NON-GAUSSIAN LIKELIHOOD FUNCTION

LUCA AMENDOLA
Osservatorio Astronomico di Roma
Viale del Parco Mellini, 84, Rome 00136 - Italy

ABSTRACT

I present here a generalization of the maximum likelihood method and the $\chi^2$ method to the cases in which the data are not assumed to be Gaussian distributed. The method, based on the multivariate Edgeworth expansion, can find several astrophysical applications. I mention only two of them. First, in the microwave background analysis, where it cannot be excluded that the initial perturbations are non-Gaussian. Second, in the large scale structure statistics, as we already know that the galaxy distribution deviates from Gaussianity on the scales at which non-linearity is important. As a first interesting result I show here how the confidence regions are modified when non-Gaussianity is taken into account.

1. Introduction

The role of statistics in large scale astrophysics is increasing at a very fast rate, barely keeping the pace with the flow of observational data from galaxy surveys and microwave background. Since we want not only to describe our Universe but also to understand it, we need quantitative ways to compare observations with theoretical models. This requires the choice of good statistical descriptors, like correlation functions, higher-order moments and similar, and the ability to determine their confidence regions (CR), i.e. the probability density function of the estimators. The general problem is that, while we certainly need some basic assumptions with respect to the statistical nature of the data, we want to keep these assumptions to a minimum. For instance, we would like to analyze the signal from the cosmic microwave background (CMB) experiments or from galaxy surveys without assuming that the data are Gaussian distributed.

To this scope I present here a general method to approach such problems, based on the Multivariate Edgeworth Expansion (MEE), an Hermite expansion around a Gaussian distribution. This method is suitable to the cases in which the data can be reasonably assumed to be mildly non-Gaussian, and we wish to estimate the region of confidence of the relevant parameters without the Gaussian assumption. I can think of several applications of the MEE to the analysis of astrophysical data. In the case of the CMB, we can use the MEE to estimate at the same time such fundamental parameters like the primordial slope $n$ and the quadrupole amplitude $Q_{\text{rms}}^{PS}$, and higher-order parameters like the skewness, along with their confidence regions. I will show that the CR may broaden or contract with respect to the Gaussian case.

*Published in Astro. Lett. and Communications, 1996, 33, 63
Similarly, one can analyse in the same manner the large scale structure of galaxy clustering. Another application is to the case of $\chi^2$ fitting when the data are not Gaussian. More details on the method and on its applications can be found in another work.

2. Formalism

Let $d_i$ be a set of experimental data (e.g., CMB fluctuations, or galaxy counts), $i = 1, \ldots, N$, and let us form the variables $x^i = d^i - t^i$, where $t^i$ are the theoretically expected values for the measured quantities. Let $e^{ij}$ be the correlation matrix

$$e^{ij} = \langle x^i x^j \rangle,$$

and let us introduce the higher-order cumulant matrices (or correlation functions)

$$k^{ijk} = \langle x^i x^j x^k \rangle$$

(skewness matrix),

$$k^{ijkl} = \langle x^i x^j x^k x^l \rangle - e^{ij} e^{kl} - e^{ik} e^{jl} - e^{il} e^{jk}$$

(kurtosis matrix).

The correlation matrices depend in general both on a number of theoretical parameters $\alpha_j$, $j = 1, \ldots, P$ and on the experimental errors. We assume the latter to be Gaussian distributed and completely characterized by the correlation matrix $e^{ij}$, to be added in quadrature to the 2-point correlation function. It is useful to define then the matrix $\lambda_{ij} = (e^{ij} + e^{ij})^{-1}$. The parameters $\alpha_j$ are fixed by maximizing, with respect to the parameters, the likelihood function $L = f(x)$, where $f(x)$ is the multivariate probability distribution function (PDF) for the random variables $x_i$. The usual simplifying assumption is then that $f(x)$ is a multivariate Gaussian distribution

$$L_g = f(x) = G(x, \lambda) \equiv (2\pi)^{-N/2} |\lambda|^{1/2} \exp(-x^i \lambda_{ij} x^j / 2).$$

where $|\lambda| = \text{det}(\lambda_{ij})$. A straightforward way to generalize the LF so as to include the higher-order correlation functions, which embody the non-Gaussian properties of the data, is provided by the MEE. An unknown PDF $f(x)$ can indeed be expanded around a multivariate Gaussian $G(x, \lambda)$ according to the formula

$$f(x) = G(x, \lambda)[1 + \frac{1}{6} k^{ijk} h_{ijk}(x, \lambda) + \frac{1}{24} k^{ijkl} h_{ijkl}(x, \lambda) + \frac{1}{72} k^{ijkl} k^{lmn} h_{i..n}(x, \lambda) + \ldots],$$

where $h_{i..}$ are Hermite tensors, a generalization of the Hermite polynomials. If there are $r$ subscripts, the Hermite tensor $h_{i..}$ is said to be of order $r$, and is given by

$$h_{i..} = (-1)^r G^{-1}(x, \lambda) \partial_{i..} G(x, \lambda),$$

where $\partial_{i..} = (\partial/\partial x_i)(\partial/\partial x_j)\ldots$. It can be shown that the MEE gives a good approximation to any distribution function provided that the cumulants obey the same order-of-magnitude scaling of a standardized mean. This condition is satisfied, for
instance, by the cumulants of the galaxy clustering in the scaling regime, which explains why the (univariate) Edgeworth expansion well approximates the probability distribution of the large scale density field.\[1,2\] In the past years, the MEE has been employed also to approximate the biased density distribution for large value of the biasing threshold, to the scope of calculating the peak correlation functions for non-G random fields\[3\] and other descriptors of excursion sets\[4\]. The same expansion has been also applied to the statistics of pencil-beam surveys\[5\], and to go beyond the Gaussian approximation in calculating the topological genus of weakly non-Gaussian fields\[6\]. Let us also note that the MEE can also be immediately generalized to the case of experimental errors not Gaussian distributed.

3. Best estimators

The best parameter estimates are obtained by maximizing Eq. (5) with respect to the parameters. To illustrate some interesting points, let us put ourselves in the simplest case, in which all data are independent, and we only need to estimate the parameters $\sigma$ and $k_3$ defined as: $c_{ij} = \sigma^2 \delta_{ij}$, $k_{ijk} = k_3 \delta_{ij}\delta_{jk}$. The maximum likelihood estimators for the variance and the skewness are then obtained by putting

$$\frac{d \log L}{d\sigma} = 0, \quad \frac{d \log L}{dk_3} = 0. \tag{7}$$

The solution reduce then to the usual sample quantities

$$\hat{\sigma}^2 = \sum_i x_i^2/N, \quad \hat{k}_3 = \sum_i x_i^3/N. \tag{8}$$

(which are asymptotically unbiassed). The same calculation can be carried out in the more general case of dependent variables, but the search for the maximum is more simply performed numerically when the situation is more complicated.

Once we have the best estimators $\hat{\alpha}_i(x)$ of our parameters, we need to estimate the confidence regions for that paramaters. The problem consists in determining the behavior of the unknown distribution $P(\hat{\alpha}_i(x))$, when we know the distribution for the random variables $x_i$. This problem is generally unsoluble analytically, and the common approach is to resort to MonteCarlo simulations of the data. However, we can always approximate $P(\hat{\alpha}_i)$ around its peak by a Gaussian distribution multivariate in the parameter space; if the number of data $N \to \infty$, this procedure can be justified by the central limit theorem. The covariance matrix of the parameters is then

$$\Sigma^{-1}_{ab} = -\frac{\partial \log L(x, \alpha_a)}{\partial \alpha_a \partial \alpha_b} \bigg|_{\alpha_a = \hat{\alpha}_a}, \tag{9}$$

where $a, b$ run over the dimensionality $P$ of the parameter space. The component $\Sigma_{22}$, i.e. the variance of $\hat{k}_3$, is then simply (dropping the hats here and below)

$$\Sigma_{22} = 6\sigma^6/N. \tag{10}$$
which, not unexpectedly, is the sample skewness variance, i.e. the scatter in the skewness of Gaussian samples. More interesting is the error in the variance parameter $\sigma$ when not only a non-zero skewness $k_3$ is present, but also a non-zero kurtosis parameter $k_4$, defined in a way similar to $k_3$ as $k_{ijkl} = k_4 s_{ijkl}$. The result is

$$\Sigma_{11} = \left(\sigma^2 / 2N\right) \left[1 + \gamma_2 / 2\right],$$

where $\gamma_2 = k_4 / \sigma^4$ is the dimensionless kurtosis. Notice that, in the mild non-Gaussianity condition we are assuming throughout this work, the mixed components $\Sigma^{-1}_{12} = \Sigma^{-1}_{21}$ are negligible. The first term in (11) is the usual variance of the sample variance for Gaussian, independent data. The second term is due to the kurtosis correction: it will broaden the CR for $\sigma$ when $k_4$ is positive, and will shrink it when it is negative. Depending on the relative amplitude of the higher-order corrections, the CR for the variance can extend or reduce. It is important however to remark that this estimate of the confidence regions is approximated, and that it can be trusted only around the peak of the likelihood function.

4. Non-Gaussian $\chi^2$ method

If our data are distributed following the MEE, then we can measure the likelihood to have found our actual dataset integrating the LF over all the possible outcomes of our experiment. Then the relevant integral we have to deal with is

$$M(\chi_0) = \int_{\chi^2 \leq \chi_0^2} L(x, \lambda) \prod_i dx_i,$$

where the region of integration extends over all the possible data values which lie inside the region delimited by the actual value $\chi_0^2$. We can then use $M(\chi_0)$ for evaluating a CR for the parameters which enter $\chi_0^2$, like the quadrupole and the primordial slope in the case of CMB. The CR will depend parametrically on the higher-order moments; however, this will not provide a CR for the higher-order moments themselves. The method of the previous section can always be employed to yield a first approximation for such moments. Fixing a confidence level of $1 - \varepsilon$, we will consider as acceptables the values of the parameters for which $M(\chi_0)$ is larger than $\varepsilon / 2$ and smaller than $1 - \varepsilon / 2$. The evaluation of (12) would require some discussion. Here, however, I only state the final result:

$$M(\chi_0) = \int L \prod_i dx_i = F_N(\chi_0) + \frac{G_N(\chi_0) \pi^{N/2} \chi_0^N}{2^{1 + N/2} \chi_0^2} \left[C_a \left(N + 2 - \chi_0^2\right) + C_b \left(-N - 2 + 2\chi_0^2 - \frac{\chi_0^4}{N + 4}\right)\right],$$

where $F_N(\chi_0)$ is the usual $\chi^2$ cumulative function, and $C_a = c_1 + 3c_2$, and $C_b = c_3 + 3c_4 + 15c_5$, and the coefficients $c_i$ are formed by summing over all the even diagonals of the correlation tensors $k^{ijkl}$ and multiplying for the Edgeworth coefficients.
(1/24) for $c_1, c_2$ and (1/72) for $c_3, c_4$ and $c_5$. Let us make some comments on Eq. (13). First, the fact that $M(\chi_0)$ is a cumulative function provides a simple way to check the consistency of our assumptions: when the higher-order moments are too large, the MEE breaks down, $M(\chi_0)$ is no longer monotonic, and can decrease below zero or above unity. Second, let us suppose that the higher-order correlation functions are positive, which is the case for the galaxy clustering. Then the non-G corrections in Eq. (13) are negative for $\chi^2_0 \gg N$. The fact that the corrections are negative for $\chi^2_0 \gg N$ implies that the value of $\chi_0 = \chi_0(\varepsilon)$ is larger than in the purely Gaussian case, in the limit of $\varepsilon \to 0$. Consequently, if the higher-order correlation functions are positive, the confidence regions are systematically widened when the non-Gaussian corrections are taken into account. Finally, it is easy to write down the result in the particular case in which all the cumulant matrices are diagonal, i.e. for statistically independent variables. In this case the variables $y^i$ are simply equal to $x^i/\sigma_i$, if $\sigma_i = (\lambda_i^2)^{-1/2}$, and we can put $k_{ii}(y) = k_{ii}(x)/\sigma^2 \equiv \gamma_{1,i}$, and likewise $k_{iii}(y) \equiv \gamma_{2,i}$ (skewness and kurtosis coefficients). Then, we have $c_1 = c_3 = c_4 = 0$, and Eq. (13) can be simplified to

$$M(\chi_0) = F_N(\chi_0) + G_N(\chi_0)q(\chi_0),$$

where

$$q(\chi_0) = \frac{6\pi^{N/2}\chi_0^N}{(N+2)\Gamma(N/2)} \left\{ \frac{\gamma_2}{24} \left[(N+2) - \chi^2_0\right] + \frac{5}{72} \frac{\gamma^2_1}{\chi^2_0} \left[-(N+2) + 2\chi^2_0 - \frac{\chi^4_0}{N+4}\right] \right\},$$

and where the average squared skewness, $\gamma^2_1 = \sum \gamma^2_{2,i}/N$, and the average kurtosis, $\gamma_2 = \sum \gamma_{2,i}/N$, have been introduced.

Let me now illustrate graphically some properties of the function $M(\chi_0)$ in its simplified version (14) above. In all this section we can think of $\chi_0$ as depending monotonically on one single parameter, for instance the overall normalization $A > 0$ of the correlation function: $\chi^2_0(A) = x^i x^j (A_{ij} + e_{ij})^{-1}$. We can then speak of a CR on $\chi_0$ meaning in fact the corresponding CR on the parameter $A$. In the general case, the relation between $\chi_0$ and its parameters can be quite more complicated. In Fig. 1a (for $\gamma_1 = 0$ and $N = 10$), I show how the function $M(\chi_0)$ varies with respect to $\gamma_2$. Schematically, for $\chi^2_0/N > 1$, the function $M(\chi_0)$ decreases when $\gamma_2 > 0$ and increases in the opposite case. As anticipated, for too large a $\gamma_2$, $M(\chi_0)$ develops a non-monotonic behavior. The consequence of the behavior of $M(\chi_0)$ on the confidence region of $\chi_0$ is represented in Fig. 1b, where the contour plots of the surface $M(\chi_0, \gamma_2)$ are shown. Consider for instance the two outer contours, corresponding to $M = .01$, the leftmost, and $M = .99$, the rightmost. The range of $\chi_0$ inside such confidence levels increases for increasing $\gamma_2$. The same is true for the other contour levels, although with a less remarkable trend. This behavior confirms the approximate result of Eq. (11). As anticipated, this means that the non-G confidence regions will be larger and larger (if the higher moments are positive) than the corresponding Gaussian regions for higher and higher probability thresholds.

The situation is qualitatively different considering $\gamma_2 = 0$ and varying $\gamma_1$, the average skewness (Fig. 2, with $N = 100$). For the outer contours, delimiting levels
Figure 1:  a) Plot of $M(\chi_0)$ as a function of $\chi_0^2/N$ and of the dimensionless kurtosis $\gamma_2$, for $\gamma_1 = 0, N = 10$. For $\gamma_2 = 0$ we return to the usual $\chi^2$ cumulative function.  b) Contour levels of $M(\chi_0)$ corresponding to $M = .01,.1,.2,.3,.7,.8,.9,.01$, from left to right. Notice how the limits for $\chi_0$ broaden for increasing $\gamma_2$.

Figure 2:  a) Same as in Fig. 1a, now with $\gamma_2 = 0, N = 100$, and varying $\gamma_1$.  b) Contour levels of $M(\chi_0)$ for the same values as in Fig. 1b.
of 1% on both tails, the CR of $\chi_0$ increases for larger $|\gamma_1|$, with a minimum for the Gaussian case. For the internal contours, however, the CR actually shrinks for larger $|\gamma_1|$, being maximal at the Gaussian point. It is clear that in the general case, $\gamma_1, \gamma_2 \neq 0$, the topography of the LF can be quite complicated.

5. Conclusions

Let us summarize the results reported here. This work is aimed at presenting a new analytic formalism for parametric estimation with the maximum likelihood method for non-Gaussian random fields. The method can be applied to a large class of astrophysical problems. The non-Gaussian likelihood function allows the determination of a full set of parameters and their joint confidence region, without arbitrarily fixing some of them, as long as enough non-linear terms are included in the expansion. The CR for all the relevant parameters can be estimated by approximating the distribution function for the parameter estimators around its peak by a Gaussian, as in Sect. 3. To overcome this level of approximation, in Sect. 4 I generalized the $\chi^2$ method to include non-Gaussian corrections. The most interesting result is then that the CR for the parameters which enter $\chi^2_0$ is systematically widened by the inclusion of the non-Gaussian terms, in the limit of $\varepsilon \rightarrow 0$. Two experiments producing incompatible results can then be brought to agreement when third and fourth-order cumulants are introduced.

There are two main limitations to the method. One is that one obviously has to truncate the MEE to some order, and consequently the data analysis implicitly assumes that all the higher moments vanish. The second limitation is that the method is not applicable to strongly non-Gaussian fields, where the MEE breaks down. This can be seen directly from Eq. (13): for arbitrarily large constants $c_1 - c_5$ the likelihood integral is not positive-definite, although always converge to unity.

Acknowledgments

I thank Stéphane Colombi, Scott Dodelson, Sabino Matarrese and Albert Stebbins for several comments and suggestions at various stages of this work.

References

[1] Chambers J. 1967, Biometrika 54, 367
[2] McCullagh P. 1984, Biometrika, 71, 461
[3] Amendola L., 1994 Fermilab-Pub-94/263-A
[4] Kendall M., Stuart, A., & Ord J. K., 1987, Kendall’s Advanced Theory of Statistics, (Oxford University Press, New York)
[5] Juszkiewicz R. et al. 1995, Ap. J.,442, 39
[6] Kofman L. & Bernardeau, F. 1995, 443, 479
[7] Matarrese S., Lucchin F. & Bonometto S. 1986 Ap. J. 310, L21
[8] Catelan P., Lucchin F. & Matarrese S., 1988 Phys. Rev. Lett. , 61, 267
[9] Amendola L. 1994 Ap. J., 430, L9
[10] Matsubara T. 1994, Ap. J. 434, 43
