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SOME APPROXIMATIVE METHODS FOR COMPUTING CROSS-SECTIONS

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Abstract

Some viable methods of computing approximatively the scattering amplitudes and cross-sections in the strong coupling case are discussed. These methods consist in combining the procedure of iteration with an extremalization, enabling to achieve best fits of some free parameters. The problem of transition from the case of scattering on an external potential to the case of a mutual scattering of two particles is discussed anew.

1. General Procedure.

A viable method of computing cross-sections from field equations or from the Schrodinger equation in the strong coupling case is unknown except for the phase shift analysis. This method is, however, cumbersome except for the limits of very low and very high energies where one may either restrict the investigation to the first few terms of the expansion into the Legendre polynomials or use the asymptotic expansions.

We shall discuss some alternative methods of approximative calculations, valid for arbitrary values of the energy and of the coupling constant. Generally speaking, these methods consist in a best fit of some free parameters introduced into the expression for the scattering amplitude. The general idea of such procedures will be explained on a simple example of elastic scattering of particles within the framework

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of non-relativistic quantum mechanics but these methods may be also extended for the case of relativistic field theories.

Let us look for a stationary solution

$$\Psi(\mathbf{r}, t) = \Psi(\mathbf{r}) e^{-i\omega t} \tag{1}$$

of the Schrodinger equation. The time-independent wave function satisfies the equation

$$\left(-\frac{1}{2m}\nabla^2 + V\right)\psi(\mathbf{r}) = \omega\psi(\mathbf{r}). \tag{2}$$

Assume ψ (r) to be of the form

$$\psi(\mathbf{r}) = \chi(\mathbf{r}) + e^{i\mathbf{p}\cdot\mathbf{r}} \tag{3}$$

where the plane wave1 satisfies the equation for a free particle, i.e.

$$\omega = \frac{p^2}{2m} \,. \tag{4}$$

Introducing (3) and (4) into (2) one gets an equation for the scattered part of the wave function

$$(\nabla^2 + p^2) \chi = 2 m \operatorname{V} (\chi + e^{i \mathbf{p} \cdot \mathbf{r}}). \tag{5}$$

The use of the retarded Green function

$$G(r) = \frac{1}{4\pi} \frac{e^{i \mathbf{p} \cdot \mathbf{r}}}{r} \tag{6}$$

enables one to replace the differential equation (5) by an integral equation

$$\chi(\mathbf{r}) = -\frac{1}{4\pi} \int d^3 \mathbf{r}' \frac{e^{i\mathbf{p}/\mathbf{r} - \mathbf{r}'/}}{/\mathbf{r} - \mathbf{r}'/} \mathbf{U}(\mathbf{r}) \left[\chi(\mathbf{r}) + e^{i\mathbf{p}\cdot\mathbf{r}} \right]$$
(7)

with

$$\mathbf{U} = 2m \, \mathbf{V}. \tag{8}$$

Representing the asymptotic solution for large r in the form

$$\chi(\mathbf{r}) = f \frac{e^{i \mathbf{p} \cdot \mathbf{r}}}{\mathbf{r}} \tag{9}$$

one obtains the scattering amplitude f whose squared absolute value denotes the differential cross-section.

^{1.} The absence of a (dimensional) factor at the plane wave means a special normalization: one particle per cm³ in the incident beam.

In the weak coupling case the equation (7) may be treated by the well known procedure of iteration starting with a suitably chosen zero-order approximation. By putting to the right-hand side of (7) $\chi^{(0)} = 0$ one obtains Born's approximation which, however, is legitimate only if the interaction is weak. A possibility of improving the approximation consists in introducing to the right-hand side of (7), instead of zero, a function dependent on a certain number of parameters

$$\boldsymbol{\chi}^{(0)} = \boldsymbol{\xi} \ (\boldsymbol{r}, \boldsymbol{p}, \alpha_1, \dots \alpha_N) \tag{10}$$

and trying to make a possibly best fit of the parameters.

The equation (7) is of the form

$$\chi = F(\chi) \tag{11}$$

where F means a linear functional. Let us consider, more generally, the linear relation

$$\eta = \mathbf{F}(\xi). \tag{12}$$

The function η may be regarded as an approximate solution of the equation (11) if it differs little from ξ . Of course, one has to define properly the sense of " η differing little from ξ ". If these functions were square integrable, then we could use, as a criterion, a small quadratic deviation in the whole space but, unfortunately, the outgoing wave, being a solution of (11), is not square integrable. The way out of this difficulty is possible due to the short range of the interaction. In fact, η depends only upon the values of ξ in the region of small r, of the order of magnitude of the range of interaction (unless one assumes ξ to increase unreasonably with r). Therefore it is sufficient to secure

$$\Delta (\xi, \eta) = \int d^3 r | \eta - \xi |^2$$

$$r \leqslant R$$
(13)

to be small, where R denotes the range of interaction, in order to guarantee η to be an approximative solution of (11), provided ξ has been chosen to be a decreasing, or at least, not increasing function for r > R.

A very simple possibility of obtaining an approximate solution of the equation (11) or (7) will consist in introducing into the right-hand side a constant

$$\xi \equiv \chi^{(0)} = \alpha, \tag{14}$$

computing $\eta \equiv \chi^{(1)}$, and trying to minimalize the integral (13) with respect to α . Another possibility is to start with a constant (14), compute the total cross-section in the first and second iterative approximation and fix the value of α from the condition

$$\sigma^{(2)} = \sigma^{(1)} \tag{15}$$

A crude but still simpler possibility consists in the following: supposing χ to be a slowly varying function in the domain r < R, we may determine the parameter α by computing $\chi^{(1)}$ at the point r=0 and equating it to α

$$\chi^{(1)}(0) = \alpha.$$
 (15')

Better approximations may be obtained with the help of suitably chosen multi-parametric functions of the type (10) and minimalizing the expression (13), i.e. determining the parameters from the equations

$$\frac{\partial \Delta^{(1)}}{\partial \alpha_j} = 0 \text{ where } \Delta^{(1)} = \int_{r \leq R} d^3 r | \chi^{(r)} - \chi^{(0)} |^2$$
 (16')

with $j=1, 2, \ldots, N$. This procedure of minimalization may be still refined by combining it with higher orders of the procedure of iteration, i.e. performing n iterations and requiring

$$\frac{\partial \triangle^{(n)}}{\partial \alpha_{j}} = 0 \text{ where } \triangle^{(n)} = \int d^{3}r |\chi^{(n)} - \chi^{(n-r)}|^{2}. \tag{16}$$

Alternatively, starting with an N-parametric function (10) the parameters may be fitted at the point r=0 by performing N iterations and demanding

$$\chi^{(o)}(0) = \chi^{(1)}(0) = \dots = \chi^{(N)}(0).$$
 (17)

It should be stressed that for large values of the coupling constant the convergence of the iterations to a solution is not guaranteed. Novertheless, the conditions (16') or (17) do provide us with approximative solutions. The question whether this approximation is good or poor depends essentially upon the proper choice of the starting-point function (10). This choice is limited by the requirement of obtaining a viable procedure. To this end the function (10) must be chosen sufficiently simple for the integrations to be performed effectively. Moreover, in order to get simple conditions (16') or (17) for the parameters it is advisable to introduce (10) in the form a linear function of the parameters. In the case of spherically symmetric potentials a plausible and sufficiently flexible form of the function (10) seems to be

$$\chi^{(o)}(r,\cos\theta) = \sum_{\mu} \sum_{\nu} \alpha_{\mu\nu} e^{-\mu \alpha r} e^{i\nu p \cdot r}$$
(18)

with $\mu=0, 1, \ldots, M, \nu=0, \pm 1, \ldots, \pm N$, and a is the reciprocal of the interaction range R^{-1} .

A drawback of the above described procedures is that they do not provide us with estimates of the limits of accuracy of the approximations but, at any rate, they yield a criterion enabling one to estimate which one of a set of approximations is the best. Considering two starting-point functions ξ and $\overline{\xi}$ of, say, quite a different form and differently parametrized, and computing η and η from the (general) formula (12) it may be claimed $\overline{\eta}$ to constitute a better approximation then η if

$$\triangle$$
 $(\bar{\xi}, \bar{\eta}) < \triangle$ (ξ, η) (19) with \triangle (ξ, η) defined by (13). Then also the value of the cross-section computed with the help of $\bar{\eta}$ will be more reliable than that computed with the help of η . Thus, \triangle (ξ, η) may be called the "index of reliability". The existence of a criterion (19) enables one to undertake a

In many cases (especially in relativistic theories) it is easier to work with Fourier transforms χ (**k**). For the Fourier transform equations of a similar type as (7) or (11) hold true as well. If we happened to choose for $\chi^{(0)}$ (**k**) the true solution, then $\chi^{(1)}$ (**k**) would be identical

more systematic search for suitable forms of starting point functions.

with $\chi^{(0)}(k)$. Herefrom it is seen that introducing a suitably chosen starting-point function

$$\chi^{(0)} = \xi \left(\mathbf{k}, \mathbf{p}, \alpha_1, \dots, \alpha_N \right) \tag{10*}$$

we shall obtain an approximation to the true solution by requiring the following conditions upon the parameters

$$\int_{k} d^{3}k |\chi^{(n)} - \chi^{(n-1)}|^{2} = \min.$$
 (16*)

These conditions correspond to the conditions (16') because the region $k \in \mathbb{R} = 1$ in the k-space corresponds roughly to the region $r \in \mathbb{R}$ in the k-space.

The condition (16*) may also be replaced by a still simpler condition for the parameter fits, namely

$$\int d\Omega \mid \chi^{(n)}(k) - \chi^{(n-1)}(k) \mid^{2} = \min$$
 (16**) at the surface of a sphere $k = 1$ or $(k + 1)^{2} = \frac{1}{2}$.

2. The Yukawa Potential.

The above described procedures may be illustrated by an example of scattering on a Yukawa potential. With the simplest choice (14) we have in this case

$$\chi^{(1)}(\mathbf{r}) = \frac{Ga}{4\pi} \int d^3r' \frac{e^{ip \mid \mathbf{a} - \mathbf{r'} \mid}}{\mid \mathbf{r} - \mathbf{r'} \mid} \frac{e^{-ar'}}{r'} \left(\alpha + e^{i \mathbf{p} \cdot \mathbf{r'}} \right) \qquad (20)$$

with

$$G = \frac{2m}{a} \frac{a^2}{4\pi} = 28 \frac{m}{a} \tag{21}$$

where m denotes the mass of the incident particle (nucleon) and a is the pion mass determining the range of nuclear forces. In this case G is very large, almost two hundreds (or, replacing m by the reduced mass, still of the order of one hundred).

From (20) we get

$$\chi^{(1)}(0) = \frac{Ga}{4\pi} \int d^3 r \, \frac{e^{(ip-a)r}}{r^2} \left(\alpha + e^{i \, \mathbf{p} \cdot \mathbf{r}} \right). \tag{22}$$

With the abbreviation

$$x = \frac{2p}{a} \tag{23}$$

the condition (15') yields

$$\alpha = iG \frac{\ln(1 - ix)}{x} \frac{1 - i\frac{x}{2}}{1 - G - i\frac{x}{2}}.$$
 (24)

The parameter α becomes infinite for G=1 and $p\rightarrow 0$ which, however, is very far from the experimental value of G in the case of scattering of nucleons subjected to nuclear forces. For large values of G the parameter α becomes actually independent of G

$$\lim_{G \to \infty} \alpha = -\frac{i}{x} \left(1 - i \frac{x}{2} \right) \ln \left(1 - i x \right) \longrightarrow -1. \tag{24'}$$

In order to compute the scattering amplitude and cross-section we have to evaluate $\chi^{(1)}$ for $ar \gg 1$ and find

$$\chi^{(i)}(r) = \chi_A^{(i)}(r) + \chi_B^{(i)}(r)$$
 (25)

where

$$\chi_{\mathbf{A}}^{(1)} = \frac{G a \alpha}{4\pi} \frac{e^{i p r}}{r} \int d^3 r' \frac{e^{-ar'}}{r'} e^{-i p r' \cos \theta'}$$
 (26)

while $x_B^{(1)}$ is the term well known from Born's approximation. The scattering amplitude defined by (9) also consists in two terms

$$f^{(1)} = f_{\mathbf{A}}^{(1)} + f_{\mathbf{B}}^{(1)} \tag{25'}$$

where $f_A^{(1)}$ follows from (26) and $f_B^{(1)}$ is the usual Born's amplitude. Hence,

$$f^{(1)} = \frac{G}{a} \left(\frac{\alpha}{1 + \frac{1}{4}x^2} + \frac{1}{1 + x^2 \sin^2 \frac{\theta}{2}} \right) \tag{27}$$

with a fitted from the condition (24).

The differential cross-section following from (27) is

$$\frac{d\sigma^{(1)}}{d\Omega} = \frac{G^2}{a^2} \left(\frac{1}{1 + x^2 \sin^2 \frac{\theta}{2}} + \frac{2 \operatorname{Re} \alpha}{\left(1 + \frac{1}{4} x^2\right) \left(1 + x^2 \sin^2 \frac{\theta}{2}\right)} + \frac{|\alpha|^2}{\left(1 + \frac{1}{4} x^2\right)^2} \right) (18)$$

where

2 Re
$$\alpha = -\frac{2G}{x} \frac{\left(G - 1 - \frac{x^2}{2}\right) \operatorname{arc} t_g x + \frac{Gx}{2} \ln(1 + x^2)}{(G - 1)^2 + \frac{x^2}{4}}$$
 (28')

and
$$|\alpha|^2 = \frac{G^2}{x^2} \frac{\left(1 + \frac{x^2}{4}\right) \left[\ln(1 + x^2)^2 + (\operatorname{arc} t_g x)^2\right]}{(G - 1)^2 + \frac{x^2}{4}} \tag{-8''}$$

From the above formulae it is seen that, contrary to the weak coupling case, where the order of iterative approximation coincides with the order of the power series expansion in G, our approximation exhibits a complicated dependence upon the coupling constant and has nothing to do with a power series expansion in G. Of course, for very small values of the coupling constant (G \leq 1) the parameter α is proportional to G so that the first terms in (27), being of the order G2, may be neglected in comparison with Born's term which is of the order G. Hence, for small G our formulae go over into Born's approximation. For $G \approx 1$ the absolute value of α becomes very large so that the crosssection would assume a resonant character (which, however, may be regarded as a sign that the assumption (14) constitutes a bad starting point in this case). For very large values of G in comparison to unity the cross-section increase again like G2 inasmuch as, according to (24'), the parameter a becomes independent of G.

By evaluating the following integrals

$$\int d\Omega \frac{1}{1+x^2 \sin^2 \frac{\theta}{2}} = \frac{4\pi}{x^2} \ln(1+x^2), \int d\Omega \frac{1}{\left(1+x^2 \sin^2 \frac{\theta}{2}\right)^2} = \frac{4\pi}{1+x^2}$$
 (29)

we get an expression for the total cross-section

$$\sigma^{(1)} = \frac{4\pi G^2}{a^2} \left\{ \frac{1}{1+x^2} + 2 \operatorname{Re} \alpha \frac{\ln (1+x^2)}{x^2 \left(1 + \frac{1}{4}x^2\right)} + \frac{\alpha \alpha^*}{\left(1 + \frac{1}{4}x^2\right)^2} \right\}$$
(30)

where Re α and $|\alpha|^2$ are given by (28') and (28''). Thus, we obtained closed formulae for small as well as medium and high values of momentum.

For small momenta our expression for the differential cross-section (28) shows that the scattering is less anisotropic than according to the corresponding formula of Born. By developing Born's expression for the differential cross-section into powers of x one encounters an anisotropic term $x^2 \sin^2 \frac{\theta}{2}$ whereas in our case (for very large G) this term is cancelled by a similar term arising from the second term in (28) so that the lowest order anisotropic term in (28) is $\left(x^2 \sin^2 \frac{\theta}{2}\right)^2$.

Of course, owing to the crudness of the assumptions (14) and (15'), it cannot be expected the formulae (8) and (30) to describe accurately the differential and the total cross-section. In order to obtain a better agreement one should introduce more sophisticated starting-point functions and more elaborate fits of the parameters. Nevertheless, this crude approximation already exhibits some qualitative and quantitative features of the elastic cross-sections in the strong coupling case.

3. Transition to the c.m.s.

In most text-books about scattering problems it is stated that the transition from the case of scattering on an external potential to the case of scattering of two particles (interacting by means of a potential of the same form) may be achieved simply by replacing the mass m by the reduced mass. The proof of this fact has been achieved by separating the relative motion from the motion of the centre of mass. However, in this case one has to do with a description of the motion of one of the two colliding particles in a non-inertial frame of reference whose origin

is fixed at the position of the other particle which gives rise to doubts as to whether this procedure remains valid also for the case of highly energetic collisions in the relativistic theory. Besides, this approach is certainly unphysical since one never measures the relative coordinates but always coordinates of the particles with respect to an inertial frame of reference.

Therefore we shall discuss the problem of transition from the case of scattering on an external potential to the case of a mutual scattering of two colliding particles anew in a more methodological fassion. To do so we may start from a Schrodinger equation for two particles

$$\left(-\frac{1}{2m_1}\nabla_1^2 - \frac{1}{2m_2}\nabla_2^2 + V\left(\mid \boldsymbol{r_1} - \boldsymbol{r_2}\mid\right)\right)\psi(\boldsymbol{r_1}, \boldsymbol{r_2}, t) = i\frac{\partial}{\partial t}\psi(\boldsymbol{r_1}, \boldsymbol{r_2}, t) \quad (31)$$

and look for a stationary solution

$$\psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi(\mathbf{r}_1, \mathbf{r}_2, t) e^{-i\omega t}$$
 (31')

Let us perform the separation of variables by going over from r_1 , r_2 to R and r where R describes, as usual, the coordinates of the mass centre but r does not mean the relative coordinates but is defined as follows

$$r = \frac{m_2}{M} (r_1 - r_2), R = \frac{m_1 r_1 + m_2 r_2}{M}$$
 (32)

where M means the total mass of the system

$$M = m_1 + m_2.$$
 (32')

The physical meaning of the new coordinates r becomes clear by remarking that

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{R} (\mathbf{r}_1, \mathbf{r}_2). \tag{33}$$

Thus, r denotes the coordinates of the first particle with respect to an inertial coordinate system whose origin coincides with the centre of mass of the system. This has great methodological advantages because one can measure directly positions, momenta, etc. of a particle with respect to an inertial frame of reference but not with respect to the other particle inasmuch as — in the latter case — we should "sit on the other particle" together with our apparatus of measurement while this particle itself undergoes an acceleration. The motion of the centre of mass being uniform, it may be brought to rest in an inertial system of reference. If

the centre of mass coincides with the origin of this inertial frame of reference, then the coordinates r denote those of the first particle in this system of reference.

From (32) we get

$$\frac{\partial}{\partial x_1} = \frac{m_1}{M} \frac{\partial}{\partial X} + \frac{m_2}{M} \frac{\partial}{\partial x}, \quad \frac{\partial}{\partial x_2} = \frac{m_2}{M} \left(\frac{\partial}{\partial X} - \frac{\partial}{\partial x} \right)$$
(34)

a**n**d

$$\frac{1}{2m_1} \frac{\partial^2}{\partial_{x_1^2}^2} + \frac{1}{2m_2} \frac{\partial^2}{\partial_{x_2^2}^2} = \frac{1}{2M} \frac{\partial^2}{\partial X^2} + \frac{1}{2M} \frac{m_2}{m_1} \frac{\partial^2}{\partial x^2}$$
(34')

whence

$$\frac{1}{2m_1} \nabla_1^2 + \frac{1}{2m_2} \nabla_2^2 = \frac{1}{2M} \nabla_R^2 + \frac{1}{2M} \frac{m_2}{m_1} \nabla_r^2$$
 (35)

while

$$r_1 - r_2 = \frac{M}{m_2} r \tag{36}$$

so that the stationary equation assumes the form

$$\left[-\frac{1}{2M} \nabla_{\mathbf{R}}^{2} - \frac{1}{2M} \frac{m_{2}}{m_{1}} \nabla_{r}^{2} + V \left(\frac{M}{m_{2}} r \right) \right] \psi(\mathbf{R}, \mathbf{r}) = \omega \psi(\mathbf{R}, \mathbf{r})$$
and is separable. (37)

At the first sight the above equation may look strange but it is certainly correct. In particular, if $m_2 \rightarrow \infty$ then $\frac{M}{m_2} \rightarrow 1$ and the above equation turns over into the usual equation for the first particle in an external potential

$$\left[-\frac{1}{2m_1}\nabla_r^2 + V(r)\right]\psi(r, \mathbf{R}) = \omega \psi(r, \mathbf{R}). \tag{37}$$

The position of the centre of mass coincides with that of the second particle in this limit and we may simply put into the above equation R=0.

By performing the separation of variables in (37) and assuming the centre of mass to be at rest (P = 0) we are left with the equation

$$\left[-\frac{1}{2M}\frac{m_2}{m_1}\nabla^2 + V\left(\frac{M}{m_2}r\right)\right]\psi(r) = \pi \psi(r)$$
(38)

describing the motion of the first particle, or

$$\left[-\frac{1}{2m_1}\nabla^2 - \omega_1\right]\psi = -\widetilde{V}(r)\psi \tag{39}$$

where

$$\omega_1 = \frac{M}{m_2} \omega, \ \widetilde{V}(r) = \frac{M}{m_2} V\left(\frac{M}{m_2}r\right). \tag{40}$$

In order to describe the scattering phenomena we assume a solution of (39) in the usual form

$$\mathbf{\psi}(\mathbf{r}) = e^{i \mathbf{p} \cdot \mathbf{r}} + \chi(\mathbf{r}). \tag{41}$$

Inasmuch as the total energy is only determined up to an arbitrary constant, we may choose this constant so that

$$\frac{p^2}{2m_1} = \omega_1. \tag{42}$$

By exchanging the indices $1 \leftarrow \rightarrow 2$ we find the following relation

$$\omega_1 + \omega_2 = \frac{M}{\mu} \ \omega \tag{42'}$$

where μ is the reduced mass. Introducing (41) and (42) into (39) we obtain an equation for χ

$$(\nabla^2 + p^2) \chi = \widetilde{\mathbf{U}} \left(e^{i \mathbf{p} \cdot \mathbf{r}} + \chi \right) \tag{43}$$

where

$$\widetilde{\mathbf{U}} = 2 \, m_1 \widetilde{\mathbf{V}}. \tag{44}$$

It is seen that the equation (43) is identical in form with the equation (5) for the scattering on an external potential, the only difference being that V is to be replaced by \widetilde{V} . Thus, the rule for going over from the scattering on an external potential to a mutual scattering of two particles is

$$V \rightarrow \widetilde{V}$$
 (45)

or

$$U=2m_1 V \rightarrow \widetilde{U}=2m_1 \widetilde{V}. \tag{45'}$$

Now, in the special case of Yukawa potential we have

$$U = -2m_1 \frac{g^2}{4\pi} \frac{e^{-r}}{r} \rightarrow \widetilde{U} = -2m_1 \frac{g^2}{4\pi} \frac{M}{m_2} \frac{e^{-a\frac{M}{m_2}r}}{\frac{M}{m_2}} = -2m_1 \frac{g^2}{4\pi} \frac{e^{-a\frac{m}{m_2}r}}{r_1}$$
(46)

where

obsident by the set of Might and set of settled that
$$\widetilde{a} = \frac{M}{m_1} a. \qquad (47)$$

Thus, the transition from the case of scattering on a external Yukawa potential to the mutual scattering of two particles interacting by means of the Yukawa potential consists, originally, in a replacement

$$a \to \widetilde{a} = \frac{M}{m_2} a. \tag{48}$$

In view of the definition (17) of G we have

$$G = \frac{2m_1}{2} \frac{g^2}{4\pi} \rightarrow \widetilde{G} = \frac{2m_1}{\widetilde{a}} \frac{g^2}{4\pi} = 2 \frac{m_1 m_2}{a M} \frac{g^2}{4\pi} = \frac{2\mu}{a} \frac{g^2}{4\pi}$$
 (49)

so that, indeed, the change of G may be viewed upon as a replacement of the actual mass of the scattered particle (appearing in the definition (17) of G) by the reduced mass. Moreover, as is seen from (20) and (24'), the scattering amplitude involves the parameter a also through the variable x which undergoes a change

$$x \to \widetilde{x} = \frac{2p}{a} = \frac{2m_2 p}{Ma} \,. \tag{50}$$

Inasmuch as (in the non-relativistic theory) $p_1=m_1 v$, the above replacement is identical with

$$\frac{m}{a} v \rightarrow \frac{m_1 m_2}{Ma} v = \frac{\mu}{a} v \tag{51}$$

which again may be interpreted as a replacement of the actual mass m by the reduced mass while keeping the actual velocity of the particle and the value of a unchanged. However, the change of mass may be regarded as apparent while the genuine physical effect consists in the change (47), i.e.

in a contraction of the range $R = \frac{1}{a}$ of nuclear forces by the factor m_2/M for the first particle

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t particle
$$\widetilde{R}_1 = \frac{m_2}{M} R \tag{52}$$

and, similarly, by the factor m_1/M for the second particle

$$\widetilde{R}_2 = \frac{m_1}{M} R. \tag{52'}$$

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COMPUTER SOLUTIONS OF NAGUMO'S EQUATION

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Abstract:

We have developed a technique to determine those values of the parameters in Nagumo's equati n which permit non-constant bounded solutions. These solutions are then obtained by using Hammings' predictor-corrector formula with the Runge-Kutta Method on a digital Computer.

Hodgkin and Huxley [1] in their fundamental work on pulses in a squid axon were the first to give a mathematical description of this process. Their model was based on a concept derived from "Kelvin's Cable Theory" that the nerve membrane is effectively an inductance free line with a constant capacitance and a non-linear current flow element. K.S. Cole et al [2] discussed the problem of Hodgkin and Huxley in detail for the squid giant axon membrane. More recently a simplified model for the process has been proposed by Nagumo, A Rimoto and Yoshizawa [3]. Now the problem is to obtain the non-constant bounded solutions for the third order non-lin ar ordinary differential equation

$$\frac{d^3U}{dx^3} - c \frac{d^2U}{dx^2} + f'(u)\frac{dU}{dx} - (b/c) U = 0,$$
 (1)

where f(U) = U(1-U)(U-a), 0 < a < 1

To the best of our knowledge no one has so for succeeded in obtaining the non constant bounded solutions for the O.D.E. (1). We shall find those values of the parameters a, b and c which permit non-constant bounded solutions of O.D.E. (1) and determine the corresponding solutions. We shall obtain the solutions in steps. Firstly we try to obtain the numerical solution when the parameter b is set equal to zero.

Solutions for b=0.

When b=0, the third order non-linear O.D.E. (1) reduces to the second order differential equation

$$\frac{d^2\mathbf{U}}{dx^2} - c \frac{d\mathbf{U}}{dx} + f = 0 \tag{2}$$

where f=U(1-U)(U-a), 0 < a < 1

Theoretical (analytical) Solution

Huxley (4) has obtained the theoretical solution of Equation (2). He has shown that when $c = \sqrt{2}(\frac{1}{2}-a)$ (called the Huxley speed) and $0 < a < \frac{1}{2}$, equation (2) has the solution

$$U(x) = [1 + \exp(-x/\sqrt{2})]^{-1}$$
 (3)

· "我只要你的,我就是一点,我们还有一个人的。" "我们就是我们的。" "我们就是我们的。" "我们的,我们就是我们的,我们就是我们的,我们就是我们的,我们就

It is obvious from (3) that for large positive values of x, the solution U(x) is approaching unity and for large negative values of x it is approaching zero.

Numerical Solution

We have to evaluate numerically for each of several values of a, the corresponding values of c for which a non-constant bounded solution of the differential equation (2) exists. This value of c can be compared with the corresponding Huxley speed and the numerical solution of equation (3).

Method of Solution

Fixing the parameter a, taking several values of c and solving (2) numerically, it is found that for some values of c the solution incaeases indefinitely (giving computer overflow) and for other values of c the solution after first increasing starts to decrease and continues decreasing indefinitely (giving computer overflow) for large values of c. Two values of c, say c_1 and c_2 , such that $c_2 > c_1$ are chosen in such a manner that if we take values of c less than c_1 the solution increases very rapidly (giving computer overflow) for large values of c and if we take the values of c greater than c_2 , the solution first increases and then decreases very rapidly (giving computer overflow) for large values of c

Now in the selected interval (c_1, c_2) a series of values of c are again tried and we thus obtain a smaller interval (c'_1, c'_2) with $c'_2 > c'_1$, such that solutions with $c < c'_1$ increase indefinitely for large values of x while solutions with $c < c'_2$ decrease indefinitely for large x. This procedure is repeated a number of times and eventually (for a fixed value of the parameter) a value of parameter c (for which the solution of the differential equation approximates the desired form) is obtained to some given accuracy.

From differential equation (2), we find that the linearised equation near U=0 is

$$\frac{d^2U}{dx^2} - c \frac{dU}{dx} - a U = 0$$
 (4)

The auxiliary equation of (4) is

$$m^2 - cm - a = 0 \tag{5}$$

(a and c being + ive (3) which has only one positive root

$$m_1 = (c + \sqrt{c^2 + 4 a})/2.$$

This root (i.e. m_1) must correspond to the solution for large negative values of x (near U=0). Therefore, for large negative values of x, the solution $U(x) \simeq A e^{m_1 x}$ and $U'(x) \simeq A m_1$. $e^{m_1 x} = m_1 U$ where $U \simeq 0$ and A is a constant. Thus taking initial conditions as U(0) = h, V(0) = mh where h is a small step size used in the numerical solution and m_1 is the only positive root of (5), we obtain the following solutions:

For a=0.125, 0.25 and 0.375, values of c are determined as c=0.52919, 0.35344 and 0.17649 respectively. The nonconstant bounded solution corresponding to one of these values is shown in Fig. 1. The numerical results are compared with the corresponding theoretical values. The method of solution explained earlier is also used for the third order non-linear differential equation by fixing parameters a and b and trying various values of c in a specified interval (upper limit is

obtained by Huxley speed and the lower limit is obtained by an equation mentioned in [4]).

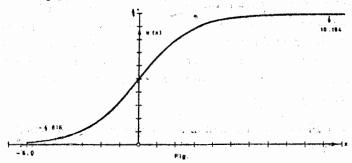


Fig. 1. Comparison of Huxley's theoretical solution with numerical solution obtained for a = 0.375, c = 0.176490

Numerical Solution for third order non-Linear O.D.E.

Solutions fo: b>0: We must now consider the full third order ordinary non-Linear differential Equation

$$U''' - c U'' + f'(U) U' - (b/c) U = 0$$
 (6)

where f(U) = U(1-U)(U-a) 0<a<1

Now the problem is to determine numerically the values of the parameters a, b ($\neq 0$) and c which permit non-constant bounded solutions and then to evaluate the corresponding solutions numerically.

McKean Jr. [4] was the first to attempt a solution of (6) and has produced the graph for the general shape of the solution. We shall try to find the various values of the parameters, a, b and c which permit the non-constant bounded solution of (6). The linearised third order equation is

$$U''' - c U' - a U' - (b/c) U = 0$$
(7)

The auxiliary equation is

$$m^3 - c m^2 - am - (b/c) = 0 (8)$$

which is solved by taking the initial conditions as U=h, V=m h and $w=m_1^2$ h where h is the small step size and m_1 is the only + ive root of the auxiliary equation (8).

Fixing the parameters a and b, the lower limit of c is obtained by considering that $b < a^2/4$, that c exceeds the largest positive root of the equation

$$(a^2-4b) c^4+2a (2a^2-9b) c^2-27b^2=0$$

and that the upper limit of c is obtained by Huxley speed discussed earlier. We now have an interval in which to restrict our search for an appropriate value of the parameter c for which the solution U(x) should attain the desired form.

Results

(I) For a = 0.125, b = 0.001, m = 0.45595 the required value of c for a non-constant bounded solution of the O.D.E. lies in the interval (0.149660, 0.149665) and to five decimal places the value of c is 0.14966. The solution curves are depicted in computer graphs shown in Figs. 2 and 3.

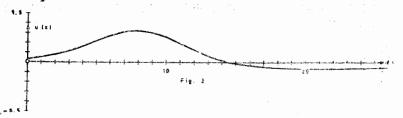


Fig. 2. Solution of third order non-linear differential equation for a=0.125, b=0.001 & c=0.149660

(for large values of x the solution U(x) is approaching to zero and there is no room in Computer to print out and drawgraph beyond the value x=26.0).



Fig. 3. Solution of third order non-liner differential equation for a=0.125, b=0.001 & c=0.1496650

(II) For a=0.25, b=0.001, c=0.135272 and $m_1=0.58475$, the solution curve is shown in Fig. 4. For a=0.25, b=0.001, c=0.135278 and m=0.58475 the solution curve is shown in Fig. 5. From the results obtained it is obvious that the required value of c (for a=0.25, b=0.001) lies in the interval (0.135272, 0.135278).

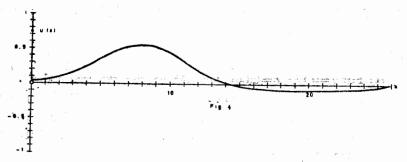


Fig. 4. Solution of third order non-linear differential equation for $a=0.2\tilde{s}$, b=0.001 & c=0.1352720

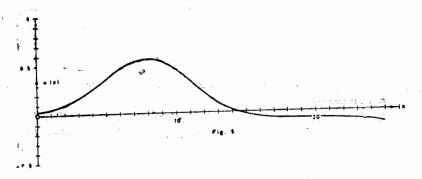


Fig. 5. Solution of third order non-linear differential equation for $a \approx 0.25$, $b \approx 0.001$ & $c \approx 0.135278$

(III) For a=0.25, b=0.002, m=0.62010925 the required value of c for a non-constant bounded solution of the O.D.E. lies in the interval (0.1894685, 0.1894690). Graphs were also obtained as in the cases of I & II.

- (IV) For a=0.375, b=0.001 the values of c are tried in the interval (0.1 to 0.8) but on each occasion the solution increases indefinitely without turning giving computer overflow.
- (V) For a=0.375, b=0.0001, m=0.69905 the required value of c for a non-constant bounded solution of the O.D.E. lies in the interval. (0.16020, 0.16025), computer graphs are obtained as in cases I & II.

For $a > \frac{1}{2}$ i.e. a = 0.75, b = 0.001, 0.0001 and calculating the proper interval for c, the solution increases indefinitely without turning, giving computer overflow every time, as shown in Tables 1, 2. These numerical calculations support the conjecture proposed by H.P. McKean JR. [4], that if a is greater than 0.5 and b is greater than zero then no nonconstant bounded solution exists for the third order O.D.E. Further support could be given to the conjecture by trying a large number of different values of b. The underlying idea is that parameter 'a' plays the role of a doping parameter and the disappearance of the nonconstant bounded solution corresponds to the physical fact that if too much of novocaine is injected, the whole nerve goes dead.

TABLE No. 1

For a = 0.75

b = 0.001

x represents that value where computer overflow occurs.

\boldsymbol{c}	: .	x	
0.001		9.0	0.895289
0.001 0.00 9		6.0	0.936587
0.015		7. 0	0.915233
0.10		7.9	0.93041
0.1350		7.0	0.94459
0.1353		7.0	0.94472
0.30		6.0	1.03099
0.40		5.0	1.09015
0.50		5.0	1.15235
0.60		5. 0	1.21726
0.70		4.0	1.28467
0.80		4.0	1.35442

TABLE No. 2

For a = 0.75

b = 0.0001

x represents that value where computer overflow occurs.

C	x	m_1
0.1	7. 0	0.92635
0.2	6. 0	0.97356
0.3	6.0	1.02936
0.4	5.0	1.08899
0.5	3 .0	1.15149
0.6	5.0	1.21724
0.7	4.0	1.28442
0.8	4,0	1.35412

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VARIOUS APPROACHES TO ESTIMATING A LINEAR FUNCTIONAL RELATION

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1. Introduction

We consider a linear functional relation $Y = \alpha + \beta x$ where X, Y are mathematical variables and α , β are unknown parameters. Suppose that X, Y are not observable but we can observe x, y where x = X + e, y = Y + f and e, f are errors of observation. The problem of estimating the parameters α , β which was possibly first investigated by Kummell (1879), has been studied by many statisticians since then. A variety of estimators of α , β proposed over the years are now available in the literature. We shall briefly review here various approaches that have been pursued from time to time for estimation of a linear functional relation.

2. Notations

Let X_i , Y_i be the values of the variables X, Y for the *i*th individual. We take our linear relationship as

Similarly
$$Y_i = \alpha + \beta X_i$$
 $(i = 1, 2, ..., n)$.
 $x_i = X_i + e_i$ $y_i = Y_i + J_i$.

where we observe x_i , y_i ; and e_i , f_i are errors of observation. If we have a replicated situation, x_{ih} and y_{ik} shall be the values on hth and kth replications of x_i and y_i , so that here the assumptions are

$$x_{ih} = X_i + e_{ih}$$
 $(h=1, 2, ..., r_i)$
 $y_{ih} = Y_i + f_{ih}$ $(k=1, 2, ..., s_i)$.

We shall use the following quantities in a replicated situation

$$\overline{\mathbf{X}} = \mathbf{R}^{-1} \sum r_i \mathbf{X}_i, \qquad \overline{\mathbf{Y}} = \mathbf{S}^{-1} \sum s_i \mathbf{Y}_i,$$

$$B_{xx} = \frac{1}{n-1} \sum r_i (\bar{x}_i - \bar{x})^2, \qquad W_{xx} = \frac{1}{R-h} \sum (x_{ih} - \bar{x}_i)^2,$$

$$B_{yy} = \frac{1}{n-1} \sum s_i (\bar{y}_i - \bar{y})^2, \qquad W_{yy} = \frac{1}{S-n} \sum (y_{ih} - \bar{y}_i)^2,$$

$$B_{xy} = \frac{1}{n-1} \sum r_i (\bar{x}_i - \bar{x})(\bar{y}_i - \bar{y}),$$

$$B'_{xy} = \frac{1}{n-1} \sum s_i (\bar{x}_i - \bar{x})(\bar{y}_i - \bar{y}),$$
where
$$R = \sum r_i \qquad S = \sum s_i$$

$$\bar{x}_i = \sum x_{ih}/r_i \qquad \bar{y}_i = \sum y_{ik}/s_i$$

$$\bar{x} = \sum r_i x_i/R \qquad \bar{y} = \sum s_i y_i/S$$

If $r_i = s_i = 1$ for each i, it may be noted that the situation is not replicated one.

3. Estimation of β

Since, without loss of generality, we can shift the origin by an introduction of a dummy variable and reduce the linear functional relation to one containing only β , we shall confine our attention only to estimation of this parameter.

3.1. Maximum Likelihood and Least Squares Method. The problem of estimation of β has been attacked through the use of maximum likelihood and least squares by Kummell (1879), Lindley (1947), Madansky (1959), Graybill (1961), Ord (1969) and other statisticians. We give below estimators as suggested by Lindley and Madansky when $r_i = s_i = 1$.

We assume that e_i , f_i are normally and independently distributed with zero means and variances σ_e^2 and σ_f^2 . The likelihood function is

$$L = f(e_1, e_2, \dots, e_n, f_1, f_2, \dots, f_n)$$

$$= (2\sigma_e \ \sigma_f \ \pi)^{-n} \ \exp\left[-\frac{1}{2} \left\{ \sum (e_i^2 / \sigma_e^2) + \sum (f_i^2 / \sigma_f^2) \right\} \right]$$

Substituting into it $e_i = x_i - X_i$, $f_i = y_i - Y_i = y_i - \alpha - \beta X_i$, and taking partial derivative of log L with respect to each of the n+4 unknowns

 $X_1, X_2, \ldots, X_n, \alpha, \beta, \sigma_e^2$ and σ_f^2 , we obtain

$$\hat{\sigma}_f^2 = \frac{1}{n} \sum (y_i - \hat{\alpha} - \hat{\beta} \hat{X}_i)^2$$

$$\hat{\sigma}_e^2 = \frac{1}{n} \sum_i (x_i - \hat{X}_i)^2,$$

from which it follows that

$$\hat{\beta}^2 = \hat{\sigma}_f^2 / \hat{\sigma}_e^2$$
.

Since this result is unreasonable, so in order to get a satisfactory result the need of making some assumptions about error variances obviously arises.

Lindley makes the assumption that $\lambda = \sigma_f^2 / \sigma_e^2$ is known and gets his estimator $\hat{\beta}$,

$$\hat{\beta} = o_1 + \sqrt{o_1^2 + \lambda}$$

where

$$o_1 = \frac{\sum (y_i - \bar{y})^2 - \lambda \sum (x_i - \bar{x})^2}{2 \sum (x_i - \bar{x})(y_i - \bar{y})},$$

provided that the denominator of o_1 does not vanish. The positive or negative sign is taken when $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. When $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. When $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. When $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. When $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. When $\sum (x_i - \bar{x})(y_i - \bar{y}) < 0$ or > 0. This method fails to estimate β if we have $\lambda = \sum (y_i - \bar{y})^2 / \sum (x_i - \bar{x})^2$.

Madansky considers several assumptions and obtains following estimates.

(i) When σ_f^2 is known

$$\hat{\beta} = \frac{\sum (y_i - \bar{y})^2 - n \sigma_f^2}{\sum (x_i - \bar{x})(y_i - \bar{y})},$$

(ii) When σ_e^2 is known

$$\hat{\beta} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x}))^2 - n\sigma_e^2},$$

- (iii) When $\lambda = \sigma_f^2 / \sigma_e^2$ is known, the estimate is the same as that of Lindley.
- (iv) When both σ_e^2 and σ_f^2 are known

$$\hat{\beta} = \frac{\sum (y_i - \bar{y})^2 - n\sigma_f^2}{\sum (x_i - \bar{x})^2 - n\sigma_e^2},$$

the sign to be taken as that of $\sum (x_i - \bar{x})(y_i - \bar{y})$.

Dorff and Gurland (1961) propose an estimator of β when λ is unknown. They consider the situation when replicated observations are available and $s_i/r_i=g$. They first take $\stackrel{\Lambda}{\lambda}=W_{yy}/W_{xx}$, and then they suggest following estimate, assuming that e_i , f_i are nomally distributed.

$$b_4 = \frac{\theta}{g} \pm \sqrt{\frac{\theta^2}{g^2} + \frac{\hat{\lambda}}{g}}$$

where

$$\theta = \frac{\mathbf{B}_{yy} - \hat{\lambda} \mathbf{B}_{xx}}{2\mathbf{B}_{xy}}$$

provided $B_{xy}=0$. The positive or negative signs are chosen according as $B_{xy}>0$ or <0. For the case $B_{xy}=0$, $b_4=0$ is taken provided $\lambda = B_{yy}/B_{xx}$. Dorff and Gurland also obtain asymptotic variance of estimator b_4 under certain assumptions about the first four moments of the distribution of errors. The expression for this is lengthy and is therefore not being given here.

3.2. Method of Grouping

Several statisticians have taken an approach to grouping of observations for estimation of β . Wald (1940) who was the first to adopt this

method, makes the assumption that the errors e_i and f_i are uncorrelated. If i is the order number when the observations are arranged ascendingly according to values of X_i , Wald gives an estimator

$$b_{\mathbf{W}} = \frac{\sum_{i=1}^{n} y_{i} - \sum_{i=1}^{m} y_{i}}{\sum_{i=1}^{n} x_{i} - \sum_{i=1}^{m} x_{i}}, m = \frac{n}{2}$$

provided n is even. This estimator has been shown to be consistent if $\lim_{n \to \infty} [(X_1 + X_2 + \dots + X_m) - (X_{m+1} + \dots + X_n)/n] > 0.$

Bartlett (1949) uses the same concept of grouping on the assumption that n is divisible by 3. His estimator is

$$b_{\mathbf{B}} = \frac{\sum_{i=1}^{n} y_{i} - \sum_{i=1}^{m_{1}} y_{i}}{\sum_{i=1}^{n} \frac{m_{1}}{m_{1}}}$$

$$\sum_{i=1}^{m_{1}} x_{i} - \sum_{i=1}^{m_{1}} x_{i}$$

$$m_{2} + 1 \qquad 1$$

where $m_1 = \frac{n}{3}$, $m_2 = \frac{2n}{3}$. He shows that this is a more efficient estimator.

Gibson and Jowett (1957), Theil and Van Yzeren, Housner and Brennan (1948) have further refined Bartlett's scheme.

Dorff and Gurland (1961) consider the estimator

$$b_{L} = \frac{\sum w_{i} y_{i}}{\sum w_{i} x_{i}}$$

where the w_i are weights such that $\sum w_i = 0$. This estimator is consistent provided the expectation of $\sum w_i x_i$ does not vanish. It is easy to see that the family of b_L includes as special cases of the estimators b_W , b_L and the one that of Housner and Brennan (1948) who suggested the use of b_H where $w_i = i - \bar{i}$. Dorff and Gurland obtain following asymptotic variance of b_L

$$\operatorname{var}(b_{L}) = (\sigma_{f}^{2} + \beta^{2} \sigma_{e}^{2}) \frac{\sum w_{i}^{2}}{(\sum w_{i}X_{i})^{2}},$$

They found that this variance is minimized by choosing.

$$w_i = c (\mathbf{X}_i - \overline{\mathbf{X}}),$$

where c is any arbitrary contant other than zero. Since the spacing of the X_i is generally unknown, we cannot find w_i and then we may use $b_{\mathbf{w}}$, or $b_{\mathbf{B}}$, or $b_{\mathbf{H}}$ for estimation of β . If the \mathbf{X}_i are equally spaced, $b_{\mathbf{H}}$ has the smallest asymptotic variance. If there are only two levels of \mathbf{X}_i such that

$$X_i = A$$
 $i = 1, \dots, \frac{n}{2}$
= B $i = \frac{n}{2} + 1, \dots, n$

then Wald's estimator is best to use. If the X_i are evenly divided among only three levels, b_B is preferred. They showed that b_H is more robust than b_W or b_B as its asymptotic variance does not greatly exceed the optimum unless the X_i are bunched or badly skewed.

All such methods of grouping should obviously be open to objection in the sense that the group limits are based on only the observed values and not on some external criterion.

3.3. Use of Instrumental Variables

Another approach to estimate β is through the use of an instrumental variable 2, that is, a variable which is correlated with X, Y but uncorrelated with errors of observation. Geary (1949) derives following estimator of β .

$$\dot{\mathbf{p}} = \frac{\sum \mathbf{Z}_i \, \mathbf{y}_i}{\sum \mathbf{Z}_i \, \mathbf{x}_i}$$

where $\sum Z_i x_i - \rightarrow 0$ as $n \rightarrow \infty$. Geary also obtains an estimate of the variance of $\hat{\beta}$.

3.4. Use of Variance Components

Dorff and Garland (1961) make the use of covariance analysis in estimating β when replicated observations are available. They assume that at least one of the r_i and atleast one of the s_i are more than unity. On the basis of results

E
$$(B_{xx}) = \frac{1}{n-1} \sum r_i (X_i - \overline{X})^2 + \sigma_e^2$$

E $(W_{xx}) = \sigma_e^2$
E $(B_{yy}) = \frac{1}{n-1} \sum s_i (Y_i - \overline{Y})^2 + \sigma_f^2$
E $(W_{yy}) = \sigma_f^2$
E $(B_{xy}) = \frac{1}{n-1} \sum r_i (X_i - \overline{X})(Y_i - \overline{Y})$
E $(B'_{xy}) = \frac{1}{n-1} \sum s_i (X_i - \overline{X})(Y_i - \overline{Y}),$

they suggest that

$$b_1 = \frac{B_{xy}}{B_{xx} - W_{xx}}, b_2 = \frac{B_{yy} - W_{yy}}{B'_{xy}}, b_3 = \sqrt{\frac{B_{yy} - W_{yy}}{g(B_{xx} - W_{xx})}}$$

are the consistent estimators of β where $g = \frac{s_i}{r_i}$ is contant for each *i*. It may be noted that the denominator cannot have vanishing expectations unless all the X_i are identical.

These results, when $r_i=s_i=N_i$ for all i, agree with those of Madansky (1959) who also uses covariance analysis to estimate β .

Dorff and Gurland also find asymptotic variances of their estimators (expressions are lengthy and are therefore being omitted here). They compare these variances of the estimators b_1 , b_2 , b_3 when $r_i = s_i = r$ for each i. They discover that

- (i) b_1 is the best estimator if $\beta^2 < r_0 \lambda$
- (ii) b_2 is the best estimator if $\beta^2 > r_0 \lambda$
- (iii) b_3 is the best estimator if $r^{-1} \lambda < \beta^2 < r_0 \lambda$,

where
$$r_o^2 = \frac{r-1}{r} + \sqrt{\left(\frac{r-1}{r}\right)^2 + 3}$$
, and $\lambda = \sigma_f^2 / \sigma_e^2$. The use of b_4 is recommended when r_o is equal or close to unity.

Up to this point we have considered the assumption that the errors e_i , f_i are independently distributed. We shall now consider below the case where e_i , f_i are correlated.

Dorff and Gurland (1961) also deal with this situation when $r_i = s_i = r$ for each i. The estimators proposed are

$$b_{1} = \frac{B_{xy} - W_{xy}}{B_{xx} - W_{xx}}$$

$$b_{2} = \frac{B_{yy} - W_{yy}}{B_{xy} - W_{xy}}$$

$$b_{3} = \sqrt{\frac{B_{yy} - W_{yy}}{B_{xx} - W_{xx}}}$$

$$b_{4} = \theta + \sqrt{\theta^{2} + L}$$

where

$$\theta = \frac{B_{yy} - \hat{\lambda}B_{xx}}{2(B_{xy} - \hat{R} B_{xx})}$$

$$L = \frac{\hat{\lambda}B_{xx} - \hat{R} B_{yy}}{B_{xy} - \hat{R} B_{xx}}$$

$$\hat{\lambda} = \frac{W_{yy}}{W_{xx}}, \quad \hat{R} = \frac{W_{xy}}{W_{xx}}$$

provided that $B_{xy} - R^{\hat{A}} B_{xx} \neq 0$,

$$b_4 = -\frac{\hat{\lambda} B_{xy} - \hat{R} B_{yy}}{B_{yy} - \hat{\lambda} B_{xx}}$$

when $B_{xy} - \hat{R} B_{xx} = 0$ and $B_{yy} - \hat{\lambda} B_{xx} \neq 0$. The estimator b_4 is not used when the expression $B_{yy} - \hat{\lambda} B_{xx}$ is also zero. All these estimators are consistent provided expectations of their denominators are nonvanishing.

They find similar results, as earlier stated in case of independent errors, when it comes to choosing the best of b_1 , b_2 , b_3 ,

3.5. Generalised Least squares Method

Sprent (1966) generalises the least squares principles to deal with the situations in which the departures e_i , f_i of the observed values x_i , y_i from the corresponding values X_i , Y_i are distributed as follows:

$$var e_i = \sigma_{11}$$

cov
$$(e_i, f_i) = \sigma_{12}$$
 for all i
var $f_i = \sigma_{22}$

He assumes that

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}$$
 is nonsingular

and e_i , f_i are uncorrelated with e_j , f_j for $i \neq j$.

$$x_i = X_i + e_i$$

$$y_i = Y_i + f_i$$

into

$$Y-\beta X=0$$
 (the origin shifted to obtain it),
 $Y_i-\beta X_i=e_i-f_i$.

Taking

$$z_i = Y_i - \beta X_i$$

it is seen that

$$var (z_i) = \beta^2 \sigma_{11} - 2 \beta \sigma_{12} + \sigma_{22}$$

$$cov (z_i, z_j) = 0 \qquad i \neq j.$$

The sum of squared residuals with weights inversely propotional to their respective variances is

$$U = \frac{\sum z_{i}^{2}}{\beta^{2} \sigma_{11} - 2 \beta \sigma_{12} + \sigma_{22}}$$
$$= \frac{\beta^{2} S_{11} - 2 \beta S_{12} + S_{22}}{\beta^{2} \sigma_{11} - 2 \beta \sigma_{12} + \sigma_{22}}$$

where S_{ij} are elements of sample covariance matrix

$$S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}.$$

The procedure for the estimation of β is to minimise U. It can be seen that

$$\frac{d\mathbf{U}}{d\mathbf{B}} = \mathbf{0}$$

gives the normal equations and an approximate estimate of β is

$$\hat{\beta} = \frac{S_{12} - \eta \ \sigma_{12}}{S_{11} - \eta \ \sigma_{11}}$$

$$\eta = -\frac{K + \sqrt{K^2 - 4 \mid \Sigma \mid \mid \mid S \mid}}{2 \mid \Sigma \mid}$$

and

$$K=2 \sigma_{12} S_{12} - \sigma_{11} S_{22} - \sigma_{22} S_{11}$$
.

Special cases.

- (i) If $\sigma_{11}=0$, the estimate of β reduces to $\frac{S_{12}}{S_{11}}$ which is an estimate of regression coefficient of y on x.
 - (ii) If $\sigma_{12} = 0$, then

$$\hat{\beta} = \frac{\sigma_{11} S_{22} - \sigma_{22} S_{11} + \sqrt{(\sigma_{11} S_{22} - \sigma_{22} S_{11})^2 + 4 \sigma_{11} \sigma_{22} S_{12}^2}}{2 \sigma_{11} S_{12}}$$

(iii) If $\sigma_{11} = \sigma_{22}$, it is interesting to see that $\hat{\beta}$ is independent of σ_{11} and σ_{22} .

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THE NUMBER OF PERMUTATIONS ON N SYMBOLS WHICH CONTAIN AT LEAST ONE CYCLE OF LENGTH i>1

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The total number of permutations on n symbols is n!. However, if we look at the permutations with the cycle-structure given by the partition.

1. $\alpha_1 + 2$. $\alpha_2 + \ldots + n$. $\alpha_n = n$ (1)

of n, their number is

$$\frac{n!}{\alpha_1! \alpha_2! \dots \alpha_n! 1^{\alpha_1} 2^{\alpha_2} \dots n^{\alpha_n}}$$
 (2)

An interesting problem that arises in this connection is to find the number of those permutations which contain at least one cycle of given length $i \ge 1$. One method of attempting to solve this problem would be to look at all the partitions of n with $\alpha_i \ge 1$ and to sum expressions of the type given in equation (2) over such partitions. This procedure does no seem to be immediately applicable. Our solution below uses difference-equation techniques.

Let the required number be represented by the symbol P_n^I . Evidently

$$P_0^i = P_1^i = \dots = P_{i-1}^i = 0$$
 (3)

We divide the n! permutations on n symbol into n sets $S_1, S_2, \ldots S_n$ such that the set S_j consists of those permutations which contain the symbol "1" in a cycle of length j. Then the set S_j ($1 \le j \le n, j \ne i$)

contributes $\frac{(n-1)!}{(n-i)!} P_{n-i}^i$ permutations to P_n^i , whereas the set S_i contri-

butes (n-1)! permutations to P_n^i . Thus P_n^i satisfies the recursion relation

$$P_{n}^{i} = (n-1)! \left[1 + \sum_{\substack{j=1 \ j \neq 1}}^{n} \frac{P_{n-j}^{i}}{(n-j)!}\right]$$
(5)

 $(:P_0^1=0)$, the sum on the right hand side is effective only upto n-1).

$$\mathbf{P}_{n}^{i}=n! \mathbf{Q}_{n}^{i}$$

We obtain from (5)

$$Q_n^i - Q_{n-1}^i = -\frac{1}{n} \left[Q_{n-i}^i - Q_{n-i-1}^i \right]$$
 (7)

The initial conditions (3) and (4) for P_n^i result in the following initial $Q_o^i = Q_1^i = \dots = Q_{i-1}^i = 0$ $Q_o^i = Q_1^i = \dots = Q_{i-1}^i = 0$ conditions for Q_n^l :

$$Q_0^i = Q_1^i = \dots = Q_{i-1}^i = 0$$
 (8)

$$Q_{1}^{i} = \frac{1}{i}$$

$$Q_{1}^{i} = \frac{1}{i}$$
(9)

Writing

$$n=mi+i', 0 \le i' \le i-1, m \ge 0$$

we obtain from equations (7) - (10)

$$Q_n^i = Q_{mi}^i = \sum_{j=1}^m \frac{(-1)^{j-1}}{i^j \times j!}$$
 (11)

for n > i. For n < i, $Q_n^i = 0$ consistent with equation (8). Thus

$$P_{n}^{i} = P_{mi+i'} = n! \sum_{j=1}^{m} \frac{(-1)^{j-1}}{i^{j} \times j!}$$

$$0 \le i' \le i-1$$
(12)

for $n \ge i$ while for n < i, $P_n^i = 0$.

Using our previous results we can also compute the number of permutations on n symbol s which contain exactly one cycle of length i. This number comes out to be

$$\frac{n!}{(n-i)!} \left[(n-i)! - P_{n-i}^{i} \right] \\
= \frac{n!}{i} \sum_{j=0}^{m-1} \frac{(-1)^{j}}{i^{j} \times j!} \tag{13}$$

for $n \geqslant i$.

The right hand side of equations (12) and (13) are equal for n=i to $P_i^i = (i-1)!$

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A NOTE ON DIRECT SUMS OF QUASI-INJECTIVE MODULES

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We shall assume throughout that R denotes an associative ring with identity and that all R-modules are unitary right R-modules. For the definitions and fundamental results on quasi-injective modules, we refer to Johnson and Wong [7].

The following two theorems give necessary and sufficient condition on modules for a finite direct sum of quasi-injective modules to be quasi-injective. It may be remarked that both these theorems are, in fact, easy deductions from a fundamental result of Johnson and Wong [7, Theorem 1.1] on quasi-injective modules. However, their proofs are also included here.

Theorem 1. Let R be any ring and $M = \bigoplus_{i=1}^{n} M_i$ be a direct sum of quasi-injective R-modules. Then M is quasi-injective if and only if M_i Hom_R (E (M_i) , E (M_j)) \subseteq M_j for each $i, j=1, \ldots, n$; where E (M_i) denotes the injective hull of M_i .

Proof. We have $M = \bigoplus_{i=1}^{n} M_i$. Let F be the injective hull of M and

 $E_i = E(M_i)$ be the injective hull of M_i . Then $E = \bigoplus_{i=1}^n E_i$. Let $\bigwedge = \operatorname{Hom}_{\mathbf{R}}$

(E, E). By Johnson and Wong [7, Theorem 1.1] M is quasi-injective if and only if $M \wedge \subseteq M$. In other words, M is quasi-injective if and only if $m\lambda \in M$ where m and λ are arbitrary elements of M and \wedge respectively.

Since $\lambda \in \Lambda$, $\lambda = (\lambda_i j)$ where $(\lambda_i j)$ denotes an $n \times n$ matrix and $\lambda_i j$ is the composition of the restriction of λ to E_i with the projection from E to E_j and so $\lambda_i j \in \operatorname{Hom}_{\mathbf{R}}(E_i, E_j)$.

If m is an element in M then we can write $m=(m_1, \ldots, m_n)$ where $m_i \in M_i$; $i=1, \ldots, n$. Then it follows easily that $m_i : \lambda = \sum_{j=1}^{n} m_i : \lambda_{i,j}$.

In order that $m \lambda \in M$, it is necessay and sufficient that $m_i \lambda_{ij} \in M_j$. In other words, for $m\lambda$ to be in M for all λ , it is necessary and sufficient that M_i Hom_R $(E_i, E_j) \subset M_j$ for all λ_{ij} . This proves the theorem.

Corollary (i). Let $M = \bigoplus_{i=1}^{n} M_i$ be a direct sum of quasi-injective modules over any ring. Then M is quasi-injective if and only if M_i Hom_R $(M_i, E(M_j)) \subseteq M_j$ $(i, j=1, \ldots, n)$.

Proof. Clearly M_i Hom_R $(M_j, E(M_j)) \subset M_j$ implies Hom_R $(E(M_i), E(M_j)) \subset M_j$. Hence by the above theorem, M is quasi-injective.

Conversely, let us suppose that M is quasi-injective. Then, by the above theorem, M_i Hom_R $(E_i, E_j) \subseteq M_j$ $(i, j=1, \ldots, n)$. Let $\theta \in \text{Hom}_R$ (M_i, E_j) , Since M_i is a submodule of E_i and E_j is injective, it follows that θ extends to an R-homomorphism ϕ from E_i to E_j . Then M_i $\theta = M_i$ $\phi \subseteq M_i$ Hom_R $(E_i, E_j) \subseteq M_j$.

Therefore, M_i Hom_R $(M_i, E_j) \subseteq M_j$ which proves the corollary.

The above theorem also yields the following two corollaries which are already known.

Corollary (ii). Let R be any ring and N a quasi-injective R-module.

If $M = \bigoplus_{i=1}^{n} M_i$, where each $M_i = N$, then M is quasi-injective (See Jane and Wu [6], Proposition 2.5).

Corollary (iii). Let M be any quasi-injective module and E=E (M) be the injective hull of M. Then $M \oplus E$ is quasi-injective if and only if M=E [See Har da [5], Proposition 2.4].

We now state the following lemma which was proved by Matlis [8].

Lemma 1. Let R be a right Noetherian ring and $M = \bigoplus M_i$ be any $i \in I$ direct sum of R-modules M_i . If E (M) is the injective hull of M then $E(M) = \bigoplus_{i \in I} E(M_i)$ where $E(M_i)$ denotes the injective hull of M_i .

Using the above lemma and arguments similar to those which we used to establish Theorem 1, we can prove the following theorem.

Theorem 2. Let R be a right Noetherian ring. If $M = \bigoplus_{i \in I} M_i$ is a direct sum of quasi-injective R-modules then M is quasi-injective if and only if M_i Hom_R (E (M_i) , E $(M_j) \subseteq M_j$ for each $i, j \in I$.

Again, the following corollary can be derived from the above theorem.

Corollary. Let R be right Noetherian and M a quasi-injective R-module. If $A = \bigoplus_{i \in I} M_i$ with each $M_i = M$ then A is also quasi-injective.

In [2], Faith and Walker called an injective R-module M Σ — (countably Σ —) injective if a direct sum of arbitrarily (countably) many copies of M is again injective. We shall call a quasi-injective R-module M Σ —(countably Σ —) quasi-injective if a direct sum of arbitrarily (countably) many copies of M is also quasi-injective.

Finally, in form of the following theorem, we formulate a result which is implicitly known in the literature (See e.g. Faith and Walker [2] and Osofsky [9] and also Chase [1, Proposition 4.1, Page 471]).

Theorem 3. Let R be a ring such that every injective R-module is countably Σ -quasi-injective then R is right Noetherian.

Proof. (Following Faith and Walker [2]). Let $O=I_1 \subset I_2 \subset \ldots$; be an ascending chain of right ideals of R Let us consider the R-modules R/I_i ; $i=1, 2, \ldots$, Let $Q_i = E(R/I_i)$ be the injective hull of R/I_i . Als, let us write $Q=\bigoplus Q_i$ and $M=\mathcal{T}Q_i$. Since any direct product of injective modules is injective, M, is injective. Therefore, $\bigoplus M_i$, where each $M_i = M_i$, is quasi-injective by our assumption.

Let
$$M_j = \pi Q_i = Q_j \oplus P_j$$
 where $P_j = \pi Q_i$.
Then $\bigoplus M_j = \bigoplus_{j \in \mathbb{N}} Q_j \oplus \bigoplus_{j \in \mathbb{N}} P_j$.

Thus Q becomes a direct summand of a quasi-injective module. Hence Q is quasi-injective.

Let $I = \bigcup_k$. Then the natural homomorphism $f_k : I \to R/I_k$ maps I into Q_k . Also, if $a \in I$, then $a \in I_t$ for some t and then f_k (a) = 0, for all $k \ge t$.

Let $f(a) = (f_1(a), \dots, f_i(a), \dots)$; $a \in I$. Then $f(a) \in Q$ since only a finite number of terms are non-zero. Also, f is an R-homomorphism from I into Q.

Since $I \subseteq R \subseteq Q_1 \subseteq Q$ and Q is quasi-injective, there exists a map $\lambda \in Hom_R(Q, Q)$ which induces f. Let us suppose that $\lambda(1) = m$, where 1 is the identity of R, then $\lambda x = mx$, for all $x \in R$.

Clearly,
$$m \in \mathbb{Z}$$
 \mathbb{Z} \mathbb{Q}_i for some t and then $f(I) \subseteq m \mathbb{R} \subseteq \mathbb{Z}$ \mathbb{Q}_i This

shows that $I_{t+1} = I_{t+2} = \dots = I$ and R is, therefore, right Neotherian. This completes the proof.

The above theorem immediately gives the following corollary which is Theorem 2.3 of Fuller [3]. (See also Fuller [4] for a correction in the proof of this theorem).

Corollary. Let R be any ring. Then each quasi-injective R-module is Σ -quasi-injective if and only if R is right Noetherian.

[43]

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A NOTE ON THE GENERALISED BATEMAN k-FUNCTION

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1. Introduction.

Recently the author published an article entitled "Some theorems on the generalised Bateman k-function" in the Punjab University Journal of Mathematics, Vol. 6, pp 35-66, (1973) in which there are a number of misprints and errors. In the present article the author has pointed out the misprints and corrected the results.

2. Corrections.

Page 47, Line 16 from the top; read equation (4.6) instead of (4.5). In the equations (3.1), (3.4), (3.7), (3.8), (4.3) to (4.8), (4.10), (4.11), (4.26) and (5.28) read \rightleftharpoons instead of =. Between the two terms inside the square bracket of the equations (2.8), (2.12), 4.6) and (5.20) read + instead of - and of the equations (5.21), (5.22), (5.23), (5.28), (5.29) and (5.30) read - instead of +.

The first term inside the square bracket of the result (2.1) should be $K_{n+u-2r\pm 1}^{\nu}$ (x), the second term on the right of the result (2.6) should

be
$$-K_n^{u+2, v}(x)$$
 and on the right of the result (2.9) $\frac{x}{2}$ should be re-

placed by
$$\left(\frac{x}{2}\right)^{\frac{\nu+1}{2}}$$
. Also on the right of the results (2.23) a and (2.23) b

read
$$K_{n-1}^{u, v+1}(x)$$
 instead of $K_{n-1}^{u, v}(x)$, the result (3.4) read $K_{2n}^{2l+2r}(x)$

instead of
$$K_{2n}^{2m+2l}(x)$$
 and that of the result (3.5) read $(-1)^{l+1}$ instead

of $(-1)^m$. In the formula (2.24) read $D_x K_n^{u, v}(x)$ instead of $D_x K_n^{u, v+2}(x)$.

In the result (3.5) and the equation (3.8) the function ϕ_2 should be read as follows.

$$\phi_2$$
 $\left[l+m+1, l+m, 1; 2l+2; t, -t, -\frac{(1+x)}{(1-x)}t\right]$

On the right of the result (4.6) read $(-1)^r$ instead of x^r and the result (4.9) should be corrected as follows.

$$e^{-\frac{x}{2}} K_{2n}^{2m, 2l} \left(\frac{x}{2}\right) = \sum_{r=0}^{m} (-1)^{n-l-1} {m \choose r} \frac{2^{-2l-2r}}{\Gamma(n+l+r+1)} D_x^{n-l-r-1} \times \left[e^{-x} \cdot x^{n+l+r}\right]$$

On account of the correction in the result (4.9) the result of Theorems 15 and 16 also need correction. But this is not difficult as these results are the particular cases of (4.9)

The left hand side of (4.23) should be $\sum_{n=1}^{\infty} \frac{(-1)^n}{2n} K_{2n}^{-2, 0} (\pm x).$

Although u has been chosen to be -2 the integral representing $K_{2n}^{-2,0}$ ($\pm x$) exists and the series under consideration is absolutely covergent.

The first term on the right of the results (5.1) and 5.5) should be $\frac{\Gamma(\nu+\frac{3}{2})}{\Gamma(\nu+2)}\pi^{-\frac{1}{2}}$ and in the last term of (5.5) x should be replaced by 0.

Under the integral sign of the result (5.14) read $K_{2n+1}^{u, v}(x)$ instead of $K_{2n-1}^{u, v}(x)$ and in the result (5.19) read y^{2l+1} instead of y^{2l} .

In the equation (5.28) the expression inside the Square Bracket on the left should be $p^{w+\frac{1}{2}(n-l-r-1)}/[1+\sqrt{p}]^{n+l+r+1}$ and on the right side the last term in the second row of the G-functions should be

read as
$$\frac{-(l+r)+w}{2}$$
 instead of $-\frac{l+r+w}{2}$.

ACKNOWLEDGEMENTS

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CONTENTS

		Page
I.	SOME APPROXIMATIVE METHODS FOR COM- PUTING CROSS-SECTIONS.	
	Jerzy Rayski	1
II.	COMPUTER SOLUTIONS OF NAGUMO'S EQ- UATION.	
	M. Iqbal	15
III.	VARIOUS APPROACHES TO ESTIMATING A LINEAR FUNCTIONAL RELATION.	
	Ahmed Zogo Memon	23
IV.	THE NUMBER OF PERMUTATIONS ON N SYMBOLS WHICH CONTAIN AT LEAST ONE CYCLE OF LENGTH $i \ge 1$.	
	M. A. Rashid	35
V.	A NOTE ON DIRECT SUMS OF QUASI-INJECTIVE MODULES.	
	Javed Ahsan	39
VI.	A NOTE ON THE GENERALISED BATEMAN k-FUNCTION.	
	T. N. Srivastava	45