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On the Lorentzian shape and the information provided by an experimental plot

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Abstract. The shape of an experimental curve is considered in the scheme of information theory. The present approach gives an explanation for the Lorentzian shape which is very commonly observed for physical systems.

1. Introduction

The aim of this paper is to show how the Lorentzian shape of an experimental curve, so frequently encountered in the analysis of line spectra, can be derived in the scheme of information theory. Information theory was developed by Shannon and Wiener (Shannon 1948, Wiener 1948) who introduced the expression:

$$U_S(P) = -\sum p_n \ln p_n \tag{1}$$

as a measure of the uncertainty, or missing information, relative to the probability distribution $P(p_1, p_2, \ldots, p_m)$. One can obtain some important probability distributions from the maximum-entropy principle (Shannon 1948, Jaynes 1957a, b), i.e. by choosing as the most probable, among all the distributions which satisfy some given constraints, the one which maximizes (1). For example, we obtain the equal probability distribution by requiring the norm to be fixed, the geometric distribution if the norm and the first moment are fixed, and the Gaussian distribution if the second moment is also supposed to be known. A similar derivation for the Poisson distribution has been obtained by Ingarden and Kossakowsky (1970) who have considered, instead of the usual Shannon information measure (1), a special case of the generalized information defined by one of the authors (Kossakowsky 1968):

$$U_K(P) = -\sum p_n \ln (p_n/w_n) \tag{2}$$

which looks like a generalization of the Kullback relative information measure (Kullback 1959). In expression (2) the quantity w_n is a 'weight' given to the nth elementary event. The Poisson distribution has been obtained as the one which maximizes (2) requiring Σp_n and Σnp_n be fixed, and assuming $w_n = 1/n!$. Powles and Carazza (1970b), who were primarily interested in the analysis of the NMR lineshape, considered a spectral line $f(\omega)$ as a distribution of many indistinguishable contributions. As in statistical mechanics, they grouped the contributions to the spectra line in ranges k with

n_k contributions at or near ω_k with 'degeneracy' g_k, considering the resulting number of configurations:

$$W_{\text{E-B}} = \prod_k \frac{(n_k + g_k - 1)!}{n_k!(g_k - 1)!}. \tag{3}$$

Then, maximizing the quantity ln $W_{\text{E-B}}$ (which was considered the suitable definition of the missing information for a probability distribution of indistinguishable objects), and requiring the total intensity and the second moment of $f(\omega)$ be fixed, they obtained for the most probable lineshape:

$$n_k = \frac{g_k}{\exp(\beta + \lambda\omega_k^2) - 1} \tag{4}$$

i.e.

$$f(\omega) = \frac{A}{\exp(\beta + \lambda\omega^2) - 1}. \tag{5}$$

The maximization of Shannon's uncertainty, or of a suitable expression, thus leads (depending on the constraints which are imposed) to some typical shapes which are very commonly observed. We note, however, that the results we have summarized before can be applied to the information theory analysis of an experimental curve only when it can be considered a distribution of some events or physical objects. As this is not always the case, we wish to consider an experimental curve from the point of view of information theory, without considering it as a distribution of some event or object.

2. The information provided by an experimental plot

Let us consider the plot $y_n = y_n(x_n)$ of some continuous and positive quantity y, which is subject to experimental error, for the $2m+1$ values of $x_n = n\epsilon$ $(n = 0, \pm 1, \pm 2, \ldots \pm m)$ of the variable x. Let us recall that we are not interested in those experimental curves one can consider as distributions of events or physical entities. We will assume the point of view of a person who is looking at the plot with no knowledge either of the system the plot refers to, or of what y and x means. A person in this situation can ask himself what information is provided by the plot as to the relationship between y and x. For any value x_n, the dependent variable is not known exactly, but can in principle assume all the possible values around the plotted value y_n within the experimental error $\pm\Delta_n$. We thus assume that any value ξ_n in the range $y_n \pm \Delta_n$ is equally probable '*a priori*', each probability distribution $\rho_n(\xi_n)$ being, moreover, independent of the others. So we can associate with the plot a distribution:

$$\rho(\xi_{-m}, \xi_{-m+1}, \ldots, \xi_m) = \prod_{n=-m}^{m} \rho_n(\xi_n) \tag{6}$$

where $\rho_n(\xi_n)$ is equal to $1/2\Delta_n$ for ξ_n varying in the range $y_n - \Delta_n \leqslant \xi_n \leqslant y_n + \Delta_n$. There is of course a lack of knowledge of the exact relationship between y and x, for the $y_n(x_n)$ are only known within the experimental error range. We propose to assume, as a measure of this lack of knowledge, the Shannon missing information $U_S(\rho)$ relative to the distribution (6). Using the missing information measure for a continuous many-dimensional distribution (Shannon 1948), we have:

$$U_S(\rho) = -\int_{y_{-m}-\Delta_{-m}}^{y_{-m}+\Delta_{-m}} \dots \int_{y_m-\Delta_m}^{y_m+\Delta_m} \rho \ln \rho \, d\xi_{-m} \dots d\xi_m \tag{7}$$

i.e., by our assumption concerning the distribution $\rho(\xi_{-m}, \dots, \xi_m)$:

$$U_S(\rho) = \sum_{n=-m}^{m} \ln 2\Delta_n. \tag{8}$$

Let us now specify the dependence of Δ_n on y_n. If the percentage error is constant, one has ($\beta < 1$)

$$\Delta_n = \beta y_n \tag{9}$$

and thus, apart from additive constants:

$$H = \sum_{n=-m}^{m} \ln y_n \tag{10}$$

is the uncertainty, or missing information, relative to the experimental plot.

3. The Lorentzian shape

Supposing now that Σy_n and $\Sigma y_n x_n^2$ have a fixed value, let us look for the values $\bar{y}_n$ which maximize H, subject to the constraints above. It can be done by means of Lagrange multipliers, maximizing:

$$I = H + \lambda \sum_n y_n + \mu \sum_n y_n x_n^2. \tag{11}$$

The condition for this is:

$$\delta I = \sum_n \left(\frac{1}{y_n} + \lambda + \mu x_n^2\right) \delta y_n = 0 \tag{12}$$

for any variation δy_n of the y_n, and consequently:

$$\bar{y}_n = \frac{a}{b + x_n^2} \tag{13}$$

where $a = -1/\mu$ and $b = \lambda/\mu$ have to be chosen so that the constraints are satisfied. We note that the values for Σy_n and $\Sigma y_n x_n^2$ cannot be fixed without limitations, if we want the $\bar{y}_n$ to be real and positive. The second variation $\delta^2 I$ of (11):

$$\delta^2 I = -\sum_n \frac{1}{\bar{y}_n^2} (\delta y_n)^2 \tag{14}$$

is evidently negative when the $\bar{y}_n$ are real, so the truncated Lorentzian shape (13) is indeed the one which maximizes H under the assumed constraints. The extension of the result for the case of continuous values of x is straightforward. We observe, moreover, that if only Σy_n is supposed to be known, by maximizing H we obtain the result that the y_n are all equal to a constant. The assumption that Δ_n is proportional to some power of y_n leads to the same results.

4. Conclusions

This simple result is of interest for physical systems. It is often the case that the total intensity and the second moment of an experimental curve are known (sum rules). Then the usual information theory approach gives a Gaussian shape (Jaynes 1957a, b, Powles and Carazza 1970a). The present approach gives an explanation for the Lorentzian shape which is very commonly observed for physical systems.

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