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ANALYSIS OF AN OBSERVED FUNCTION INTO COMPONENTS, USING ITS SECOND DERIVATIVE

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A method is described which uses the second derivative to estimate the parameters of components of an observed function. The method is programmed for a computer and the results can be used either directly, giving a rough description of the function, or they may be taken as an initial estimate for a least-squares fit. The method has been applied to the analysis of 21-cm profiles into Gaussian components.

1. Introduction

Several authors (see e.g. LINDBLAD 1967; TAKAKUBO and VAN WOERDEN, 1966; TAKAKUBO 1967; VAN WOERDEN, 1967) have shown that the decomposition of 21-cm profiles into Gaussian components can be a powerful method in the study of the kinematics of neutral hydrogen. This decomposition, however, encounters some difficulties in that (i) the computer analysis starts from an initial estimate which has so far been made by hand and (ii) its intrinsic ambiguity requires a careful judging of the results (see KAPER *et al.*, 1966, section 5). Both difficulties tend to make the decomposition very time consuming, even when one neglects the time actually needed on the computer.

The method to be described here allows automation of the initial estimates, which removes difficulty (i). Besides, the results of the method can be used directly in a discussion of observations, if one is only interested in the main features of the profiles.

The method can be summarized by the flow-diagram in figure 1. The observed profile is represented by intensities, y_k, expressed as a function of the independent variable, x, at equal intervals $\Delta x \equiv h$. A second-order polynomial is fitted at each x_k by the method of least squares, using q_i points distributed symmetrically around x_k. The coefficient of the second-order term is an approximation of the second derivative of the observed profile. Assuming that the observed profile can be approximated by the sum of a few Gaussian functions:

$$f(x_k) = P \exp\left[-(x_k - X)^2/2\sigma^2\right], \qquad (1.1)$$

the parameters X, σ are calculated from the main minima of the second derivative, whereas the P are estimated from the observed profile. Tests using different threshold values, make it possible to discriminate against spurious components; the threshold values depend, among other things, on q_i and on the r.m.s. noise of the observed profile. The Gaussian components are then subtracted from the observed profile, and the residual profile, mainly the sum of a few remaining broader components, is handled in the same way as the original. The method is, therefore, applied in iteration, always using a larger number of points for the next least-squares fit of a polynomial, in order to reduce the statistical fluctuations of the second derivative. An example is shown in figure 3.

This method could also be easily used for functions $f(x)$ other than Gaussians.

The method reveals the main features of a profile even if it has a complex structure with various components of different dispersions. The method does not claim to be effective in detecting weak components; these must be found by other techniques. A possible procedure would be to improve the fit of the estimated set of components by means of a least-squares analysis and to estimate the additional components on the basis of the distribution of the residuals; the quantity, K_s, proposed by KAPER *et al.* (1966, section 5) could serve as an indicator.

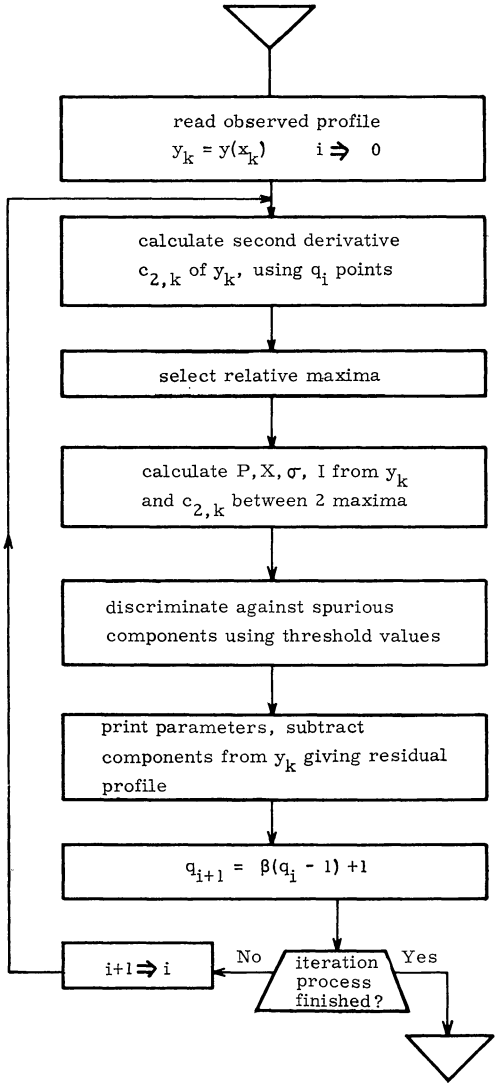

Figure 1. Schematic flow-diagram. For details of the procedure, see sections 1 and 2.

2. Description of the method

2.1. *Calculation of the second derivative*

For each x_k a second-order polynomial

$$e_k(x) = c_{0,k} + c_{1,k}(x - x_k) + \tfrac{1}{2}c_{2,k}(x - x_k)^2 \quad (2.1)$$

is fitted to the observed profile, according to the method of least squares. For this fitting process q_i points are used, distributed symmetrically around x_k, and all receiving equal weight. One then finds that

$$c_{2,k} = -Ah^{-2} \sum_{\lambda} [y_\lambda (1 - B\lambda^2)], \quad (2.2)$$

with the summation extending from $\lambda = k - (q_i - 1)/2$ to $k + (q_i - 1)/2$, and

$$A = 30/[q_i(q_i^2 - 4)],$$
$$B = 12/(q_i^2 - 1).$$

2.2. *Reconstruction of the parameters, X, σ from the second derivative*

A Gaussian function f of the form (1.1) has a second derivative f'' which is shown in figure 2. The points a

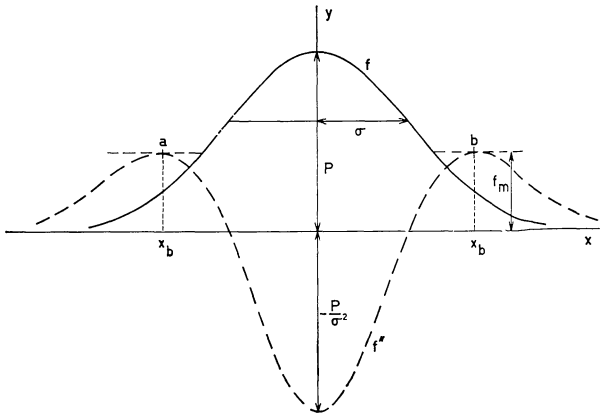

Figure 2. Gaussian function (full line) and its second derivative (dashed line). Arbitrary scale.

and b are the maxima of f'' at $x = X \pm \sigma\sqrt{3}$. The ratio of the ordinate of the minimum to the ordinate f_m of the maxima is $-\frac{1}{2}e^{\frac{3}{2}} = -2.241$. The depth of the minimum is P/σ^2.

If several Gaussians are superimposed, then the second derivatives are also superimposed. In general, the narrow components will give rise to the most pronounced minima; these may be superimposed on the second derivatives of several broad components, thereby being lifted or lowered. Therefore, if one wishes to calculate σ from the depth and width of the minima, it is best to consider the minima only with respect to the neighbouring maxima. The two integrals

$$M_0 = \int_{x_a}^{x_b} (f'' - f_m)\,dx = -2.32\frac{P}{\sigma}$$
$$M_1 = \int_{x_a}^{x_b} (f'' - f_m)x\,dx \quad (2.3)$$

give

$$X = M_1/M_0. \quad (2.4)$$

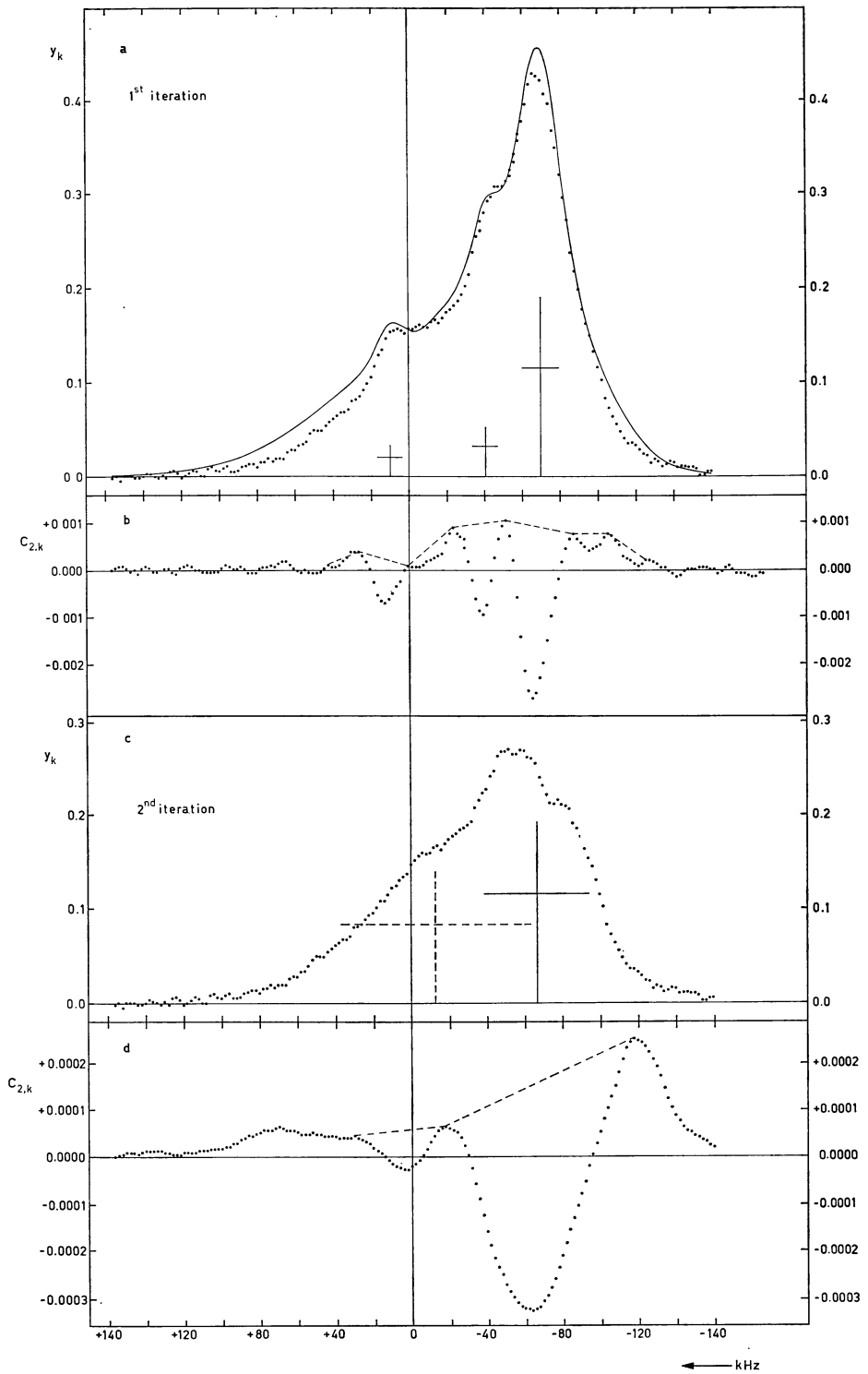

Figure 3. Example of an analysis. The observed function is a 21-cm line profile of neutral hydrogen in the Orion region; the ordinates are optical depths. Two iterations ($i = 1, 2$) are illustrated, in figures 3a, 3b and 3c, 3d respectively. For each, y_k (dots in a and c) and the second derivative ($c_{2,k}$; dots in b and d) are given. The dashed lines in b and d link consecutive relative maxima of $c_{2,k}$, cf. section 2.3. From the original function, plotted in a, three estimated components (drawn as crosses) are subtracted, resulting in c. From this a broader component is estimated.

The first run ($i = 0$) gave no component. This is exceptional; it is due to the fact that the bandwidth of observations was quite small compared to the width of profile details. The last one ($i = 3$) gave a component which is represented in d by a dashed cross. The superposition of all five components is represented in a by a full line.

And using the second moment

$$M_2 = \int_{x_a}^{x_b} (f''-f_m)(x-X)^2\,dx = -0.81\,P\sigma, \quad (2.5)$$

one finds:

$$\sigma = 1.69\,(M_2/M_0)^{\frac{1}{2}}. \quad (2.6)$$

P, too, could be deduced from M_0 and M_2; however, to minimize the effects of statistical fluctuations, it is preferable to derive P from the observed profile as described in the following paragraph.

2.3. *Analysis of the second-order curve*

The coefficients $c_{2,k}$ of the second-order term of the polynomial [eq. (2.1)], which are an approximation to the second derivative of the observed function, are analyzed as follows. Each point with

$$c_{2,k-1} < c_{2,k} > c_{2,k+1} \quad \text{and} \quad c_{2,k} > 0 \quad (2.7)$$

is considered as a relative maximum of $c_{2,k}$. Through adjacent relative maxima straight lines are drawn and $c'_{2,k}$ calculated, that is the difference between the $c_{2,k}$ and the straight lines (see figure 3). Then the function $c'_{2,k}$ is treated separately in each interval between two maxima. The $c'_{2,k}$ are considered as approximations of the terms $(f''-f_m)$ in eqs. (2.3) and (2.5). The integrals M_0, M_1, M_2 are calculated with the integration being approximated by summation. From these integrals X and σ are derived according to eqs. (2.4) and (2.6).

P is estimated from the observed profile*. The relation

$$y(X)-y(X \pm \sigma\sqrt{3}) = P\{1-\exp(-3\sigma^2/2\sigma^2)\} \quad (2.8a)$$

is approximated by

$$P = \{y_c-\tfrac{1}{2}(y_{c+t}+y_{c-t})\}/\{1-\exp(-t^2h^2/2\sigma^2)\} \quad (2.8b)$$

where c is the index of the point x_k closest to X, and t the integer closest to $\sigma\sqrt{3}/h$. If $P > y_c$, one assumes that $P = y_c$.

In order to discriminate against spurious or highly uncertain components, a series of tests is applied using the following threshold values: M_{0m}, I_m, σ_{min}, σ_{max} and M_{0m}^-. Only those components are used which fulfil the following criteria:

(i) $|M_0| > M_{0m}$,

(ii) $I(\equiv P\sigma\sqrt{2\pi}) > I_m$,

(iii) $\sigma_{min} < \sigma < \sigma_{max}$,

(iv) $|M_0^-| > M_{0m}^-$, with M_0^- equal to the integral of the $c_{2,k} < 0$.

The threshold values may depend on q_i, β and on the r.m.s. fluctuations of the observed intensities, y_k. For a discussion of the purpose of these tests and for a suitable choice of the threshold values see section 3.2.

2.4. *Correction against smoothing*

In general the σ derived from the $c_{2,k}$ are overestimated, depending on $(q_i-1)h$, as if the profile had been smoothed. This effect has been studied numerically by applying the method with different q_i to Gaussians of different dispersions. It turns out that the important parameter is

$$s \equiv (q_i-1)h/\sigma_0, \quad (2.9)$$

where σ_0 is the true dispersion of the Gaussian. In figure 4 σ/σ_0 is plotted against s. The deviations from the horizontal $\sigma/\sigma_0 = 1$ are small in the range of s from 0 to 4; from the straight line drawn through the points the following correction formula is deduced:

$$\sigma_{corr} = \sigma[1-0.05(q_i-1)h/\sigma]. \quad (2.10)$$

In the range $s > 4$, $\sigma/\sigma_0 = 0.3s = 0.3(q_i-1)h/\sigma_0$ or, in other words, σ is independent of σ_0. The smallest

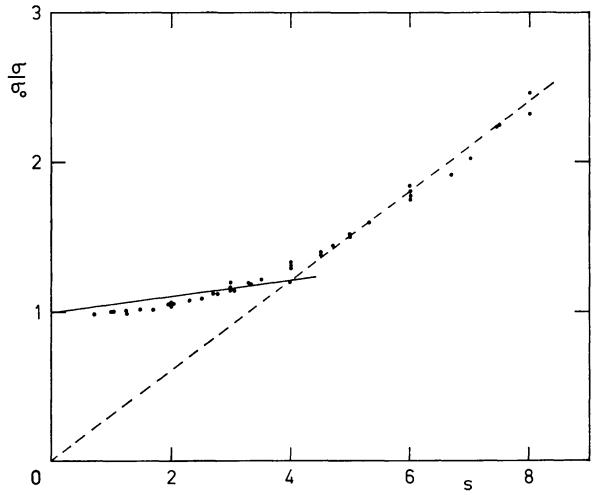

Figure 4. Effect of "smoothing", see section 2.4. σ_0 is the true, σ the estimated dispersion; s is defined by eq. (2.9). Dots show the results of numerical calculations; the full line [eq. (2.10)] is used to correct estimated dispersions.

* The use of a smoothed version of the observed profile y_k, namely $c_{0,k}$ [eq. (2.1)], gave less satisfactory results.

true dispersion which gives a meaningful result is therefore (from $s = 4$):

$$\sigma_{\min} = (q_i - 1)h/4. \tag{2.11}$$

Components with true dispersions smaller than this receive the constant estimate $\sigma_{\text{corr}} \approx \sigma_{\min}$.

2.5. *Iterations*

As mentioned in section 1, the narrowest components are picked out first. After subtracting these components, the same method is applied again to the remaining profile, but now using $q_{i+1} = \beta(q_i - 1) + 1$ points to calculate $c_{2,k}$; a suitable choice of the parameter β is discussed in section 3.2. At the same time the threshold values are altered according to eqs. (3.4) to (3.8). The iteration process may be stopped if the number of points used to derive $c_{2,k}$ surpasses, say, half the number of observed points, or if $\sigma_{\max}$ exceeds a given upper limit of the dispersions to be expected in the profile.

The calculations can be simplified by replacing $h\ (= \Delta x)$ by $\beta \cdot h$ in successive iterations.

3. Error estimates

3.1. *The statistical errors of the estimated component parameters*

It is obvious that in cases where components are close together, systematic errors will occur which may be considerably greater than the statistical errors. On the other hand, if components are well separated, the errors are statistical in nature and determine the size of the weakest components detectable with this method.

Theoretical estimates of the errors of X and I lead to the following results:

$$\begin{aligned} \mu^2(X)/\sigma^2 &\approx 50(q_i - 1)^{-3.5}(\sigma/h)^3\,(\mu/P)^2, \\ \mu^2(I)/I^2 &\approx [2 + 200(q_i - 1)^{-3.5}(\sigma/h)^3]\,(\mu/P)^2, \end{aligned} \tag{3.1}$$

where μ is the r.m.s. deviation of an observational point y_k. The method is more sensitive to narrow components than to broad ones. The smallest errors are attained for those components which have an estimated dispersion $\sigma_{\min}$ [eq. (2.10)]. Using eq. (2.11) one finds then:

$$\begin{aligned} (\mu^2(X)/\sigma^2)_{\min} &\approx 0.4(\sigma_{\min}/h)^{-0.5}\,(\mu/P)^2, \\ (\mu^2(I)/I^2)_{\min} &\approx [2 + 1.6(\sigma_{\min}/h)^{-0.5}]\,(\mu/P)^2. \end{aligned} \tag{3.2}$$

These theoretical estimates of the errors have been roughly checked by means of Monte Carlo calculations ($n = 50$).

The errors found from eqs. (3.1) and (3.2) may be compared with the mean errors attainable in Gaussian analysis by least-square methods [KAPER *et al.* (1966), eqs. (5.8) and (5.9)]:

$$\begin{aligned} (\mu^2(X)/\sigma^2)_{\text{l.sq.}} &= 1.1(\sigma/h)^{-1}\,(\mu/P)^2, \\ (\mu^2(I)/I^2)_{\text{l.sq.}} &= 0.84(\sigma/h)^{-1}\,(\mu/P)^2. \end{aligned} \tag{3.3}$$

As the comparison shows, the minimum error attainable in X [eq. (3.2)] is of the same order as in the least-squares fit. The mean relative error for I, on the other hand, is considerably larger than in the least-squares method.

3.2. *The threshold values*

a) $\sigma_{\max}$ and $\sigma_{\min}$

$\sigma_{\max}$ discriminates against too large dispersions and is related to β in the following way. If in successive iterations q_i, respectively $\beta(q_i - 1) + 1$ points, are used to calculate $c_{2,k}$, then the minimum dispersions [eq. (2.11)] are: $(q_i - 1)h/4$, resp. $\beta(q_i - 1)h/4$. In order to cover the whole range in σ, $\sigma_{\max}$ must be chosen so that

$$\sigma_{\max} = \beta\sigma_{\min} = \beta(q_i - 1)h/4. \tag{3.4}$$

Occasionally the dispersion of a component is estimated larger than $\sigma_{\max}$ in one iteration and smaller than $\sigma_{\min}$ in the next. To avoid rejection of a component in a situation like this, the test $\sigma > \sigma_{\min}$ is done only for components for which $I < 5I_{\text{m}}$. In the last iteration the test $\sigma < \sigma_{\max}$ is dropped.

b) I_{m}

This is the minimum of the area $I \equiv P\sigma\sqrt{2\pi}$; its relation to q_i and to the r.m.s. fluctuation of y_k is derived by using eq. (3.1), which gives the mean error of I. Define a quantity $I_T(\sigma)$, which is the value of I of a component for which the relative error $\mu(I)/I$ equals T. Putting the left-hand side of the second one of eqs. (3.1) equal to T^2, introducing $\sigma_{\min}$ [eq. (2.11)], and solving for I, one finds

$$I_T(\sigma) = 2\sqrt{\pi}\,\mu\sigma T^{-1}[1 + 1.6(q_i - 1)^{-\frac{1}{2}}(\sigma/\sigma_{\min})^3]^{\frac{1}{2}}. \tag{3.5}$$

I_{m} could be made equal to $I_T(\sigma)$; but then components with σ slightly greater than $\sigma_{\min}$ (of each iteration) would be in a favourable position. To avoid this, I_{m} is taken as σ times the average of $I_T(\sigma)/\sigma$, which gives:

$$I_m \approx 7\mu\sigma/T. \quad (3.6)$$

If one defines P_{min} by $I_m = P_{min}\sigma\sqrt{2\pi}$ it follows that

$$P_{min} \approx 3\mu/T. \quad (3.7)$$

This value can in some cases be lowered for broad components, cf. section 4.2.

c) M_{0m}

The test involving M_{0m} is done before M_1 and M_2 are calculated and is of a more formal nature. From eq. (2.3) and from eq. (3.7) one gets $M_{0m} = 2.32P_{min}/\sigma$. Since σ is not known at the stage of the program where M_{0m} is used, we use $\sigma = \sigma_{max}$ to calculate a lower limit of M_{0m} which gives, with an extra factor $\frac{1}{2}$ in order not to discriminate too strongly:

$$M_{0m} = 14\mu/[\beta(q_i-1)hT]. \quad (3.8)$$

d) M_{0m}^-

M_{0m}^- is used to discriminate against "satellite" components, which can appear on both sides of high, narrow components. These are a consequence of the adopted method of connecting maxima by straight lines and considering c_2' instead of c_2. Experience has shown, that M_{0m}^- should be a small positive quantity; in other words, only components causing negative curvature in the profile are allowed.

4. Practical experience

4.1. *The basic constants*

In the preceding section some constants were introduced which are basic to the performance of the method. These constants are:

(i) q_0, the number of points used to calculate $c_{2,k}$ in the first run,

(ii) β, the factor by which q_i-1 is multiplied for successive iterations,

(iii) T, the maximum allowable relative error in I, the area of the component.

(i) In order to reduce statistical fluctuations, one should make q_0 as large as possible (it must also be uneven). However, the value of q_0 should still allow the estimation of the narrowest components present in the profile. This depends on the resolution of the observing method. If the instrumental profile can be approximated by a Gaussian of dispersion σ_{instr}, then $\sigma_{instr} \geq \sigma_{min} = (q_0-1)h/4$, which gives

$$q_0 \leq 1+4\sigma_{instr}/h. \quad (4.1)$$

Normally, $\sigma_{instr} \approx h$ which gives as the highest possible value $q_0 = 5$.

(ii), (iii). The influence of the other constants has been investigated by applying the method to artificial profiles, see section 4.2.

4.2. *Tests of the method with artificial profiles*

Applications of the method to artificial profiles have served to test its performance and to determine experimentally the two basic constants β and T, which could not be fixed a priori. The profiles used for this purpose are the sum of several Gaussians (parameters P_0, X_0, σ_0), each chosen at random in a given interval, with noise superimposed. Several series of profiles, representing a variety of profile structure, with and with-

TABLE 1

Types of profiles analyzed (see section 4.2)

Series	Number of profiles	Number of components	Specification
A	100	0	pure noise, length of interval 20 h
B	20	1	one S or one M or one L ($P_0 \approx P_{min}$, see table 2)
C	30	2	one S, and one M or one L ($5 < P_0/\mu < 20$)
D	20	3	three M ($5 < P_0/\mu < 30$)
E	20	4	two S ($P_0/\mu < 10$), one M ($P_0/\mu < 30$), one L ($P_0/\mu < 20$), all blend-free and with $P_0/\mu > 5$
F	22	4	two S, blend-free ($10 < P_0/\mu < 30$), one M ($P_0/\mu = 60$), one L ($3 < P_0/\mu < 20$)
G	10	4	three S ($5 < P_0/\mu < 15$), one L ($0.5 < P_0/\mu < 15$)

Symbols: S : narrow component, $1 < \sigma_0/h < 2$.
M: medium component, $3 < \sigma_0/h < 6$.
L : broad component, $8 < \sigma_0/h < 20$.

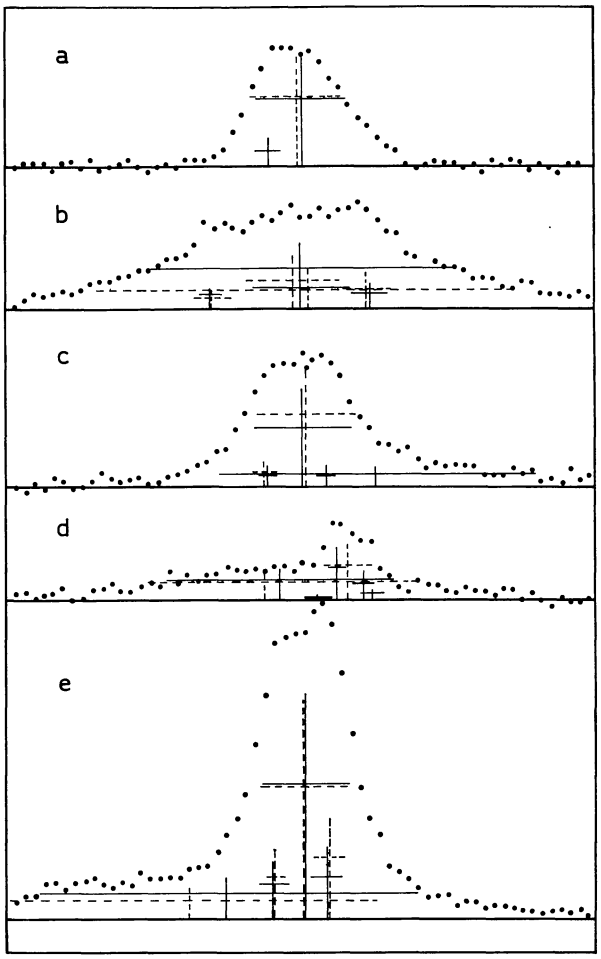

Figure 5. Examples of artificial profiles, discussed in section 4.2. The solid crosses are the given components, the dashed crosses are the estimated components. Not the full interval in x is illustrated. The profiles a to e are taken from the series: C, E, E, G and F, cf. table 1.

out blends*, have been analyzed; the characteristics of these are summarized in table 1. Examples are illustrated in figure 5. Each profile has been analyzed with one or more of the following sets of constants:

a) $\beta = 2$, $T = \frac{2}{3}$;
b) $\beta = 2$, $T = \frac{1}{2}$;
c) $\beta = 3$, $T = \frac{2}{3}$;
d) $\beta = 3$, $T = \frac{1}{2}$.

For broad components in series B the value $T = 2$ has been used.

(i) The series A, B, C, E have been used to determine the detection probability for weak components, depending on P_0 and σ_0 (see table 1).

Series A (no component): The analysis has resulted in *no* spurious components. The discrimination against these is very effective, because P is derived from the observed profile, and is required to be greater than $P_{\min}$, which is in the present cases at least 4.5 μ.

Series B (one component): The results are summarized in table 2. $\beta = 2$ is slightly more effective in detecting weak components.

* A blend is defined as a set of two or more components with small differences in X_0 and σ_0.

TABLE 2

Results of profile analysis; series B (cf. table 1)

Type of component	P_0/μ \ T	$\beta = 2$ 2	2/3	1/2	$\beta = 3$ 2	2/3	1/2
S	4	—	30	—	—	20	—
	4.5	—	60	—	—	40	—
	5	—	75	—	—	75	—
	5.5	—	—	45	—	—	45
	6	—	—	60	—	—	60
	6.5	—	—	60	—	—	60
M	4.5	—	35	—	—	25	—
	5	—	35	—	—	35	—
	6	—	—	40	—	—	30
	6.5	—	—	45	—	—	40
L	2	15	—	—	(15)	—	—
	3	70	—	—	60	—	—

The numbers given are percentages of detected components. The symbols S, M, L are explained in table 1.

TABLE 3

Results of profile analysis; series C and E (cf. table 1)

Series	C				E			
parameter set	a	b	c	d	a	b	c	d
percentage of detected S	95	95	100	90	80	70	90	85
percentage of detected M, L	90	80	95	80	90	80	85	80
number of failures	2	0	1	2	2	3	1	2

Parameter sets: a, $\beta = 2$, $T = \frac{2}{3}$; b, $\beta = 2$, $T = \frac{1}{2}$; c, $\beta = 3$, $T = \frac{2}{3}$; d, $\beta = 3$, $T = \frac{1}{2}$.

TABLE 4

Results of profile analysis; series D, F, G (cf. table 1)

Series	D				F				G			
parameter set	a	b	c	d	a	b	c	d	a	b	c	d
class												
V	0	0	0	0	2	2	0	0	0	0	0	0
G	11	12	10	11	5	5	9	9	4	5	3	4
F	6	6	2	2	4	6	4	5	2	2	1	2
M_S	—	—	—	—	3	3	1	1	1	1	1	1
M_{ML}	0	0	5	5	3	4	4	4	1	1	1	1
X	3	2	3	2	5	2	4	3	2	1	4	2
$Q_0 < 5$	18	16	11	10	11	9	8	8	7	7	6	7
$Q_0 < 2$	10	8	7	6	1	1	1	1	2	2	5	4

The symbols for the classes are explained in the text (section 4.2); those for the parameter set in table 3.

Series C and E (two respectively four blend-free components): The tests contained in these two series are less complete than those in series A and B. The detection limit of weak, narrow components superimposed on broader components depends on their relative position. In table 3 the percentage of the detected components is given, together with the number of failures of the analysis (spurious components or very poor estimates).

(ii) The series D, F and G may contain blends of components. Depending on the amount of blending and on the noise, it may not be possible to separate the components by any method. After inspection of the profiles by eye, the results of the analysis have been put into the following classes: very good (better than would have been expected) (V), good (G), fair (F), bad —at least one narrow component missing (M_S), bad— a medium or broad component missing (M_{ML}), very bad (spurious component, wrong structure or unexpected blend) (X). The quantity Q_0, derived from the sum of squares of residuals as follows:

$$Q_0 = \frac{1}{\mu^2} \sum [res(x_k)]^2 , \qquad (4.2)$$

also gives an indication of the quality of the estimate of the components. In the ideal case Q_0 should be about unity. The statistics of the results are summarized in table 4.

From these experiments it follows that two different cases may be distinguished:

a) For profiles containing no blends, the values $T = \frac{2}{3}$ and $\beta = 2$ or 3 give the best results. A special case is that of profiles (or parts of profiles) with isolated broad components ($\sigma/h \geq 10$); the discrimination against spurious broad components by the tests (i), (ii) and (iv) (cf. section 2.3) is already very effective; the value $T = 2$ can be tolerated. Components with $P/\mu \geq 3$ are then detectable in the majority of cases.

b) For profiles containing blends, the values $T = \frac{1}{2}$ and $\beta = 2$ give the best results.

It must be stressed that the experiments presented here are not sufficient in number (and in variety of profile structure) to allow absolute and general conclusions.

Figure 5 illustrates some results obtained with the method. The profiles are taken from the artificial profiles discussed above. Although a few unfavourable cases were purposely included, the figure already shows that the results of the method are quite satisfactory.

4.3. *Application to analysis of 21-cm profiles*

I have used the method on a large scale in a preliminary, unpublished discussion of a 21-cm survey of neutral hydrogen in the Camelopardalis region. The results proved to be a very useful description of the profile structure. More recently, I have also used the method to obtain initial estimates for a subsequent least-squares fit.

4.4. *Modifications of the method*

There is a rich variety of possibilities to adapt the method to special problems.

(i) To avoid components of similar σ and X in an initial estimate for a least-squares fit, tests may be applied at the end of the analysis.

(ii) If the presence of *one* weak, broad component is

highly probable, it is more reliable to derive its parameters from the values Σy_k, $\Sigma y_k x_k$, $\Sigma y_k {x_k}^2$ of the residual profile. The necessity of such a component may be based on a test of Q_0; very high values of Q_0 are mostly due to the lack of broad components among the estimated ones.

(iii) For a further automation of a program for Gaussian analysis, different sets of β and T may be used, resulting in possibly different initial estimates.

The method is programmed in the algorithmic language ALGOL; a copy of the program is available on request.

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