


Display of probability densities for data from a continuous distribution

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Based on cumulative distribution functions, Fourier series expansion and Kolmogorov tests, we present a simple method to display probability densities for data drawn from a continuous distribution. It is often more efficient than using histograms.

Keywords: Display of data, Histograms, Probability densities

1. Introduction

We address the simple problem of displaying an empirical probability density (PD) $f(x)$ from data for a *continuous* variable x . Commonly this is done using histograms. This is appropriate when x is discrete, because there is then a natural scale. But in case of a continuous variable x , one is faced with choosing binsizes. This is a frustrated problem: One would like to keep the binsize small for a high resolution, but big to suppress statistical fluctuations. Here we present a method [1] to by-pass the problem. It is based on the cumulative distribution function (CDF)

$$F(x) = \int_{-\infty}^x dx' f(x'). \quad (1)$$

Given a time series of n real numbers (data), a parameter free empirical estimate (ECDF), is well-known: The step function $\bar{F}(x)$ defined by increasing by $1/n$ at each data point. This does not help directly in getting an estimate of the probability density, because the derivative is a sum of Dirac delta functions.

One needs some kind of interpolation of the CDF. This is no fun, as one has to decide whether the interpolation of 2, 3, 4, or k points will work best. In contrast, plotting a histogram is simple and robust, but not a smooth function. Our way out relies on *Fourier expansion* of the ECDF $\bar{F}(x)$. This leads to the desired smooth approximation as long as the expansion is sufficiently short, but will imitate every wiggle of the data, when carried too far. Therefore, one needs a cut-off criterion. We base this on the *Kolmogorov test*, which tells us whether the difference between the ECDF and an analytical approximation of the CDF is explained by chance. *Fortran code* for our procedure [1] is available from the CPC Library.

2. (Peaked) Cumulative Distribution Functions

Assume we generate n random numbers x_1, \dots, x_n . We re-arrange the x_i in increasing order (π_1, \dots, π_n a permutation of $1, \dots, n$):

$$x_{\pi_1} \leq x_{\pi_2} \leq \dots \leq x_{\pi_n} \quad (2)$$

An estimator for the distribution function $F(x)$ is the ECDF

$$\bar{F}(x) = \frac{i}{n} \quad \text{for } x_{\pi_i} \leq x < x_{\pi_{i+1}}, \quad i = 0, 1, \dots, n-1, n, \quad (3)$$

and by definition $x_{\pi_0} = -\infty$, $x_{\pi_n} = +\infty$. Fig. 1 shows an ECDF from 100 Gaussian distributed random numbers generated for the probability density

$$g(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \quad (4)$$

together with the exact CDF. The CDF is in this case determined by the error function:

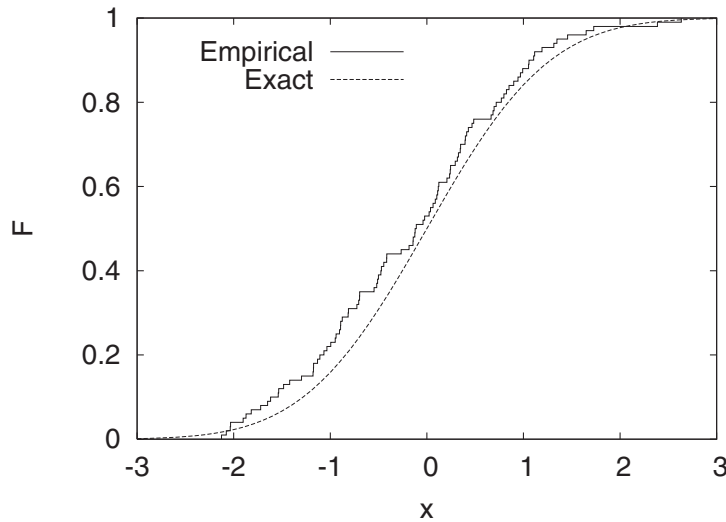


Figure 1: ECDF from 100 Gaussian distributed random numbers together with the exact CDF.

$$G(x) = \int_{-\infty}^x dx' g(x') = \frac{1}{2} + \frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{2}}\right). \quad (5)$$

The probability density of events is encoded in the slope of the ECDF. This makes it often difficult to read off high probability regions and, in particular, the median. This can be improved by switching to the peaked CDF [2]:

$$F_p(x) = \left\{ \begin{array}{l} F(x) \text{ for } F(x) \leq \frac{1}{2} \\ 1 - F(x) \text{ for } F(x) > \frac{1}{2} \end{array} \right. \quad (6)$$

By construction the maximum of the peaked CDF is at the median $x_{\frac{1}{2}}$ and $F_p(x_{1/2}) = 1/2$. Therefore, $F_p(x)$ has two advantages: The median is clearly exhibited and the accuracy of the ordinate is doubled. It looks a bit like a PD, but is in essence still the integrated PD. An example from 10,000 Gaussian random numbers is shown in Fig. 2.

3. Kolmogorov Test

Do empirical and exact CDFs of our two figures agree? The Kolmogorov test answers this question (for a review see [2]). It returns the *probability Q, that the difference between the analytical CDF and an ECDF from statistically independent data is due to chance*. If the analytical CDF is known and the data are sampled from this distribution, Q is a uniformly distributed random variable in the range $0 < Q < 1$. Turned around, if one is not sure about the exact CDF, or the data, or both, and Q is small (say, $Q < 10^{-6}$) one concludes that the difference between the proposed CDF

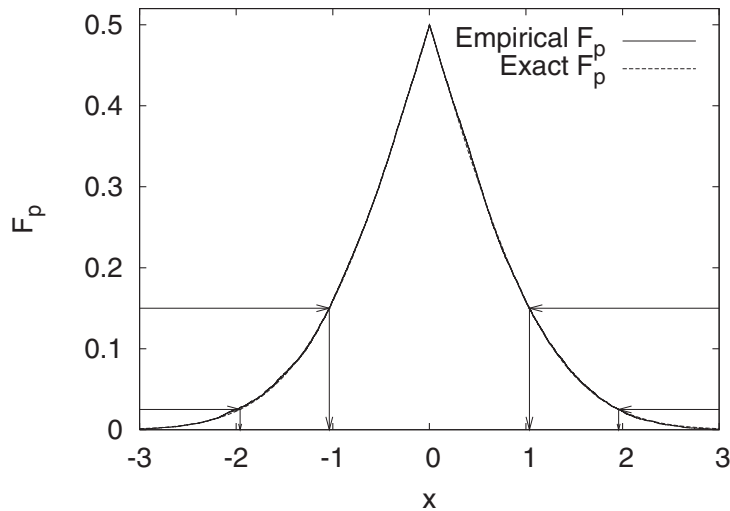


Figure 2: Peaked ECDF from the 10,000 Gaussian random numbers versus exact Gaussian peaked CDF. The arrows indicate 70% and 95% confidence intervals.

and the data is presumably not due to chance. Kolmogorov’s ingenious test relies just on the maximum difference between the ECDF and the CDF:

$$\Delta = \max_x |F(x) - \bar{F}(x)| . \tag{7}$$

The test yields, respectively, $Q = 0.19$ and $Q = 0.78$ for the samples used in Fig. 1 and 2. Both values signal consistency between CDF and data.

4. Probability Densities

Our method [1] to construct an empirical probability density (EPD) from an ECDF consists of two steps:

1. Define as an initial approximation to $\bar{F}(x)$ a differentiable, monotonically increasing function $F_0(x)$.
2. Fourier expand the remainder until the Kolmogorov test yields $Q \geq Q_{\text{cut}} = 1/2$ (there may be some flexibility in lowering Q_{cut}).

For $F_0(x)$ we require

$$F_0(x) = 0 \text{ for } x \leq a \text{ and } 1 \text{ for } x \geq b , \tag{8}$$

where $[a, b]$ has to lie within the range of the data. For PDs with support on a compact interval, or with fast fall-off like for a Gaussian distribution, the natural choice is $a = x_{\pi_1}$ and $b = x_{\pi_n}$. In case of slow fall-off, like for a Cauchy distribution, or other distributions with outliers, one has to restrict the analysis to $[a, b]$ regions, which are well populated by data.

We denote the ECDF of the range $[a, b]$ by $\bar{F}_{ab}(x)$. As for $F_0(x)$, by construction $\bar{F}_{ab}(x) = 0$ for $x \leq a$ and 1 for $x \geq b$. Our aim is to construct a PD estimator $\bar{f}_{ab}(x)$ from $\bar{F}_{ab}(x)$. In the following we restrict our choice of $F_0(x)$ to the straight line,

$$F_0(x) = \frac{x - a}{b - a} \text{ for } a \leq x \leq b , \tag{9}$$

which keeps the approach simple. More elaborate definitions will likely give improvements in a number of situations, but may discourage applications. Once $F_0(x)$ is defined, the remainder of the ECDF is given by

$$R(x) = \bar{F}_{ab}(x) - F_0(x) . \tag{10}$$

We expand $R(x)$ into the Fourier series

$$R(x) = \sum_{i=1}^m d(i) \sin\left(\frac{i\pi(x-a)}{b-a}\right). \quad (11)$$

The cosine terms are not present due to the boundary conditions $R(a) = R(b) = 0$. The Fourier coefficients follow from

$$d(i) = \sqrt{\frac{2}{b-a}} \int_a^b dx R(x) \sin\left(\frac{i\pi(x-a)}{b-a}\right) \quad (12)$$

In our case $R(x)$ is the difference of a step function and a linear function. The integrals over the flat regions of the step function are easily calculated, and the $d(i)$ obtained by adding them up.

The Fourier expansion is useless for too large values of m , because it will then reproduce all statistical fluctuations of the data. To get around this problem, we perform the Kolmogorov test first between $\bar{F}_{ab}(x)$ and $F_0(x)$ ($m = 0$), and then each time m is incremented from $m \rightarrow m + 1$. Once $Q \geq Q_{\text{cut}} = 1/2$ is reached, we know that the information left in the data is statistical noise and the expansion is terminated. The thus obtained smooth estimate of the CDF,

$$F_{\text{estimate}}(x) = F_0(x) + R(x), \quad (13)$$

yields $\bar{f}_{ab}(x)$ by differentiation.

We attach *error bars* to the estimate of the PD by dividing the (unsorted) original data into *jackknife* blocks and repeat the analysis for each block. Comparing the thus obtained function values, error bars follow in the usual jackknife way. An example for the Gaussian distribution follows. See [1] for more examples: The Cauchy distribution and autocorrelated data from U(1) lattice gauge theory. The histogram for the Gaussian distribution is shown in Fig. 3

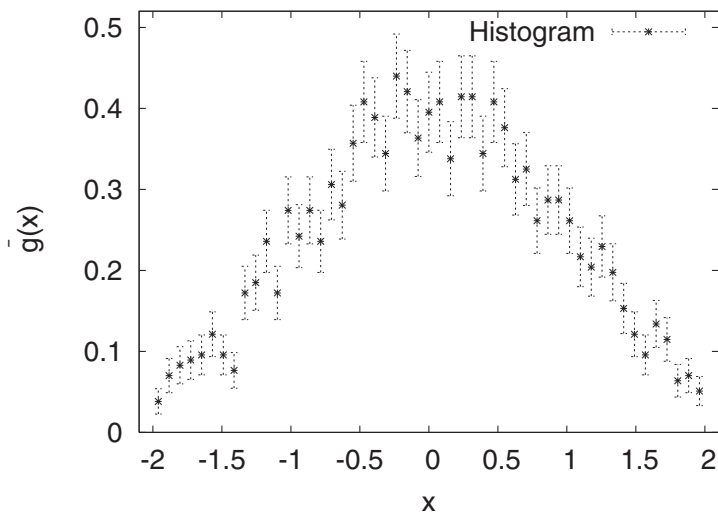


Figure 3: Histogram of 51 bins for 2000 random numbers generated according to the Gaussian distribution.

(the error bars follow from the variance $p(1-p)$ of the bimodal distribution with $p = h(i)/n$). Fig. 4 gives our estimate $\bar{g}(x)$ of the PD obtained from the same data with the described method. We used $a = x_{\pi_1}$ and $b = x_{\pi_n}$. $Q = 0.97$ was reached with $m = 4$ ($Q = 0.056$ with $m = 3$). Twenty jackknife blocks were used to calculate the error bars.

5. Summary and Conclusions

Based on Fourier expansion and Kolmogorov tests, we introduced a method for constructing continuous probability density functions from data. We did not develop a statistically rigorous approach. We address physicists and others, who do not hesitate to use whatever works.

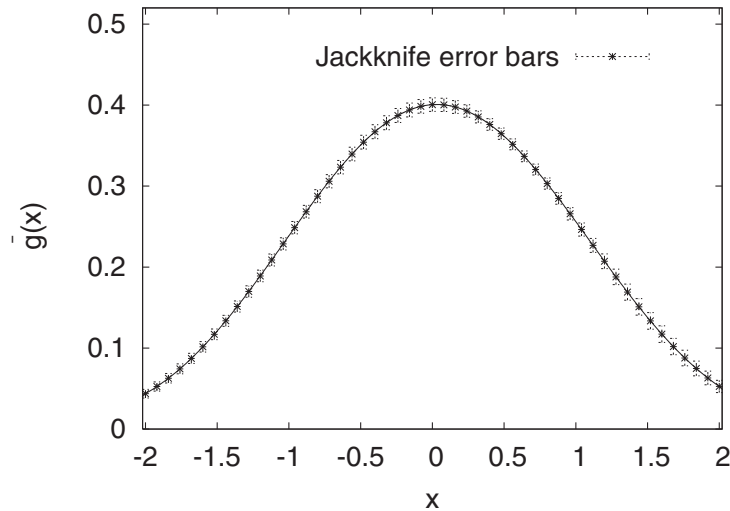


Figure 4: Estimate $\bar{g}(x)$ for the data of the previous figure.

Our results were obtained with a straight line as initial approximation for the CDF. There is certainly space for improvement at the price of giving up some of the simplicity. With our $Q_{\text{cut}} = 1/2$ rule, we are slightly overexpanding the Fourier expansion. In the average Q should be $1/2$, but all our values are $Q \geq 1/2$. That gives some flexibility to lower Q_{cut} when the m of the Fourier expansion appears to be too large.

There are many open questions. Given the initial approximation, we construct a smooth Fourier expansion of the remainder, that is consistent with the data, using the ordering in which the long wave lengths modes come first. Obviously, the result of this procedure is not the only analytical function, which is consistent with the data. Which ordering of the serious expansion or other complete function system gives the smoothest approximation (smallest number of terms) consistent with the data? Do systems of monotonically increasing functions exist, which are complete for the expansion of monotonically increasing functions?

Kernel density estimates [3, 4] are in spirit similar (but by no means identical) to our method. A comparison remains to be carried out.

Acknowledgments

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- [1] B.A. Berg and R. Harris, *Comp. Phys. Commun.* 179 (2008) 443-448.
- [2] B.A. Berg, *Markov Chain Monte Carlo Simulations and Their Statistical Analysis*, World Scientific, 2004.
- [3] P.K. Janert, *Gnuplot in Action: Understanding Data with Graphs*, Manning Publications, 2009. See section 13.2.2.
- [4] More references can be found in Wikipedia under *Kernel density estimation*. The *Earth mover's distance* might be of interest as a replacement of the Kolmogorov test, if one likes to attempt a generalization of the method to more than one dimension.