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Histogram analysis by use of L-moments, linear functions of order statistics

HISTOGRAM ANALYSIS BY USE OF L-MOMENTS, LINEAR FUNCTIONS OF ORDER STATISTICS

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Abstract

It is current statistical practice to summarize observed data by the moments or cumulants of the distribution. In comparison with conventional moments, L-moments, linear combinations of an ordered data set, are of considerable interest in defining an experimental data set because no assumption is made concerning the probability distribution of the data. The aim of this publication is to demonstrate the advantages as well as to explain the properties of L-moments as features of histograms. We use a pattern recognition approach in order to interpret and analyse histograms which are defined in a new vectorial space which is determined by Legendre polynomials.

ANALYSE D'HISTOGRAMME PAR LES L-MOMENTS, FONCTIONS LINEAIRES DE STATISTIQUES D'ORDRE.

Résumé

La description de données expérimentales par les moments ou les cumulants de la distribution sous-jacente est une pratique statistique classique. Par rapport aux moments conventionnels, les L-moments, combinaisons linéaires de l'ensemble des données ordonnées, sont d'un intérêt certain pour décrire les données sans faire d'hypothèses sur la loi de distribution. Dans cet article, nous montrons l'intérêt et les propriétés des L-moments comme descripteurs d'un histogramme, représentation graphique de données expérimentales. L'analyse et l'interprétation de ces histogrammes sont abordées comme un problème de reconnaissance des formes, dans le but de décrire ces histogrammes dans un nouvel espace de primitives engendré par les polynômes orthogonaux de Legendre.

Key words :
Pattern recognition. Histogram. Legendre polynomials. L-moments. High order statistics.

Classification AMS : 7-40. 13-25. 12-05-3

HISTOGRAM ANALYSIS USING L-MOMENTS, LINEAR FUNCTIONS OF THE ORDER STATISTICS

It is current statistical practice to summarize observed data by moments or cumulants. In comparison with conventional statistical moments, L-moments are of considerable interest to define an experimental data set, because no assumption need be made on the probability distribution of the data [HOS90]. Furthermore, vectorial data is normally defined in reference to a polynomial transformation. This publication reports on the use of L-moments and certain properties of Legendre orthogonal polynomials for the analysis of histograms. Several examples will be given.

Image analysis of DNA ploidy pattern has become of vital diagnostic interest since the discovery in the 1950s that tumour cells possess elevated quantities of DNA. DNA histograms are classical representations of the cellular DNA quantities in a tumour sample. The development of numerous statistical methods to interpret these histograms has progressed since 1980. The majority of these methods are based on the computation of a single parameter such as the index or percentage of cells containing a given quantity of DNA [OPF87]. To date, however, the analysis of biological samples by the statistical methods presently available does not necessarily correlate with the pathological status. This paper proposes a new statistical approach, based on the theoretical results of Hosking [HOS90], in order to improve DNA histogram interpretation. We propose to replace univariate distribution by the corresponding set of L-moments, which can subsequently be used in factorial analysis

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I.INTRODUCTION

The L-moments, analogous to conventional moments, can be estimated by linear combinations of an ordered data set, i.e by L-statistics. These L-moments have the theoretical advantage over conventional statistical moments in that they characterize a wider range of distributions. Moreover, they are robust when outliers are present in the sample. Greenwood et al.[GRE79] defined the probability of weighted moments of a variable in terms of order statistics from a random sample of size n. However, these moments are less adapted for use in the pattern recognition approach than L-moments, and they have therefore not been used in this study. On the other hand, Hosking

[HOS86] developed a unified theory covering the characterization of statistical distributions, the representation of data samples, the fitting of the data to probability distributions with data and an hypothesis for testing the fitted distributions. We use some of his theoretical results to extract certain features from the DNA distributions and to study their properties.

By definition, a histogram is dimensioned by a certain number of classes. In this study histogram analysis is treated as a problem of pattern recognition. Since it is usual to define vectorial data by a polynomial transformation, we use Legendre orthogonal polynomials to define the histogram in a new vectorial space.

Pattern recognition can be divided into two steps [YOU74]. In the first step the most prominent features of the histogram are extracted. The second step concerns the classification of this histogram based on the new features. With q L-moments, it is possible to reconstruct the original histogram using the reduction property of the Legendre polynomials [SIL69]. The quality of the reconstructed histogram is then compared with the original. The two first conventional moments are sufficient to describe a Normal distribution pattern, but when dealing with an unknown probability density, the conventional moments are of limited value in defining the distribution.

II. DEFINITIONS AND ALGORITHMS

II.1 Preliminary Notations

Let X be a continuous random variable with a distribution function F. Let x_i be the value of the variable X for different objects i, for i = 1, ..., N. Let x(F) be the quantile function or inverse distribution function of X. x(F) is defined by N points. Let f be the notation of the original histogram. The component f(i) is the relative frequency of objects belonging to class i, for i = 1, ..., K, where K is the number of classes by which the histogram is defined. g(i) is defined as the relative frequency of objects belonging to class i for a reconstructed histogram.

II.2 L-moments : definitions and properties

This method (illustrated in flow diagram 1) parametrizes an original distribution function by its L-moments and this distribution function is reconstructed using only a few of these L-moments.

* first, the L-moments are computed [HOS89] :

$$\lambda_r = \int_0^1 x(F) \; P^*_{r-1}(F) \; dF , \quad r = 1, 2, ..., \quad (1)$$

$P^*_r(x)$ is the rth shifted Legendre polynomial, derived from the Legendre polynomial $P_r(x)$, and given by $P^*_r(x) = P_r(\frac{x+1}{2})$. The Legendre polynomials are orthogonal for the interval $[0,1]$ with unit weight function. These polynomials can be used to define vectorial data by a polynomial transform. The selection of the number of L-moments will be developed below.

** then using the inversion theorem, proposed by Sillitto [SIL69], x(F) is approximated by a quantile function x*(F) given in terms of L-moments by equation (2) :

$$x^*(F) = \sum_{r=1}^{\infty} (2r-1)\lambda_r P^*_{r-1}(F) \quad 0<F<1 \quad (2)$$

x*(F) is convergent to x(F) in mean square sense, i.e.

$$R_s(F) \equiv x(F) - \sum_{r=1}^{s} (2r-1)\lambda_r P^*_{r-1}(F)$$

the remainder after stopping the infinite sum after s terms, satisfies

$$\int_0^1 \{R_s\}^2 dF \to 0 \text{ as } s \to \infty \quad (3)$$

This theorem is valid for discrete random variables, provided that the quantile function is normalized, i.e. that

$$\lim_{\varepsilon \to 0} \frac{1}{2} \{ (x(F+\varepsilon) + x(F-\varepsilon) \} = x(F) \text{ for all } F \in (0, 1)$$

*** finally a new distribution function F* can be generated from the quantile function x*(F). The relative frequency of each class i can be estimated from this distribution by the integration between two values a and b, which are extremities of the

class i. Since a density function is the derivative of the distribution function, it follows that :

$$g(i) = F^*(a) - F^*(b) \quad \text{for } i = 1 \rightarrow K$$

II.3 Specific algorithm.

The L-moment properties described above are adapted to the present problem; but since the analytical formula of the quantile functions are unknown, we use numerical computing algorithms to resolve the different equations.

- Let X be a continuous random variable, with N observations $x_1, x_2, \ldots, x_N$.

- Let F be the distribution function of the variable X, defined on N points.

- Let f be a histogram, a graphical representation of the variable X, represented by $f(i)$ for $i = 1, \ldots, K$, with K classes.

- empirical distribution function F can be plotted

$$F(x) = Pr(X \leq x)$$

$$F(x_j) = \sum_{z=1}^{j} Pr(x_z), \text{ for } j = 1 \text{ to } N$$

- and q L-moments (Simpson method) be computed:

$$\lambda_r = \int_0^1 x(F) \, P^*_{r-1}(F) \, dF, \quad r = 1, 2, \ldots, \quad (1)$$

From the N values of the empirical distribution function F, this integral is computed by means of the Simpson's algorithm.

- Restoration phase :

compute $x^*_q(F)$ the reconstructed quantile function by using the q first L-moments :

$$x^*_q(F) = \sum_{r=1}^{q} (2r-1)\lambda_r P^*_{r-1}(F) \quad 0 < F < 1 \quad (4)$$

plot the approximated distribution function curve F^*_q from $x^*_q(F)$,

compute $g_q(i)$ the restored histogram with the q first L-moments, from F^*_q

$$g_q(i) = F^*_q(a) - F^*_q(b) \quad \text{for } i = 1 \rightarrow K \quad (5)$$

with a and b extremities of the class i.

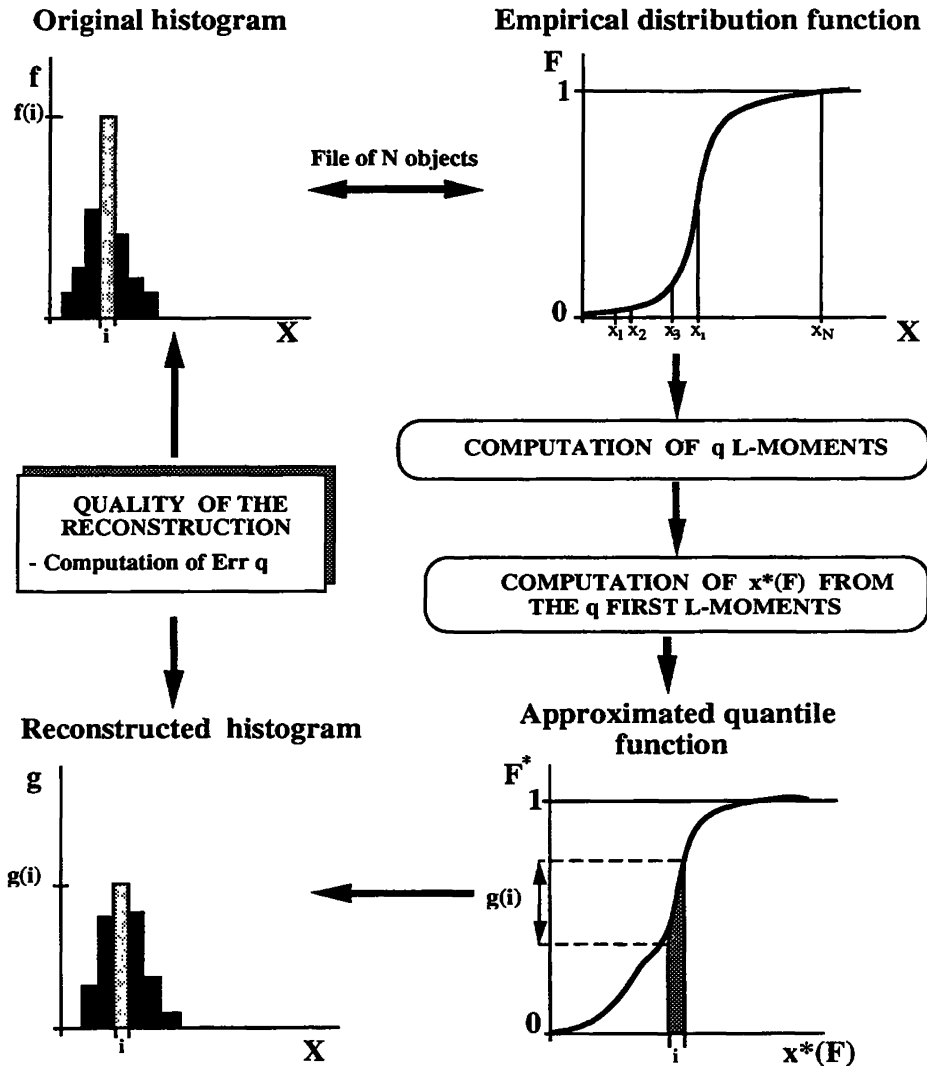$F^*(a)$ and $F^*(b)$ are computed by dichotomy.

Remarks : This algorithm permits the reconstruction of the original distribution function F, from the formula (4). However, we have chosen to study the reconstruction of histograms using formula (5). In the present biological situation, distributional analysis is less informative than the form of the histogram itself. In this respect, the quality of histogram reconstruction depends entirely on the characteristics of the original distribution function F : a histogram is merely a graphical representation of the sample.

II.4 Choice of the number of L-moments.

The choice of the number of L-moments needed to describe the distribution F depends on the quality of the inversion. The process is terminated when a criterion error, called Err, reaches a minimum. The most obvious criterion is given by relation (3). However, Hosking leaves a number of questions unanswered about the convergence of Rs(F) to 0. Thus we prefer to compute a stop criterion based directly on the quality of the reconstructed histogram. We note Err_q as the quadratic error associated with the reconstruction of the original histogram f(i) by $g_q(i)$ using the q first L-moments. For a histogram defined by K classes, Err_q is defined by the relation :

$$Err_q = \sum_{i=0}^{K} \frac{(f(i) - g_q(i))^2}{f(i)^2}$$

The best reconstruction is obtained with q L-moments when Err_q is a minimum. Nevertheless, we are also interested in the evolution rate of the reconstructed histogram in order to study the contribution and the significance of each L-moment. Oja [Oja81] studied this problem for the four first conventional moments using a theoretical approach.

Original histogram

Empirical distribution function

File of N objects

COMPUTATION OF q L-MOMENTS

QUALITY OF THE
RECONSTRUCTION

- Computation of Err q

COMPUTATION OF x*(F) FROM
THE q FIRST L-MOMENTS

Reconstructed histogram

Approximated quantile
function

FLOW DIAGRAM 1 : Illustration of the algorithm : The original histogram may be reconstructed by using the q first l-moments in order to study the quality of these features.

III. RESULTS

Some results of using L-moments in synthetic and real situations will now be given. L-moments will be calculated for synthetic distributions with a mixture of normal sub-populations and real distribution of biological populations. Some histograms will be reconstructed by using an ascending number of the L-moments.

III.1 Analysis of normal distribution by L-moments.

In the case of a few known continuous distributions Hosking [HOS90] has given some analytical relations between the first four L-moments and the first two conventional moments. These relations are listed in table 1 for a simulated normal distribution of 300 objects. We can verify that the analytical relations remain correct through the use of numeric algorithms. The differences between the computed results and expected results are due to approximation errors of the successive integrations. As expected, these differences decrease as the sample size increases (results not shown).

In Figure 1, the histogram of the former distribution has been reconstructed according to our algorithm. The histogram A is the original, represented on 30 classes. We used successively 1, 2, 3, 4, 5, 7, 11 and 16 L-moments to reconstruct the histograms B, C, D, E, F, G, H and I respectively .

The first-order L-moment gives the location of the distribution, i.e the mean or the median in the case of a symmetric distribution. The second-order L-moment gives the shape of the distribution while the third-order L-moment gives the degree of skewness. In a normal distribution, the third-order L-moment is approximately equal to 0, so the reconstructed histogram is also approximately the same as the former reconstructed with two L-moments. The fourth-order L-moment gives the degree of kurtosis of the distribution. The interpretation of these four L-moments is identical to that obtained from conventional moments. The reconstructed histogram using the first four L-moments is already a good approximation to the original histogram. The contribution of the fifth to the sixteenth-order L-moment (which gives the best reconstruction according to our criterion) is not significant and it is difficult to interpret each one for this normal distribution. Indeed, in this case, for which two first conventional moments are sufficient to define the probability density function, the use of L-moments (16 L-moments!!!) seems to be of little interest. But, when the distribution law is unknown, the use of L-moments to define any kind of distribution is, on the contrary, of prime interest.

Conventionnal moments	Computed L-Moments	Expected L-moments from	analytical relations
μ = 2007,97	λ_1 = 2006,12	2007,97	$(\lambda_1 = \mu)$
σ^2 = 43689	λ_2 = 118,20	117.04	$(\lambda_2 = 0.56\sigma)$
	λ_3 = 0.06	0	$(\lambda_3 = 0)$
	λ_4 = 13.6	14.42	$(\lambda_4 = 0.069\sigma)$

Table1. Comparison between the two first conventional moments (mean μ and variance σ^2) and the two first computed L-moments λ_1 and λ_2 for a simulated normal distribution (mean μ = 2007, standard deviation σ = 209, objects = 300). The first four expected L-moments from Hosking's analytical relations, given in the third column, are similar with the four first computed L-moments.

III.2. Detection of sub-populations in some multimodal distributions.

Figures 2, 3, 4 and 5 illustrate the analysis of simulated bimodal histograms in which the two sub-populations are weighted differently. The proportion of the two subpopulations, are respectively 0.9/0.1, 0.75/0.25, 0.5/0.5, 0.25/0.75.

In Figure 2, where the initial histogram (Figure 2A) corresponds to the sum of two normal distributions with probability 0.90 and 0.10, the first-order L-moment corresponds to the central tendancy and the second-order L-moment corresponds to the dispersion of the distribution. The third-order L-moment represents the skewness of the distribution whereas degree of kurtosis of the distribution is represented by the fourth-order L-moment. After the sixth-order L-moment, which is not represented here, the principal sub-population is well represented. With eight L-moments (Figure 2G), reconstructed histogram shows a normal population with a long tail to the right. Progressively, with other L-moments up to twelfth-order L-moment, an increasing number of classes to the right of the principal population (which remains stable) are represented. It is necessary to use 19 L-moments (Figure 2I) to obtain the best reconstructed histogram with the second sub-population correctly represented.

In Figures 3, 4 and 5, the evolution of reconstructed histogram is approximatively the same as for the former histogram. Nevertheless, it should be noted that the number of L-moments required to detect the small sub-population varies inversely with the weight of this sub-population. Indeed the subpopulation of probability 0.10, 0.25, 0.50 are detected respectively by using 19, 10, and 5 L-moments (Figures 2I, 3H, and 4F).

Moreover, the original histogram of Figure 5 can be considered to be symmetric when compared to that of Figure 2. The difference between the two is the result of differences in distributions. Indeed the coefficient of variation is the same for the two distributions so the standard deviation varies as a function of the subpopulation mean value. It should be noted that both of these reconstructions evolve similarly, i.e the main population is detected first then the minor population is detected.

The bimodal histogram of Figure 4 indicates that the fifth-order L-moment characterizes the bimodality of the distribution. This observation has also been made by other authors [HOS90].

III.3. Problem of outliers in real histogram.

In a mixture of two normal distributions, the first detected distribution is the one which is more weighted, of course. The speed of reconstruction convergence depends on the size of the minor distribution. But in real distributions as DNA histograms, histograms are not so simple.

In Figure 6, a real DNA histogram built on 30 classes is shown which has been generated from 30 classes (with 346 objects). A major sub population can be easily detected. Moreover this histogram shows some successive irregularities, due to very low weighted sub-populations, and especially an isolated class (one object) at the tail of the distribution. The best reconstruction is obtained with 16 L-moments. The approximation is more or less accurate but the reconstruction "forgets" the smallest classes at the end of the distribution. The presence of the outlier in class 29 is responsible for the smooth tail that can be seen in Figure 6I at the right of the distribution. Indeed, even if the outlier is not detected, the polynomial approximation is sensitive to this value and tends to show it . Thus the tail of the distribution is not well represented.

We are faced with a fundamental problem. In order to solve it, we propose to modify this histogram. Indeed, the existence of empty classes between the majority of the distribution and the outlier is an element of the unsatisfactory representation of the extremely low size classes. What is proposed here is to transform the initial histogram of Figure 6 by adding a same number of objects in each of the original histogram classes. This new histogram is represented by Figure 7A. It has no more empty classes. In comparison with the six first reconstructed histograms of Figure 6, the six first reconstructed histograms (Figure 7B-7F) evolve in the same way. The difference concerns a stronger skewness of the reconstructed histograms of Figure 7, in response to the increase of objects number in the distribution tail. 21 L-moments are needed to obtain

the best reconstruction (Figure 7I) and even if a class has been created at the end of the distribution, the rise in number of L-moments needed to improve the quality of reconstruction seems to be relatively high.

III.4.Problem of degradation.

When the number of Legendre polynomials is too high, a degradation of the reconstruction appears due to the non-monotonic increment in the approximated quantile function. In fact, the problem of degeneration is common with all polynomial approximations encountered in many inverse problems such as image restoration [AND77]. In Figure 8, the evolution of criterion Err in terms of number of L-moments used for the reconstruction is shown. This degradation does not appear when the distribution has a regular and smooth tail, as in the case of a normal distribution (Figure 8A). But when the distribution is irregular (heterogeneous), the phenomenon appears (Figure 8B).
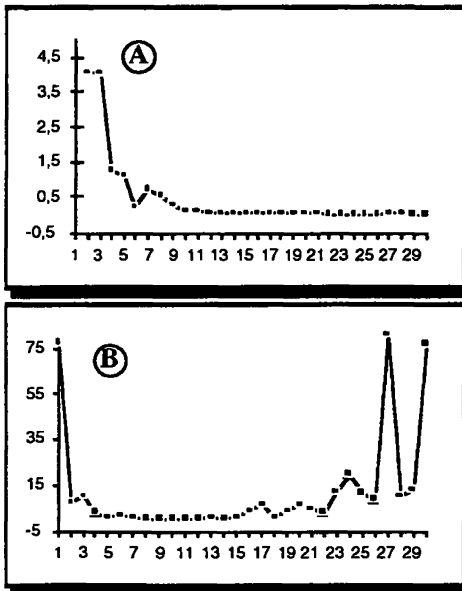

Figure 8. Evolution of stop criterion Err (ordinate) as a function of the number of L-moments (abscissa) used to approximate the original histogram. A : simulated normal distribution, B: real heterogeneous distribution.

Complete reconstruction remains an open problem and we only propose to detect the appearance of degradation in order to stop the reconstruction.

III.5. Dependency on class number.

The dependency on number of classes associated with the best representation has also to be considered. Depending on the application, this choice is often arbitrary. In our problem we have chosen to keep the same number of classes regardless of the range of the sample. Figure 9 shows three histograms A, B and C of the same distribution but generated from respectively 10 classes (Figure 9-A1), 20 classes (Figure 9-B1) and 30 classes (Figure 9-C1). The best representation is obtained with 10 L-moments. It is satisfactory for the 10 classes histogram (Figure 9-A3) but not for the 30 classes histogram (Figure 9-C3). Here it is clear that the lower the number of classes, the better the reconstruction. But, the ratio of the number of L-moments associated with the best reconstruction to the number of classes is better for histogram C (1:3) as compared with histogram A (1:1). Thus a compromise has to be found between the quantity of information present in a histogram and the quality of the reconstruction.

IV.DISCUSSION

In each pattern recognition problem , feature extraction is a crucial step. In this paper, we have shown that L-moments are the principal features of a histogram. Two important points can be deduced from these results.

Firstly, a histogram initially represented by K classes has been transformed into a Q point (Q L-moments) representation, with Q inferior to K. Thus the dimensions of the representation space has been reduced with little or no loss of information. Furthermore, this new features are independent contrary to histogram classes.

Secondly, it follows from the inversion theorem that the quality of the reconstruction can be is consistent.

These two main points show that the method of analysis of any distributional pattern can be demonstrated without the need to have defined a probability law. These results demonstrate therefore the limitations to the inverse quantile theorem in pattern reconstruction. The lack of quality in pattern reconstruction when too many L-moments are used is not a problem encountered only when Legendre polynomials are used. Many studies have demonstrated that this problem is still unresolved [AND77]. The detection of rare objects, in relation to empty classes, is limited by the large number of polynomial

approximations needed. Nevertheless, these problems can be handled as long as there are few histogram classes.

The number of L-moments satisfying the stop criterion is sometimes high. In our opinion, this criterion can be more efficiently replaced by a different test. Indeed, it would be sufficient to retain the number of L-moments which provide a reconstructed histogram "biologically equivalent" to the original histogram. In this respect it is possible to compare the distributions using, for instance, the Kolmogorov test or the Khi2 test. The first kind error can thus be fixed at a value depending on the appropriate quality of reconstruction.

It is usually sufficient to determine 20 to 30 classes in order to correctly reproduce a set of data in the form of a DNA histogram. Moreover, it is unlikely that the presence of rare objects at the extremities of the distribution will alter the resulting diagnosis. DNA histograms can be grouped into a limited number of diagnostic groups [AUE80]. As far as this application is concerned, it is apparent that the quality of pattern reconstruction is not hindered by a low number of L-moments. These results demonstrate a novel application of L-moments in DNA histogram analysis. Future work should lead to the classification of histograms from biological samples at different pathological stages as a function of L-moment values.
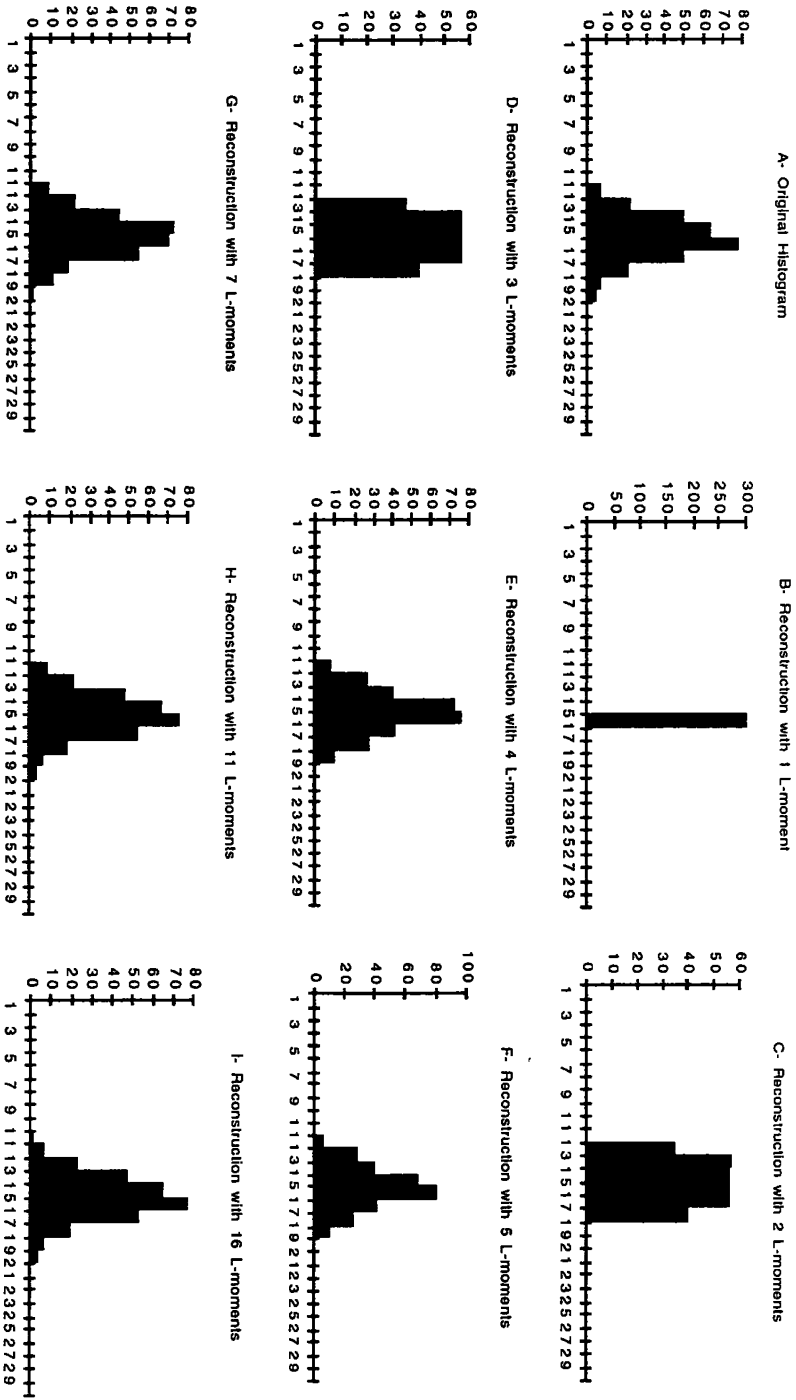
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FIGURE 1 : Reconstruction of an original histogram (A) of 30 classes and 300 objects (Normal distribution, mean = 2000, CV = 10%) with respectively 1, 2, 3, 4, 5, 7, 11 et 16 L-moments. The best reconstruction is obtained by using 16 L-moments (I).

FIGURE 2 : Reconstruction of an original histogram (A) of 30 classes and 300 objects (Normal distribution 1, mean1 = 2000, CV1 = 10%, P1 = 0,90; Normal distribution 2, mean2 = 4000, CV2 = 10%, P2 = 0,10) with respectively 1, 2, 3, 4, 5, 8, 12 et 19 L-moments. The best reconstruction is obtained by using 19 L-moments (I).
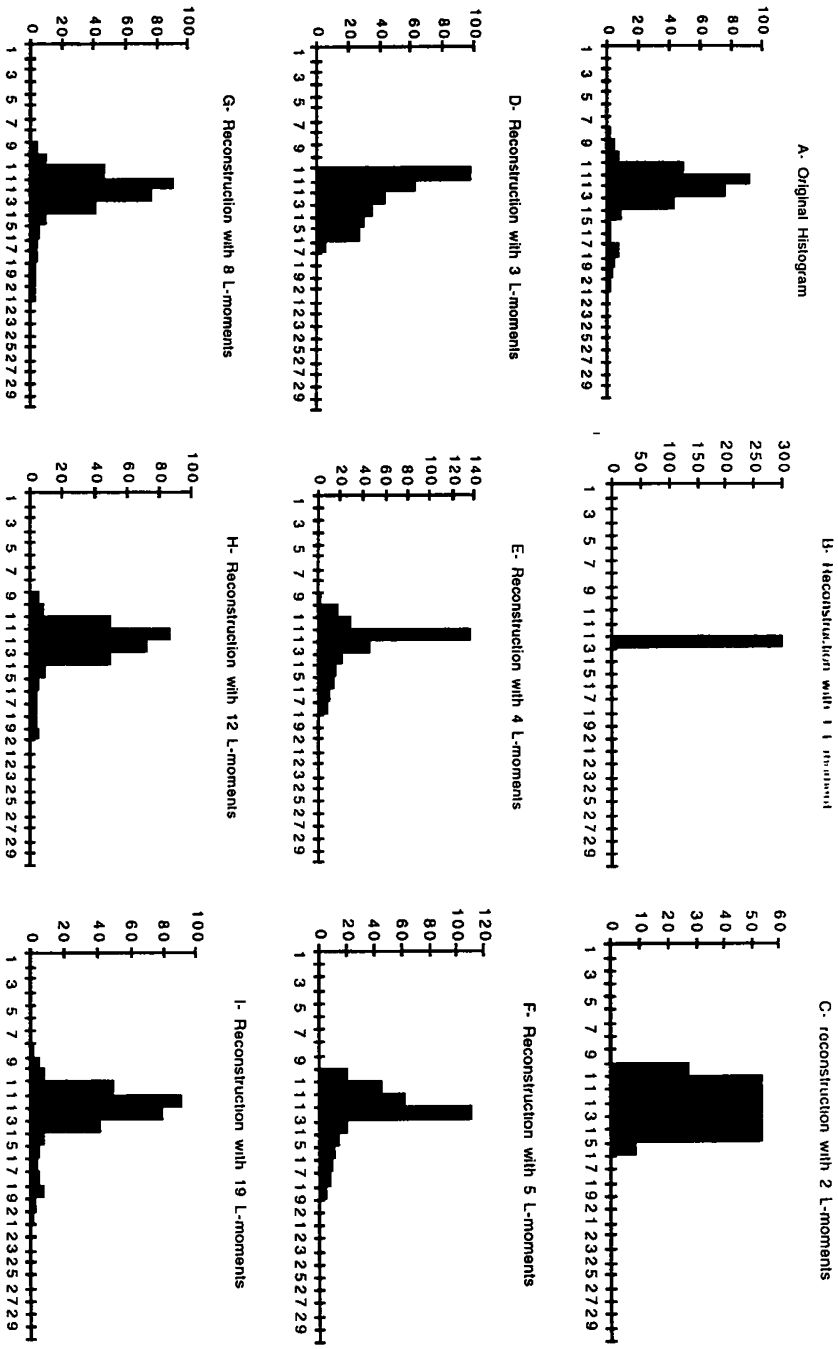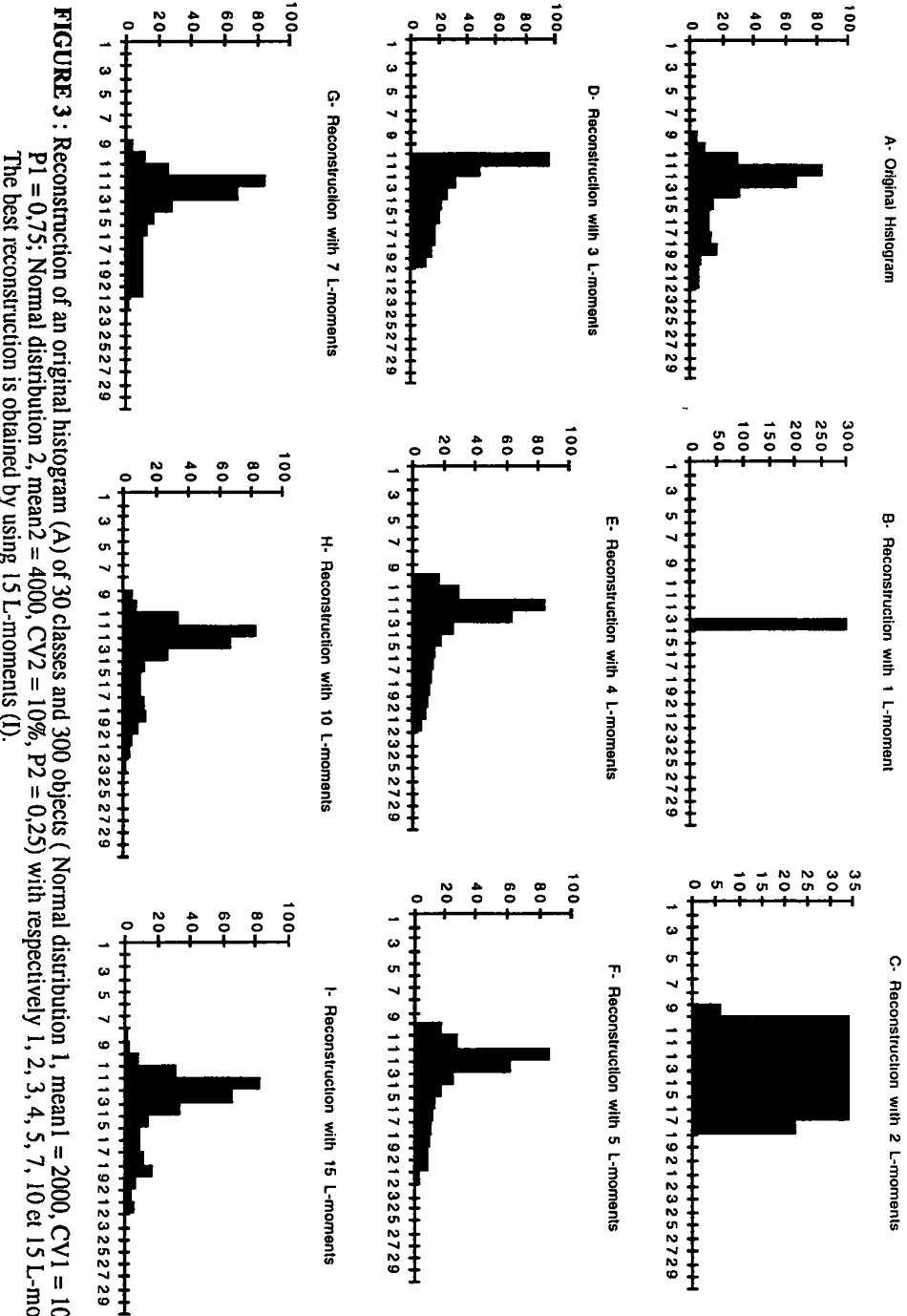
FIGURE 3 : Reconstruction of an original histogram (A) of 30 classes and 300 objects (Normal distribution 1, mean1 = 2000, CV1 = 10%, P1 = 0,75; Normal distribution 2, mean2 = 4000, CV2 = 10%, P2 = 0,25) with respectively 1, 2, 3, 4, 5, 7, 10 et 15 L-moments. The best reconstruction is obtained by using 15 L-moments (I).

A- Original Histogram

B- Reconstruction with 1 L-moment

C- Reconstruction with 2 L-moments

D- Reconstruction with 3 L-moments

E- Reconstruction with 4 L-moments

F- Reconstruction with 5 L-moments

G- Reconstruction with 7 L-moments

H- Reconstruction with 10 L-moments

I- Reconstruction with 15 L-moments

A- Original Histogram

B- Reconstruction with 1 L-moment

C- Reconstruction with 2 L-moments

D- Reconstruction with 3 L-moments

E- Reconstruction with 4 L-moments

F- Reconstruction with 5 L-moments

G- Reconstruction with 6 L-moments

H- Reconstruction with 11 L-moments
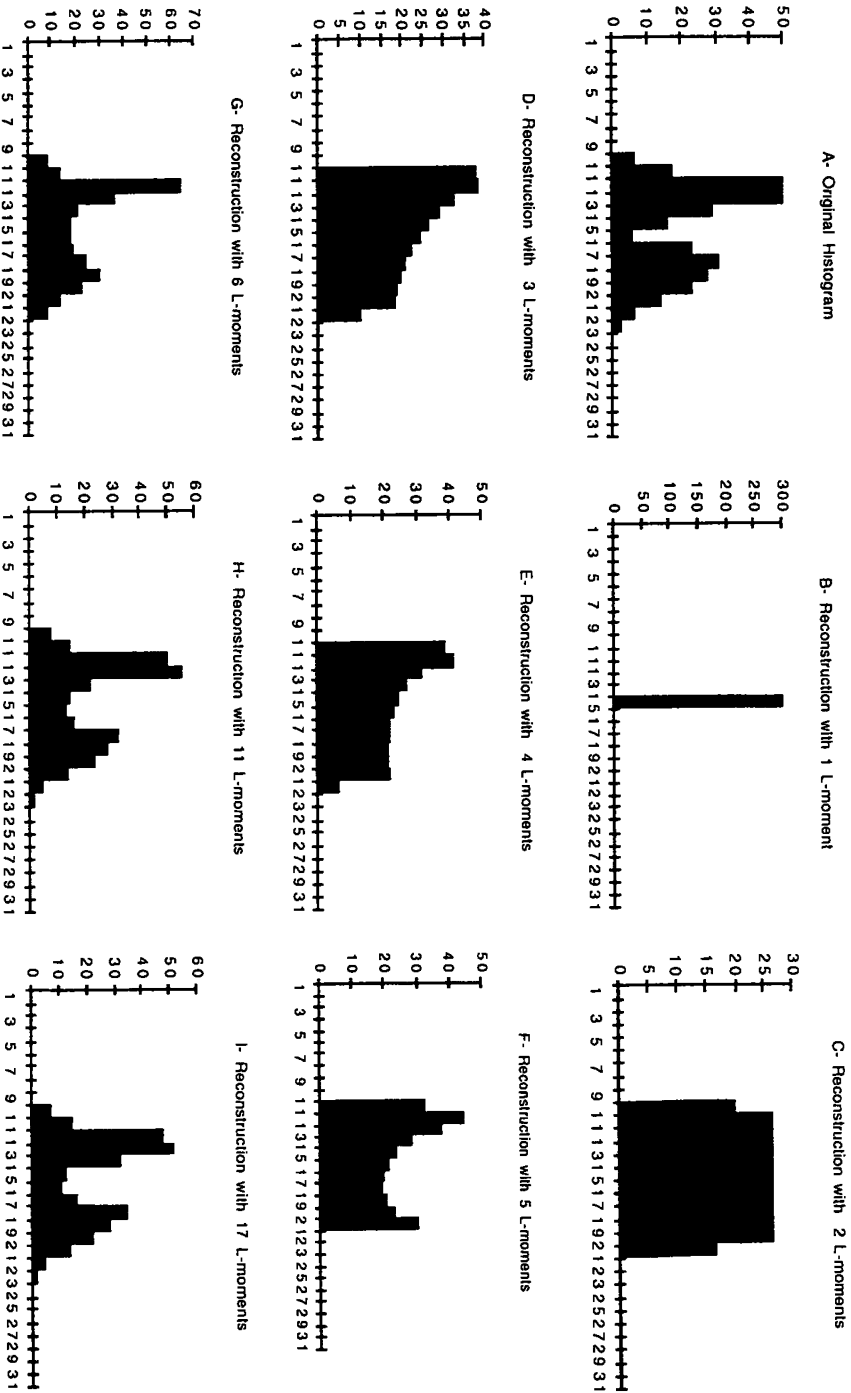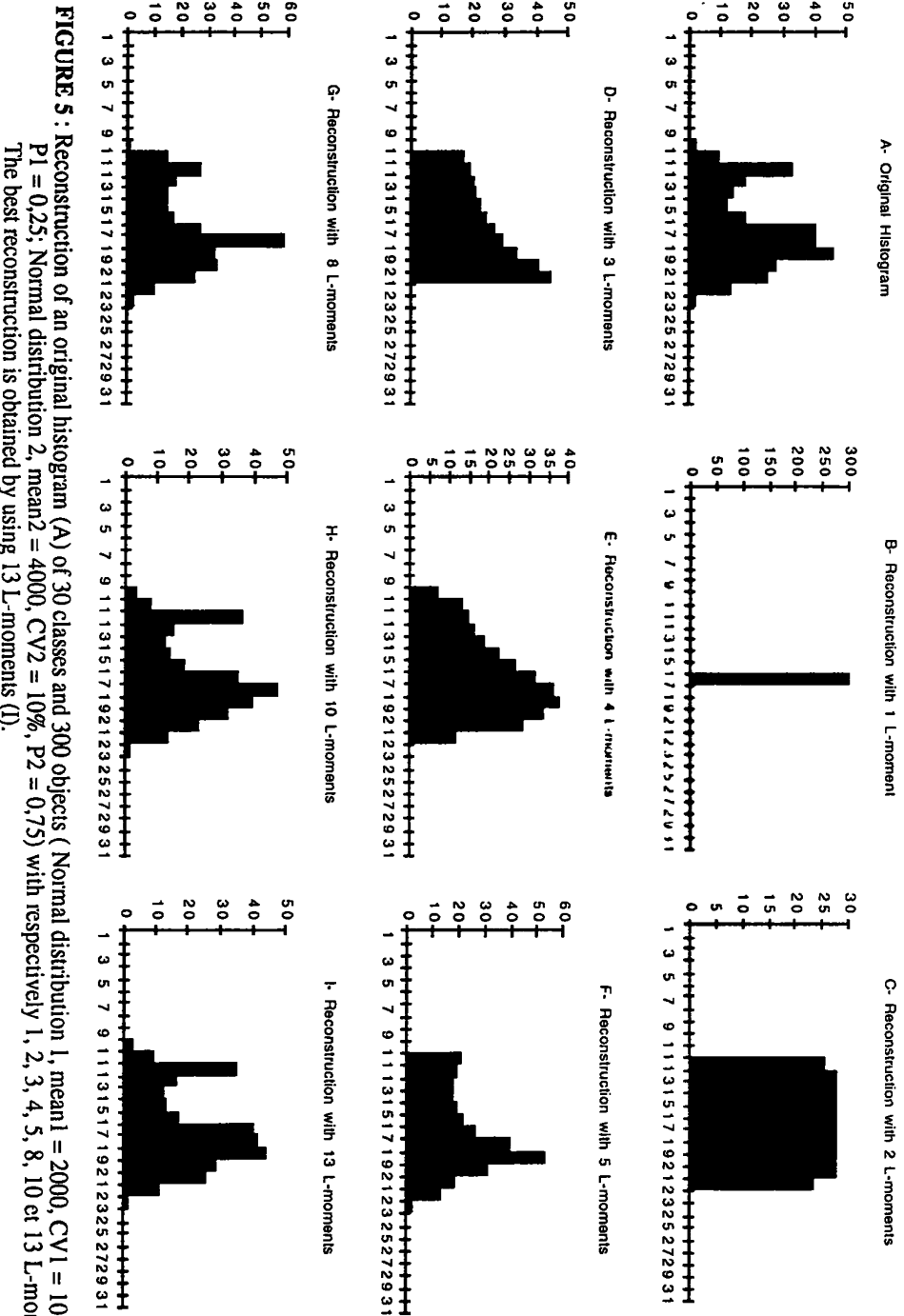
I- Reconstruction with 17 L-moments

FIGURE 4 : Reconstruction of an original histogram (A) of 30 classes and 300 objects (Normal distribution 1, mean1 = 2000, CV1 = 10%, P1 = 0,50; Normal distribution 2, mean2 = 4000, CV2 = 10%, P2 = 0,50) with respectively 1, 2, 3, 4, 5, 6, 11 et 17 L-moments. The best reconstruction is obtained by using 17 L-moments (I).

FIGURE 5 : Reconstruction of an original histogram (A) of 30 classes and 300 objects (Normal distribution 1, mean1 = 2000, CV1 = 10%, P1 = 0,25; Normal distribution 2, mean2 = 4000, CV2 = 10%, P2 = 0,75) with respectively 1, 2, 3, 4, 5, 8, 10 et 13 L-moments. The best reconstruction is obtained by using 13 L-moments (I).
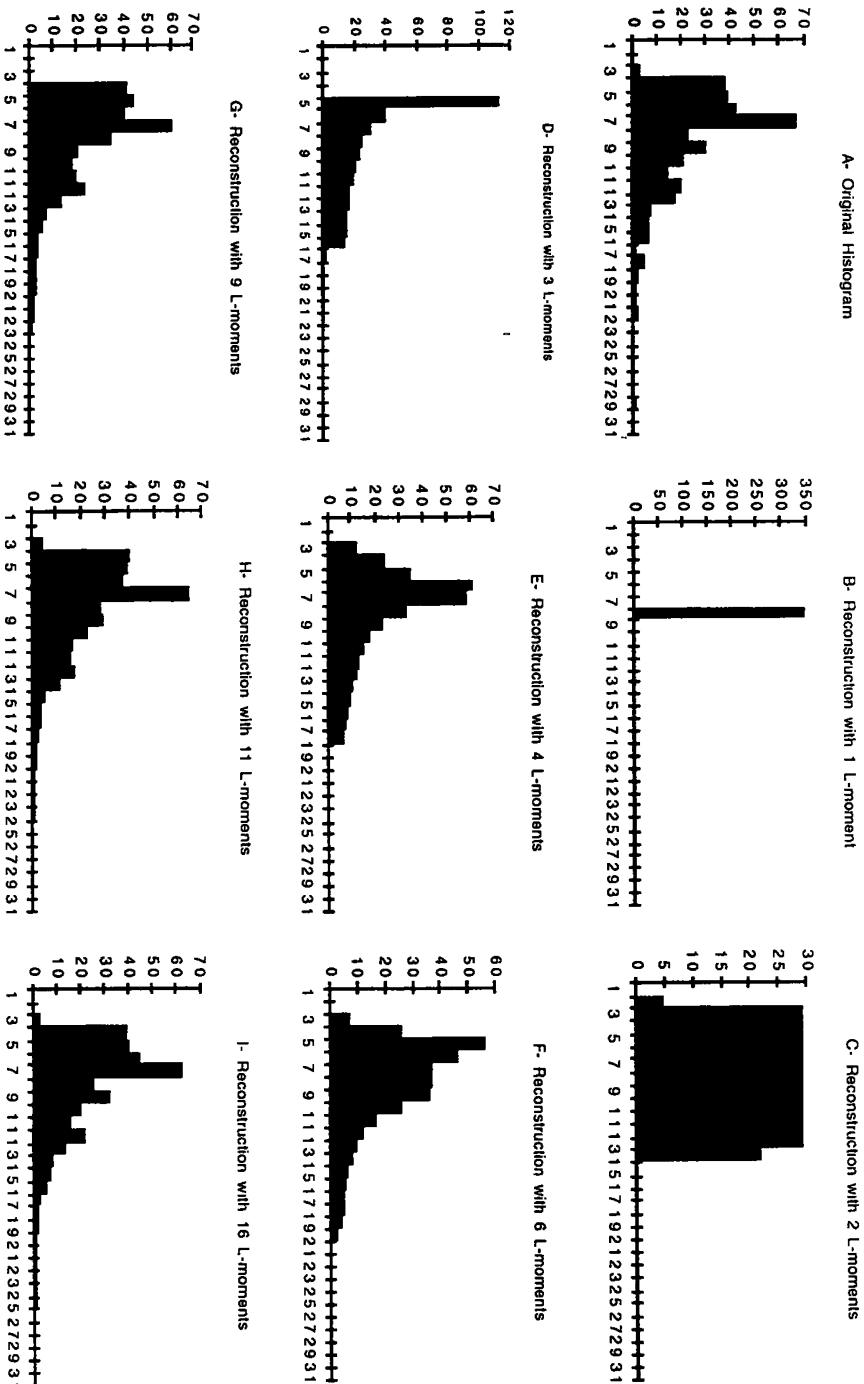
FIGURE 6 : Reconstruction of an original real ploidy histogram (A) of 30 classes and 346 objects with respectively 1, 2, 3, 4, 6, 9, 11 et 16 L-moments.The best reconstruction is obtained by using 16 L-moments (I).

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A - Original Histogram

B - Reconstruction with 1 L-moment

C - Reconstruction with 2 L-moments

D - Reconstruction with 3 L-moments

E - Reconstruction with 4 L-moments

F - Reconstruction with 6 L-moments

H - Reconstruction with 11 L-moments

H - Reconstruction with 16 L-moments

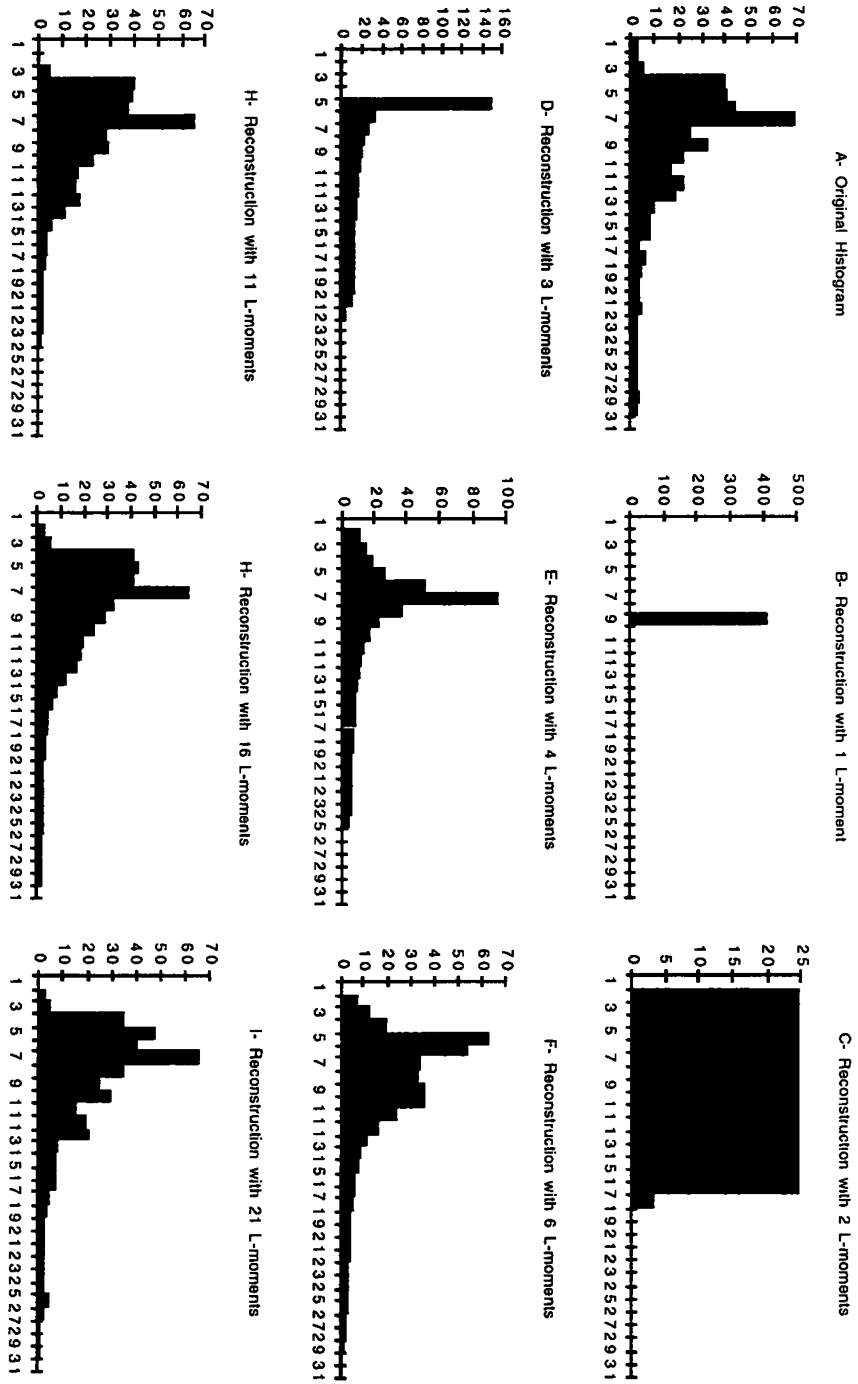I - Reconstruction with 21 L-moments

FIGURE 7 : Reconstruction of an original modified ploidy histogram (A) of 30 classes and 406 objects with respectively 1, 2, 3, 4, 6, 11, 16 et 21 L-moments.The best reconstruction is obtained by using 21 L-moments (I).
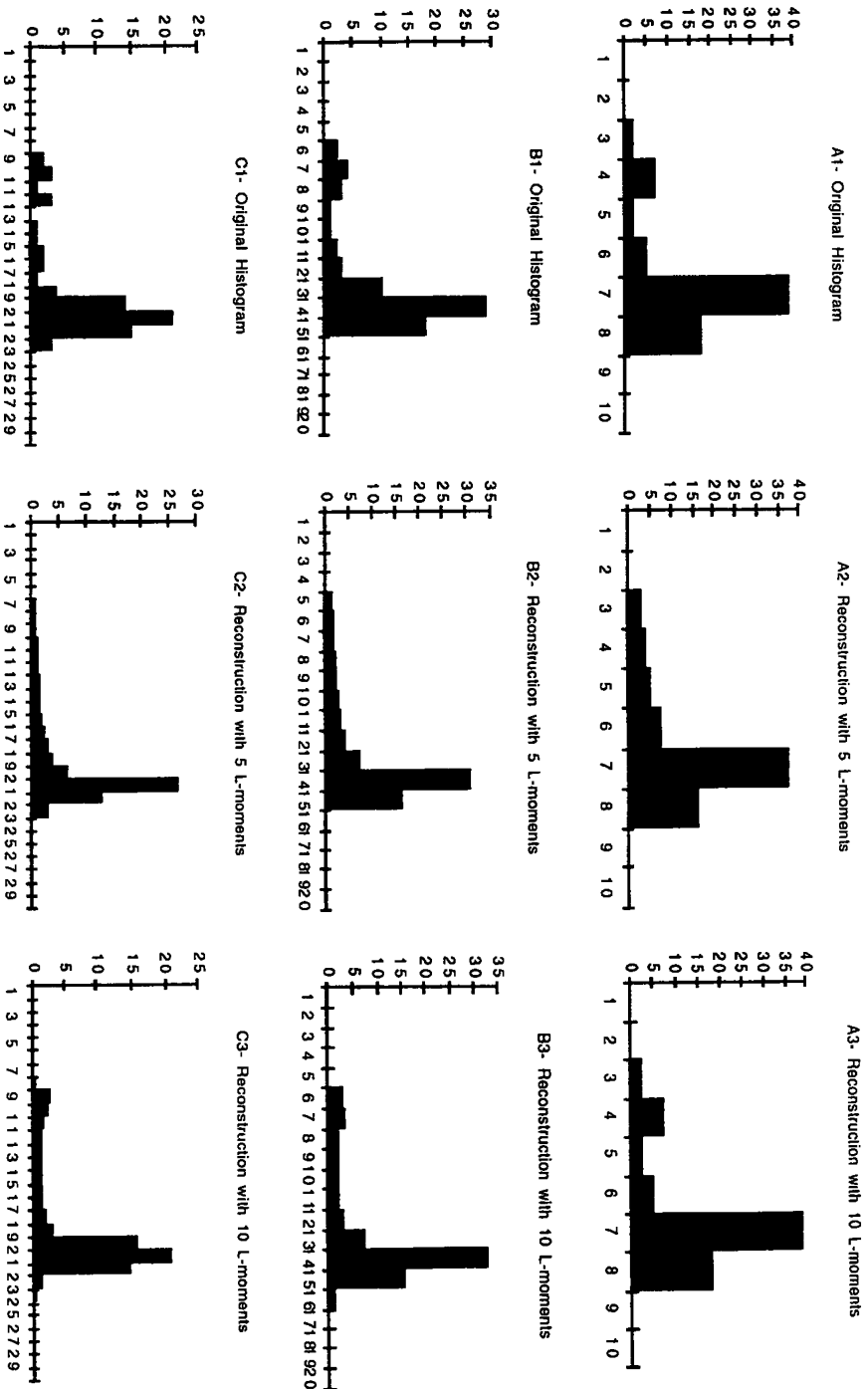
FIGURE 9 : Reconstruction of the same real ploidy histogram defined on 10 classes (A1), 20 classes (B1), 30 classes (C1) and 300 objects using respectively 5 (A2, B2, C2) and 10 L-moments (A3, B3, C3). The best reconstructions are obtained by using 10 L-moments.

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