{ij}, \end{aligned} \quad (22)$$

do not vanish even if $f''_i(\theta)$ is equal to zero. Meanwhile, the bias due to the estimator nonlinearity is small comparing with the estimator standard deviation. Since $1/D_M^M \approx \langle X^2 \rangle \approx -a$, the bias of estimator with multiplicative systematic errors is

$$B_M^M(\hat{\theta}) \approx \sqrt{D_M^M(\hat{\theta})} \left[\frac{\langle X \rangle}{\sqrt{-a}} + \frac{\langle XY \rangle - b/2}{(-a)^{3/2}} \right]. \quad (23)$$

The first term in the brackets of Eq. (23) is

$$\frac{\langle X \rangle}{\sqrt{-a}} \approx -\frac{\phi_3}{\phi_1} \frac{\rho z_3}{1 + \rho^2} \sqrt{\xi_M} \sim O(\eta \sqrt{\xi_M}). \quad (24)$$

The contribution to the second term in brackets of Eq. (23) from $\sum f'_i(\theta^0) E'_{ij} f'_j(\theta^0)$ is proportional to

$$\frac{\phi_3}{\phi_1} \frac{\rho z_1}{(1 + \rho^2)} \left(\frac{\rho^2}{1 + \rho^2} z_1 z_3 - z_{13} \right) \xi_M^{3/2}$$

and hence it is $\sim O(\eta \xi_M^{3/2})$. As one can conclude from Eqs. (21,24), the contribution to the same term from $\sum E''_{ij} C_{ij} \cdot \sum E'_{ij} C_{ij}$ is $O(\eta^3 \xi_M^{3/2})$. And, finally, since

$$\frac{1}{2} \sum_{i,j=1}^N E'''_{ij} C_{ij} = \frac{\rho z_1 \phi_3^3}{(1 + \rho^3)^2} [\rho^4 (z_3^2 - 1) + \rho^2 (1 - 3z_3^2) + 2],$$

the contribution to Eq. (23) coming from this term is $O(\eta^3 \xi_M^{3/2})$. In summary, for the linear data model the estimator bias is a sum of terms $O(\eta^p \xi_M^q) D_M^M$ with $p \geq 1$ and $q \leq 3/2$. Besides, at small ρ all the four contributions to the bias which survive for the linear data model are $\sim \rho$, while at large ρ they are $\sim 1/\rho$. Summarizing, one can conclude that the estimator bias is negligible in comparison with its standard deviation excluding the extreme cases with very large ξ_M .

The explicit estimate of the bias can be obtained from Eqs. (22,23). Meanwhile, it requires rather lengthy calculations and a simpler tool for the bias evaluation is admirable. A convenient way for this is to trace the net residual

$$R = -\frac{1}{N} \sum_{i=1}^N \frac{f_i(\hat{\theta}) - y_i}{\sqrt{\sigma_i^2 + s_i^2}}.$$

Expanding $f_i(\theta)$ near θ_0 and keeping only the first term in Eq. (4), one obtains for sample (7)

$$R \approx -\frac{1}{N} \sum_{i=1}^N \frac{\mu_i + \lambda \rho_i}{\sqrt{1 + \rho_i^2}} + (\hat{\theta} - \theta_0) \frac{1}{N} \sum_{i=1}^N \frac{\phi_1^i}{\sqrt{1 + \rho_i^2}}.$$

If the estimator is unbiased, the value of R averaged over the samples is equal to zero. Nevertheless, the particular values of R may be not equal to zero due to fluctuations. For the limited ξ_M the dispersion of R is

$$D(R) = \frac{1}{N^2} \sum_{i,j=1}^N \frac{\delta_{ij} + \rho_i \rho_j}{\sqrt{1 + \rho_i^2} \sqrt{1 + \rho_j^2}} + O(1/N). \quad (25)$$

If the analyzed data come from a single experiment with dominating systematics (i.e with $\rho > 1$), then $D(R) \sim 1$. In particular, for the BCDMS data of Refs. [15,16] $D(R) \approx 0.5$. For N_{exp} independent experiments involved in the analysis $D(R) \sim 1/N_{exp}$. Comparing the net residual R with this value allows one to get a guess about the estimator bias. A more definite conclusion can be drawn after the comparison of R with its dispersion calculated using Eq. (25).

3. PLANNING THE COUNTING EXPERIMENTS

In a particular case, when the differential cross section on the variable x is measured, the predicted average number of events in the i -th bin of data is

$$\langle N_i \rangle = L f_i \Delta x_i \beta_i,$$

where L is the integral experiment luminosity, β_i is the registration efficiency, and Δx_i is the bin width. Neglecting the fluctuations of N_i the statistical error on the i -th measurement is

$$\sigma_i = \frac{\sqrt{\langle N_i \rangle}}{L \Delta x_i \beta_i}$$

and

$$\frac{1}{\sigma_i^2} = \frac{L \beta_i}{f_i} \Delta x_i.$$

The scalar product of the vectors $\vec{\rho}$ and $\vec{\phi}$ is

$$(\vec{\rho} \cdot \vec{\phi}) = L \sum_{i=1}^N \frac{f'_i s_i}{f_i} \beta_i \Delta x_i$$

and

$$\phi^2 = L \sum_{i=1}^N \frac{[f'_i]^2}{f_i} \beta_i \Delta x_i, \quad \rho^2 = L \sum_{i=1}^N \frac{[s_i]^2}{f_i} \beta_i \Delta x_i.$$

For the concise measurements these scalars can be reduced to the integrals over the measurements region Ω :

$$(\vec{\rho} \cdot \vec{\phi}) = L \int_{\Omega} f'(x) s(x) d\tilde{x}$$

and

$$\phi^2 = L \int_{\Omega} [f'(x)]^2 d\tilde{x}, \quad \rho^2 = L \int_{\Omega} [s(x)]^2 d\tilde{x},$$

where $d\tilde{x} = \beta(x)/f(x)dx$. The latter expressions can be used in the equations for the estimators dispersions³. This approach is convenient for the future experiment optimization since it allows

³As a result, one obtains the Fisher's information for the correlated data case.

one to analyze the integrated expression in order to search for the optimal region of measurements. For the simple functions $f(x)$, $\beta(x)$, and $s(x)$ such analysis can be surely performed analytically.

Particular attention should be paid to the connection between the obtained estimator dispersion and the confidence interval. For a known distribution of the estimator the confidence interval can be easily calculated (e.g. it is well known that for the Gaussian distribution one standard deviation corresponds to the 67% confidence level). Unfortunately, due to the possible non-Gaussian nature of the systematic errors, one cannot prove that an estimator accounting for systematics is Gaussian distributed. However, for a large number of systematic errors of comparable scale, the estimator should obey the Gaussian distribution just to the central limit theorem of statistics. Otherwise the robust estimates of the confidence intervals, e.g. Chebyshev's inequality, should be used.

4. CONCLUSION

In conclusion, the CME is a convenient tool for the analysis of the data sets with account for correlations due to systematic errors. The CME is consistent for the realistic cases (when systematic errors on the fitted parameters are not extremely large comparing with the statistical ones) and its dispersion is always smaller than the dispersion of the χ^2 estimator without account for correlations. The estimator bias is negligible for the realistic cases if the covariance matrix is calculated during the fit iteratively using the parameter estimator itself. Analytical formula for the covariance matrix inversion allows one to perform fast and precise calculations even for very large data sets. The latter is especially important in view of numerical instabilities occurring in the fits to precise data in the case of large correlation between the fitted parameters (see in this connection Ref. [17]).

Acknowledgments

I am indebted to S.Keller for valuable discussions and comments. The work was supported by RFBR grant 00-02-17432.

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Received May 26, 2000

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Статистические свойства оценивающей функции построенной на основе ковариационной матрицы.

Оригинал-макет подготовлен с помощью системы \LaTeX .

Редактор Е.Н.Горина.

Технический редактор Н.В.Орлова.

Подписано к печати 29.05.2000. Формат $60 \times 84/8$. Офсетная печать.

Печ.л. 1.5. Уч.-изд.л. 1.2. Тираж 160. Заказ 160. Индекс 3649.

ЛР №020498 17.04.97.

ГНЦ РФ Институт физики высоких энергий
142284, Протвино Московской обл.

