Spline histogram method for reconstruction of probability density functions of clusters of galaxies

Dmitrijs Docenko and Kārlis Bērziņš

1 Institute of Astronomy, University of Latvia, Raina blvd 19, Riga LV-1586, Latvia; e-mail: dima@latnet.lv
2 Ventspils International Radio Astronomy Center, Akademijas laukums 1-1503, Riga LV-1050, Latvia; e-mail: kberzins@latnet.lv

Abstract. We describe the spline histogram algorithm which is useful for visualization of the probability density function setting up a statistical hypothesis for a test. The spline histogram is constructed from discrete data measurements using tensioned cubic spline interpolation of the cumulative distribution function which is then differentiated and smoothed using the Savitzky-Golay filter. The optimal width of the filter is determined by minimization of the Integrated Square Error function.

The current distribution of the TCSplin algorithm written in f77 with IDL and Gnuplot visualization scripts is available from www.virac.lv/en/soft.html.

1 Introduction

Whenever one makes a physical measurement one obtains a discrete result, starting from spatial measurements and ending with classification of some set of objects by some quantity. Particular measured value follows from the statistical properties of the system strictly following the probability distribution function, hereafter PDF. The PDF, in its turn, is determined by the physical properties of the system. If a measured data set is statistically complete then its PDF contains information about the system’s physical properties. The PDF shows a character of unimodal or multimodal systems. It is natural to assume that the PDF of unimodal physical systems contain only one global maximum and several maxima indicate the multimodality of a data set. Therefore the shape of the PDF allows one to classify the measured data points, e.g. to find structure in case of positional measurements.

In statistics it is widely accepted to use histograms as the PDF approximations. It is also well known that ordinary histograms being dependent on two free parameters (bin size and its location) give very subjective results. Many methods have been developed trying to solve this problem [5]. However, most of them are still dependent on some parameters in a non-objective manner.

Generally, the probability density estimation methods can be divided into two main groups: parametric and non-parametric. The first ones assume some definite type of the PDF function (e.g. Gaussian or their superposition) and try to find the best-fit parameters for it. A good such example is the KMM mixture modelling algorithm [2]. A main disadvantage of these methods is that not all
data sets can be well fitted with any chosen function. Rather often the real PDF of physical system has significant difference from a chosen best-fit function, and in many cases it is not known a priori what function it should be at all.

Non-parametric methods try to construct PDF estimates as compromise of two opposite demands. First, the estimate should be as close as possible to the measured PDF. Second, statistical noise due to a finite volume of the selection should be filtered out. There are several ways how to do it.

It is possible to minimize a functional that is a sum of two terms – the statistical noise and the one increasing with a difference between data points and the PDF estimate (Vondrak’s method) [21]. Unfortunately, there is still one free coefficient responsible for the smoothing degree. This coefficient is not determined in any automated way and usually is found from good-looking conditions. Another method is to convolve the initial guess of the PDF with some kernel (kernel methods) for data smoothing. Also in this case there remains a free coefficient – the kernel width, that is responsible for smoothing of the function in an “optimal way”, besides the result is weakly dependent on the chosen kernel shape [5], [20].

There is, however, a method that allows one to choose an optimal smoothing width: the PDF should not be over-smoothed and lose its true features, and the noise level should be diminished as far as possible on the other hand. This method is described e.g. in [20]. Its main idea is to define an Integrated Square Error ($ISE$) function that shows the difference between the real PDF and its estimate, and then to minimize it. The $ISE$ function method is implemented for kernel methods in e.g. [15], and results are encouraging. However, the $ISE$ function itself is often rather noisy.

In this paper we propose another approach to estimate PDF of a given one-dimensional data set in automatic and optimal way. This is the spline histogram method. We have found that the tensioned cubic splines are suitable for this task and the corresponding algorithm has been called TCSplin. The current version of the TCSplin code is freely available in the internet, it is also included in the CD-ROM.

For demonstration purposes in this article we will use the spline histogram algorithm to find a “well determined” redshift structure of galaxies within clusters Abell 2256 and Abell 3626.

This paper has the following structure. The spline histogram algorithm will be discussed in section 2. Bootstrapping simulations, discussed in section 3, help to evaluate errors of the PDF estimates. In section 4 the spline histogram application to data sets of clusters of galaxies A2256 and A3526 will be shown as examples. Finally, some concluding remarks will be given in section 5.

2 The spline histogram algorithm

The spline histogram method is a non-parametric approach for reconstruction of probability density function underlying statistical selection. It was first discussed in [4] as one of possible methods to detect substructure in clusters of galaxies.
Recently it was further developed in [9] and these results are summarized in this paper.

From spectroscopic observations we obtain redshifts of galaxies in clusters. Let us denote redshift of the $i$th galaxy by $z_i$ and order them ascendently ($z_i \leq z_{i+1}$). Next step is to construct a step-like cumulative distribution function (CDF) obtained purely from observational data: $F_{\text{obs}}(cz) = N(z_j < z)/N_{\text{gal}}$, where $N(z_j < z)$ is a number of galaxies with redshift smaller than $z$, and $N_{\text{gal}}$ is a total number of detected galaxies, $c$ is the speed of light. At this stage we assume that the data set is statistically complete being representative of the physical situation. The PDF $f(x)$ by definition is the derivative of $F_{\text{obs}}(cz)$ in respect to $cz$. If CDF is constructed as shown before then $f(x)$ is a sum of Dirac $\delta$-functions.

In the spline histogram method the points $z_i$ with ordinates $F_{\text{obs}}(cz_i)$ are consequently connected by non-decreasing smooth analytical spline $S(cz)$. After construction of $S(cz)$ the latter is analytically differentiated leading to the PDF estimate $\hat{f}(cz)$. This procedure guarantees that the obtained continuous PDF is in agreement with the discrete distribution of the data points. The PDF contains all initially observed information about the cluster and it has a lot of noise as a consequence. To diminish the noise, $\hat{f}(cz)$ has to be smoothed.

Trying to utilize usual cubic splines for interpolation of the CDF, one encounters the problem that they will generally have negative derivative intervals if both first and second derivatives in the data points are put to be equal. Although there is an infinite amount of possibilities how to construct a smooth continuous spline that has non-smooth first derivative at data points.

We have found that tensioned cubic splines (hereafter TCS) nicely fit all spline histogram needs. They are defined such that the cubic polynomial spline length between two data points is minimal, and only the interpolating function and its first derivative are continuous in data points. Also in this case sometimes a derivative of the TCS is negative. Then in order to exclude a non-physical decreasing of the CDF estimate, we use non-tensioned splines increasing accordingly the spline length within these regions.

To reduce the statistical noise, the algorithm has been symmetrized. For the same purpose there was added a possibility to unite close points in the data set, that would otherwise give unphysical high PDF peaks. Nevertheless the resulting PDF is noisy and due to this the next step of the algorithm is a smoothing procedure.

In our case the noise is seen as narrow high peaks in the PDF arising from high CDF derivatives between close data points. The Savitzky-Golay filters [16] have been chosen for the smoothing remembering that PDF construction without any a priori knowledge about the system character was one of the main reasons for developing the spline histograms. These filters locally conserve first moments of the smoothed function. The remaining problem is to define the optimal width of the filter such that it reduces the noise but not over-smoothes the real PDF features.
This is done using the Integrated Square Error (ISE) function [20]:

\[
ISE(\hat{f}(cz)) = \int_{cz_{\min}}^{cz_{\max}} \left( \hat{f}(cz) - f(cz) \right)^2 d(cz),
\]

where \(f(cz)\) is a true PDF underlying the observed selection, and \(\hat{f}(cz)\) is a PDF estimated from the observed data, i.e. the smoothed spline histogram in our case. As we are using digital filters to smooth the data, this should be rewritten for case of discrete points. It follows from the theory [18], [9], [20] that quantity \(P(h)\) will have minimum for the same smoothing width \(h\) as \(ISE(\hat{f}(x))\):

\[
P(h) = \sum_{i=1}^{N} \left( \hat{f}(cz_i)^2 - 2\hat{f}(cz_i) + 2C_0^{(h)} \right),
\]

where \(C_0^{(h)}\) are the smoothing filter zeroth coefficients, and it was taken into account that \(\sum_{i=1}^{N} \hat{f}(cz_i) = N\). In contrary to the equation defining the ISE function, \(P(h)\) can be easily calculated from the data.

The filter width that gives the minimal \(P(h)\) value is the optimal one because the corresponding deviation between the true and estimated PDFs is also minimized. As a result the spline histogram is obtained but it says nothing about the remaining statistical noise level in it. To find it out we use a bootstrapping technique described in the next section.

3 Simulated data analysis

Simulated data are produced and analysed as follows. Using the obtained spline histogram as a true PDF, we generate the same amount \(N\) of random numbers. Then from this selection we compute another smoothed spline histogram. Repeating this sufficient number of times (say 100), one can calculate the average of the simulated spline histograms and its scattering. It is useful to characterize the scattering by the distribution quartiles. The upper quartile shows that the estimated PDF has 75% probability to be below it. For the lower quartile, accordingly, this probability is 25% (see Fig. 1).

To estimate the quality of the approximation, the first moments of several simulated distributions were computed and compared with the original values (see Table 1). It can be seen that the average values are the same within statistical error bars (1\(\sigma\)), whereas the standard deviations are about 10% larger than the original values because of the smoothing effect. For Gaussian distributions the asymmetry and excess are significantly different from zero, although in non-Gaussian cases they are rather close to original values.

Dependence of the smoothing size on the selection volume was also analysed. From theoretical considerations [18], [20], [15], we know that the optimal smoothing size depends on the selection volume \(N\) in the following way: \(h_{opt} \propto N^{-1/5}\). Analysing different volume random number selections for the same initial distribution, we have empirically found that for our algorithm \(h_{opt} \propto N^{-0.195}\), that shows an excellent agreement with the theoretical prediction.
Fig. 1. Result of the simulated distribution analysis. Original PDF is shown by the thick solid line, the thin solid line represents the average value of 100 smoothed spline histograms using 500 point selection each, and the lower and upper dashed lines are the first and third quartiles, respectively.

4 Galaxy cluster data analysis

As example we show the implementation of the algorithm on two clusters of galaxies – Abell 2256 and 3526.

Table 1. Moments of the initial distribution from simulations of the 500 point selection

|                         | General distribution | 2 equal dispersion Gaussians | 2 different dispersion Gaussians |
|-------------------------|----------------------|-------------------------------|----------------------------------|
|                         | Average | St.Dev. | Asymmetry | Excess  | Average | St.Dev. | Asymmetry | Excess  | Average | St.Dev. | Asymmetry | Excess  |
| General distribution    | 0.500   | 0.089   | 0.000     | -0.006  | 0.475   | 0.190   | 0.190     | -0.718  | 0.565   | 0.190   | -0.112     | -0.836  |
| Average from simulations | 0.499   | 0.093   | -0.486    | 2.287   | 0.474   | 0.192   | 0.153     | -0.676  | 0.564   | 0.192   | -0.165     | -0.704  |
| St.Dev. from simulations | 0.004   | 0.003   | 0.109     | 0.355   | 0.009   | 0.005   | 0.068     | 0.104   | 0.009   | 0.004   | 0.064      | 0.105   |
Abell 2256 is a rich regular cluster at \( z \approx 0.06 \) (\( \alpha \approx 17^h03.7^m, \delta \approx +78^\circ43' \), equinox 2000.0 [1]). It has similar properties to the Coma cluster (similar X-ray luminosities, both have optical and X-ray substructure and a radio halo), but is situated approximately 2.5 times farther.

A2256 has been previously studied in x-rays, optical and radio by several authors, e.g. [10], [6], [7]. It is accepted and understood, that Abell 2256, being one of the best studied clusters of galaxies, exhibit complex inner structure.

Result of the implementation of the TCSplin algorithm to the data of [10], consisting of 89 galaxy redshift measurements, is shown in Fig. 2. From the figure one can obviously see that the cluster is unrelaxed and has strongly non-Gaussian velocity PDF. Most likely it consists of two or more merging parts that currently are undergoing a final stage of unification.

Centaurus cluster A3526 (\( z \approx 0.011, \alpha \approx 12^h48.9^m, \delta \approx -41^\circ18' \), equinox 2000.0 [1]) has been extensively studied, as it is a nearby rich cluster of galaxies. It is intermediate between Coma and Virgo clusters in richness and in distance and has richness class 1 or 2 (e.g. [17]). Centaurus is irregular in appearance, like Virgo. The cluster core has two apparent centres of concentration, one being centred on NGC 4696 and the other being 0.5\(^\circ\) further east ([12], [3]).

Extensive study of this cluster is made in [8], [13] and [14]. The research included determination of redshifts for 259 galaxies and photometry for 329 galaxies within 13\(^\circ\) field centred on the cluster, and the following analysis of data. The bimodal galaxy velocity distribution and extensive substructure in both subclusters have been found. Mean heliocentric velocities and line-of-sight dispersions of two main cluster components, within 3\(^\circ\) of the cluster centre, are 3041 and 586 km sec\(^{-1}\) (denoted Cen30), and 4570 and 262 km sec\(^{-1}\) (denoted
Cen45), respectively. The projected distributions of members of each component overlap on the sky. Other small galaxy groups also have been found in this study.

Recently bimodality of the cluster has been confirmed in [19]. The authors used it to test a non-parametric method of the PDF estimation proposed by [11] and the same two main features of the cluster were noticed.

Our result of processing the data set of [8] is shown in Fig. 3. We find the same two main structures as in the original analysis. Clearness of these features demonstrates the quality of the algorithm. Shape of each of these components is close to Gaussian indicating their relatively relaxed state. Besides that the spline histogram shows additional left “shoulder” of the Cen30 group at around $cz \approx 2100 \text{ km sec}^{-1}$. This probably is one of separate groups noticed by [14]. Possibly this as well as those features around 6200 and 8300 km sec$^{-1}$ are not spatially real but just the redshift space caustics artefacts.

We see that a direct implementation of the algorithm leads to a good estimate of the PDF of clusters of galaxies. The only difference is the dispersions of the group velocities that are overestimated due to our PDF smoothing. One should keep that in mind and calculate the dispersion directly from the original data if needed.
5 Concluding remarks

This paper has demonstrated the usefulness of the spline histogram algorithm in statistical studies of 1D data sets. It has all advantages over the well known ordinary histogram approach estimating the probability density functions. In principle the spline histograms may be expanded to higher dimensional cases but that introduces higher effect of the sampling noise. Unfortunately enlargement of a data set size does not necessarily guarantee larger signal to noise ratio. More generally it is dependent on the distribution character.

The latest version of the spline histogram algorithm TCSplin code is freely available online from http://www.virac.lv/en/soft.html. Presently it is written in f77 with IDL and Gnuplot visualization scripts.

Acknowledgments. DD is grateful to the European Physical Society EWTF that has provided a travel grant and the LOC of Research centre of Astronomy of Academy of Athens for possibility to participate in the Workshop. DD and KB also thank Bernard Jones for the fruitful discussions. The work of KB was supported by grant No.01.0024.4.1 of the Latvian Council of Sciences.

References

1. G.O. Abell, H.G. Corwin, Jr, and R.P. Olowin: ApJSS, 70, 1 (1989)
2. K.A. Ashman, C.M. Bird, and S.E. Zepf: AJ, 108, 2348 (1994)
3. N.A. Bahcall: ApJ, 193, 529 (1973)
4. K. Berzins: in Generation of Cosmological Large-Scale Structure ed. by D.N. Schramm and P. Galeotti (Kluwer Academic Publishers, 1997) pp.283-288
5. K. Berzins: Substructure of clusters of galaxies: Methodology, Master Thesis, University of Copenhagen and University of Latvia, Copenhagen, Riga (1998), http://www.virac.lv/papers/kberzins_msc.tar.gz
6. U.G. Briel, et al.: A&A, 246, L10 (1991)
7. T.E. Clarke, and T.A. Ensslin: astro-ph/0106137 (2001)
8. R.J. Dickens, M.J. Currie and J.R. Lucey, MNRAS 220, 679 (1986)
9. D. Docenko: Spline histograms and their application to analysis of clusters of galaxies (in Latvian), Master Thesis, University of Latvia, Riga (2002), http://www.virac.lv/papers/ddocenko_msc.pdf
10. D.G. Fabricant, S.M. Kent, and M.J. Kurtz: ApJ, 336, 77 (1989)
11. D. Fadda, E. Slezak, and A. Bijaoui: A&ASS 127, 335 (1998), astro-ph/9704096
12. A.R. Klemola: AJ, 74, 804 (1969)
13. J.R. Lucey, M.J. Currie and R.J. Dickens: MNRAS, 221, 453 (1986)
14. J.R. Lucey, M.J. Currie and R.J. Dickens: MNRAS, 222, 427 (1986)
15. A. Pisani: MNRAS 265, 706 (1993)
16. W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P. Flannery: Numerical Recipes in FORTRAN, Cambridge University Press, Cambridge (1992)
17. A. Sandage: ApJ, 183, 731 (1973)
18. B.W. Silverman: Density Estimation for Statistics and Data Analysis, Chapman & Hall, London (1986)
19. P. Stein, H. Jerjen, and M. Federspiel: A&A 327, 952 (1997), astro-ph/9707211
20. R. Vio, G. Fasano, M. Lazzarin, and O. Lessi: A&A, 289, 640 (1994)
21. J. Vondrak: Bulletin of Astronomical Institute of Czechoslovakia, 20, 349 (1969)