CERN 64 - 13
28 February 1964

ORGANISATION EUROPÉENNE POUR LA RECHERCHE NUCLÉAIRE
CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

PROCEEDINGS OF THE 1964 EASTER SCHOOL FOR PHYSICISTS

Using the CERN Proton Synchrotron
and Synchro-Cyclotron

Herceg-Novi, May 18 - 31, 1964

by invitation of the

YUGOSLAV FEDERAL NUCLEAR ENERGY COMMISSION

Volume I. Contributions by:

D. Hudson
L. Jauneau
D. Morellet
B. Ronne
A. Werbrouck

GENEVA

CERN 64 - 13
28 February 1964

PROCEEDINGS OF THE 1964 EASTER SCHOOL FOR PHYSICISTS

Using the CERN Proton Synchrotron
and Synchro-Cyclotron

Herceg-Novi, May 18 - 31, 1964

by invitation of the

YUGOSLAV FEDERAL NUCLEAR ENERGY COMMISSION

Volume I. Contributions by:

D. Hudson
L. Jauneau
D. Morellet
B. Ronne
A. Werbrouck

G E N E V A

SCIENTIFIC ORGANIZING COMMITTEE

Dr. R. Armenteros	(CERN)
Prof. E.H.S. Burhop	(University of London)
Dr. J.C. Combe	(CERN)
Prof. M. Juric	(University of Belgrade)
Dr. W.O. Lock	(CERN)
Dr. M. Nikolic	(CERN)
Miss E.W.D. Steel	(CERN)
Prof. L. Van Hove	(CERN)

EDITORIAL BOARD FOR THE PROCEEDINGS

Dr. W.O. Lock	(CERN)
Dr. M. Nikolic	(CERN)
Prof. L. Van Hove	(CERN)

7863/p/cm

TABLE DES MATIERES - CONTENTS

L. Jauneau et D. Morellet

CONTENTS OF VOLUME II.

CONTENTS OF VOLUME III.

PREFACE

This report contains the first set of contributions for the 1964 CERN Easter School which will be held at Herceg Novi, Yugoslavia in May. This school is primarily intended for young experimental physicists engaged in the analysis of bubble chamber pictures and of events in nuclear emulsions. These notes and those in Volumes II and III deal with topics that are relevant for their work. This Volume contains three papers dealing with statistics and its applications, kinematical analysis of pictures and the Monte Carlo Method.

We wish to express our gratitude to the authors for their collaboration in the preparation of these papers. We also wish to thank Mrs. V. Cooper, who has kindly assisted in this work, the Documents Typing and Reproduction Services whose efforts with the help of the Scientific Information Service made it possible to produce three volumes of the Proceedings within a short time, and to Miss M. Hutin and Miss C. Mason for their careful typing of the text.

Editorial Board

11th March, 1964
Geneva.

NOTIONS DE STATISTIQUE ET APPLICATIONS

L. Jauneau et D. Morellet
Ecole Polytechnique, Paris

INTRODUCTION

Le but de ces notes est de regrouper sous une forme aussi simple que possible les principales notions et méthodes statistiques habituellement utilisées dans la Physique des Hautes Energies. Les démonstrations qu'on y trouvera sont destinées à mieux faire comprendre l'enchaînement et le domaine d'application des diverses lois de probabilité, des "tests statistiques" et des méthodes d'estimation. Elles ne prétendent nullement à la rigueur.

Les deux premiers chapitres s'inspirent largement, rigueur en moins, du cours de Probabilités de Monsieur George Darmois, le dernier chapitre sur l'estimation par la méthode des moindres carrés (fits) des excellents résumés que l'on peut trouver dans les rapports spécialisés du CERN.

7863/p/mh

I. RAPPELS DE PROBABILITES

DEFINITIONS

VARIABLE ALEATOIRE ET VARIABLE CERTAINE

On appelle VARIABLE ALEATOIRE une grandeur pouvant prendre une suite finie ou infinie de valeurs, avec une certaine loi de probabilité.

Ex.: Le nombre de grains d'une trace d'une particule dans l'émulsion sur un intervalle de 100 microns varie d'un intervalle à l'autre et n'est déterminé qu'en moyenne.

L'énergie d'une particule dont on observe la trace est une variable certaine, mais le résultat de la mesure est une variable aléatoire.

Une particule subit des diffusions dans la traversée d'un écran : la déviation latérale et l'angle de sortie sont des variables aléatoires.

La variable aléatoire X peut être :

- DISCONTINUE : valeurs $x_1 \quad x_2 \ldots x_i \ldots$

  probabilités $p_1 \quad p_2 \ldots p_i \ldots$, avec $\sum_i p_i = 1$

- CONTINUE :

probabilité de trouver la variable entre x et x + dx = f(x)dx, avec $\int f(x)dx = 1$.

Que la variable soit continue ou discontinue, l'expérience fournit une suite de n valeurs ($x_1 \ldots x_n$) appelée ECHANTILLON ou STATISTIQUE.

On cherche à caractériser cet ensemble de valeurs par certains paramètres :

MOYENNE : $\langle x \rangle = \dfrac{\sum x_i}{n}$

MODE ou valeur la plus probable

MEDIANE : terme milieu de la suite des n valeurs rangées

D'autres parametres caracterisent la manière dont la distribution s'écarte de la valeur moyenne.

ESPERANCE MATHEMATIQUE (généralisation de la moyenne)

Pour une variable discontinue : $E(X) = \sum_i p_i x_i$

pour une variable continue : $E(X) = \int x f(x) dx$

Propriétés :

$$E(X + Y) = E(X) + E(Y)$$

$E(X Y) = E(X) E(Y)$, si les variables X et Y sont indépendantes (c'est-à-dire si la probabilité p_{ij} d'avoir x_i et y_j est égale au produit des probabilités p_i et p_j d'obtenir x_i et y_j - ou si la densité de probabilité $F(x,y)$ peut se mettre sous la forme : $F(x,y) = f(x)\ g(y)$).

On appelle VARIABLE CENTREE $\xi = X - E(X)$

$E(X)$ n'est que le premier terme d'une suite :

$$E(X)\ \ E(X^2)\ \ E(X^3)\ \ \ldots\ E(X^h)\ \ \ldots \text{ MOMENTS DE X}$$

On caractérise la largeur de la distribution par :

$$E(\xi^2) = E[X - E(X)]^2 \quad \text{(moment "centré")}$$

soit : $$E(\xi^2) = E(X^2) - [E(X)]^2$$

$\sigma^2 = E(\xi^2)$ est la VARIANCE de la loi de distribution de X.

σ est l'ECART-TYPE (ou écart quadratique moyen, ou déviation standard)

On appelle VARIABLE REDUITE l'expression $\frac{X - E(X)}{\sigma_X}$.

Problème général de la statistique

On ne connaît de la variable aléatoire X qu'un échantillon $(x_1, x_2, \ldots x_n)$. Souvent la forme analytique de la loi de distribution est connue. L'échantillon fournit une estimation des paramètres de cette loi (ESTIMATION PARAMETRIQUE) :

E(X) est estimée par la moyenne $\langle x \rangle = \frac{\Sigma x_i}{n}$

σ^2 est estimée par la moyenne des carrés des écarts par rapport à $\langle x \rangle$.

Propriétés de σ^2

1°/ Additivité des variances

soit : $X = Y + Z$

d'où : $E(X) = E(Y) + E(Z)$

$\xi = \eta + \zeta$ variables centrées

$E(\xi^2) = E(\eta^2) + E(\zeta^2) + E(\eta\,\zeta)$

Si les variables Y et Z sont indépendantes : $E(\eta\,\zeta) = E(\eta)\,E(\zeta) = 0$

d'où :

$$\sigma_X^2 = \sigma_Y^2 + \sigma_Z^2$$

Exemple : si la détermination d'une grandeur est entachée d'erreurs, les erreurs partielles s'ajoutent quadratiquement.

2°/ Ecart-type de la moyenne d'un échantillon

D'une population constituée par l'ensemble de toutes les valeurs de la grandeur X, on a extrait un échantillon de n valeurs $x_1, x_2, \ldots x_n$, la moyenne $\langle x \rangle$ est aussi une variable aléatoire.

soit : $E(X) = \Theta$

$$\sigma^2_{<x>} = E\left[<x> - \Theta\right]^2 = E\left[\frac{x_1 + \ldots + x_n}{n} - \Theta\right]^2 = \frac{1}{n^2} E\left[(x_1 - \Theta) + \ldots + (x_n - \Theta)\right]^2$$

$$= \frac{1}{n^2} \sum_i \underbrace{E(x_i - \Theta)^2}_{\sigma^2}$$

en supposant les n valeurs x_i indépendantes

variance de x

d'où :

$$\boxed{\sigma_{<x>} = \frac{\sigma}{\sqrt{n}}}$$

3°/ Estimation de la variance d'après un échantillon

La dispersion dans la population totale, $\sigma^2 = E(x - \Theta)^2$, se compose

- de la dispersion des n valeurs x_i autour de leur moyenne (dispersion intérieure a l'échantillon),

soit : $\sum \frac{[x_i - <x>]^2}{n}$

- de la dispersion de la moyenne autour de $E(X) = \Theta$, soit $\frac{\sigma^2}{n}$.

La propriété d'additivité des variances conduit à :

$$\sigma^2 = \sum \frac{(x_i - <x>)^2}{n} + \frac{\sigma^2}{n} .$$

D'où :

$$\boxed{\text{Estimation de } \sigma^2 = \frac{\sum (x_i - <x>)^2}{n - 1}}$$

Remarque

Nous avons vu que la variance σ^2 de la somme algébrique de variables aléatoires indépendantes est égale à la somme des variances. Il n'existe malheureusement pas de définition aussi simple de la variance du produit ou du quotient de deux variables aléatoires, ou plus généralement d'une fonction de variables aléatoires. Il faut se contenter d'expressions approchées (voir "PROPAGATION DES ERREURS").

LES LOIS DU HASARD

Le HASARD est défini ici comme un ensemble de causes très nombreuses, indépendantes, et ayant chacune une influence très faible.

Nous considérerons 3 cas :

1°/ REALISATION D'UN EVENEMENT A

p est la probabilité pour que A se réalise, q = 1 - p la probabilité pour que A ne se réalise pas, ou que l'événement contraire B se réalise. C'est le probleme classique de l'urne contenant deux espèces de boules, des naissances masculines ou féminines... On fait une série de n épreuves indépendantes : l'événement A se produit k fois. On choisit comme variable aléatoire le nombre des succès, k, ou la fréquence des succès, $f_n = \frac{k}{n}$. La loi de probabilité de k est :

$$P_k = C_n^k \, p^k \, q^{n-k} \qquad \text{avec} \quad C_n^k = \frac{n\,!}{k\,!(n-k\,!)}$$

Loi binômiale (Bernoulli)

Affectons chaque épreuve d'une variable aléatoire prenant les valeurs 1 ou 0 :

X_i → 1 probabilité p ; 0 probabilité q

donc : $E(X) = p$

Le nombre des succès (réalisation de A) est :

$$k = X_1 + X_2 + \ldots X_n$$

D'où :

$$\boxed{E(k) = np \quad \text{et} \quad E(f_n) = p}$$

et $\sigma^2 = E[k - E(k)]^2 = E[X_1 - p + X_2 - p + \ldots + X_n - p]^2$

$= E[\xi_1 + \xi_2 + \ldots + \xi_n]^2 = n\, E(\xi^2)$

puisque les épreuves sont supposées indépendantes.

X	$\xi = X - p$	Probabilité
1	q	p
0	- p	q

Or, $E(\xi^2) = p(q^2) + q(p^2) = pq$;

D'où :

$$\boxed{\sigma_k = \sqrt{n\,p\,q} \qquad \sigma_{f_n} = \sqrt{\frac{p\,q}{n}}}$$

p = probabilité de réalisation d'un événement A, q = 1 - p

n épreuves indépendantes

Variable aléatoire	Nombre des succès	Fréquence des succès
	k	$f_n = \frac{k}{n}$
Espérance mathématique	np	p
Ecart-type	$\sqrt{npq}$	$\sqrt{\frac{pq}{n}}$

Si $n \to \infty$, $f_n \to p$ LOI DES GRANDS NOMBRES

2°/ VARIABLE DISCONTINUE NE PRENANT QUE DES VALEURS ENTIERES

Exemple : des points sont distribués au hasard sur une droite (cas idéal des grains qui matérialisent la trajectoire d'une particule dans l'émulsion). On compte ceux qui se trouvent dans un intervalle pris au hasard sur la droite.

k = nombre de points sur l'intervalle ΔL

g = densité des points

$m = g\Delta L$

Nous montrerons que la loi de probabilité de k est :

$$P_k = e^{-m} \frac{m^k}{k!}$$ LOI DE POISSON

P_k représente aussi la probabilité d'observer k événements, alors qu'on s'attend à en obtenir m,

$$E(k) = \sum_{k=1}^{\infty} kP_k = e^{-m}\, m \sum_{k=1}^{\infty} \frac{m^{k-1}}{(k-1)!} = m$$

$$\sigma_k^2 = m$$

En effet :

$$E(X^2) = \sum_{k=1}^{\infty} k^2 P_k = \sum_{k} (k^2 - k + k)\, P_k \qquad \text{avec} \quad P_k = e^{-m} \frac{m^k}{k!}$$

(k=0 ne contribue pas)

D'où :

$$E(X^2) = e^{-m} \left[\sum_{k=0}^{\infty} k(k-1) \frac{m^k}{k!} + \sum_{k=1}^{\infty} k \frac{m^k}{k!} \right]$$

(k=1 ne contribue pas)

$$= e^{-m} \left[m^2 \underbrace{\sum_{k=2}^{\infty} \frac{m^{k-2}}{(k-2)!}}_{e^m} + m \underbrace{\sum_{k=1}^{\infty} \frac{m^{k-1}}{(k-1)!}}_{e^m} \right] = m^2 + m$$

$$\sigma^2 = E(X^2) - [E(X)]^2 = (m^2 + m) - (m)^2 = m$$

3°/ VARIABLE CONTINUE

Nous montrerons qu'une variable continue dépendant d'une infinité de causes, indépendantes, ayant toutes une action infiniment petite, obéit à une LOI DE LAPLACE-GAUSS :

La probabilité d'observer une valeur de X comprise entre x et x + dx est,

$$f(x)dx = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-\Theta)^2}{2\sigma^2}} \frac{dx}{\sigma}$$

Θ = valeur centrale
σ^2 = variance

Exemple : Dans la traversée d'un écran, une particule chargée subit une diffusion coulombienne multiple : l'angle de sortie obéit à une loi de Gauss.

Les lois de Gauss et de Poisson sont également des cas limites de la loi binômiale :

LOI BINOMIALE

n épreuves

GRANDES SERIES

La probabilité de réalisation de l'événement A reste finie.

n, k → ∞

$f_n = \frac{k}{n}$ → variable continue

LOI DE GAUSS

de valeur centrale p

d'écart-type $\sqrt{\frac{pq}{n}}$

m grand

PETITES SERIES

n → ∞, mais la probabilité de réalisation de l'événement devient extrêmement petite; de sorte que :

m = E(k) = np reste fini

LOI DE POISSON

E(k) = np = m

$\sigma_k = \sqrt{m}$

D'autre part, si m devient grand, k tend vers une variable continue et on montre que la loi de Poisson tend asymptotiquement vers une loi de Gauss : On considère alors $\sqrt{m}$ comme l'écart-type d'une variable gaussienne (valable pour m > 30).

QUELQUES DEMONSTRATIONS

La façon la plus simple d'étudier l'origine et les propriétés des lois du hasard que nous venons d'énoncer consiste à introduire la TRANSFORMEE DE FOURIER de la loi de probabilité, appelée FONCTION CARACTERISTIQUE.

On définit donc : $\varphi_X(t) = E\, e^{it\,X}$

c'est-à-dire : $\varphi_X(t) = \sum_i pi\, e^{it\,x_i}$ pour une variable discontinue

$\varphi_X(t) = \int e^{it\,x} f(x)\,dx$ pour une variable continue.

La fonction caractéristique de la somme de variables aléatoires indépendantes est égale au produit de leurs fonctions caractéristiques.

D'autre part, on peut développer $\varphi_X(t)$:

$$\varphi_X(t) = 1 + it\,E(X) + \frac{(it)^2}{2!}\,E(X^2) + \ldots + \frac{(it)^h}{h!}\,E(X^h) + \ldots$$

Les coefficients du développement sont les "moments" de la distribution de X.

Un changement de variable et d'échelle s'exprime simplement sur la fonction caractéristique :

$$\text{si} \quad \xi = \frac{X - a}{b} \qquad \varphi_\xi(t) = e^{-i\frac{a}{b}t}\,\varphi_X\left(\frac{t}{b}\right) .$$

Exemples :

LOI BINOMIALE

X	Prob.
1	p
0	q

$$\varphi_X(t) = p\, e^{it} + q$$

$$\boxed{\varphi_k(t) = \left(p\, e^{it} + q\right)^n}$$

LOI DE POISSON $\qquad P_k = e^{-m}\,\frac{m^k}{k!}$

$$\varphi_k(t) = \sum_k P_k\, e^{itk} = \sum_k e^{-m}\,\frac{(m\, e^{it})^k}{k!} = e^{-m}\, e^{me^{it}}$$

$$\boxed{\varphi_k(t) = e^{m(e^{it}-1)}}$$

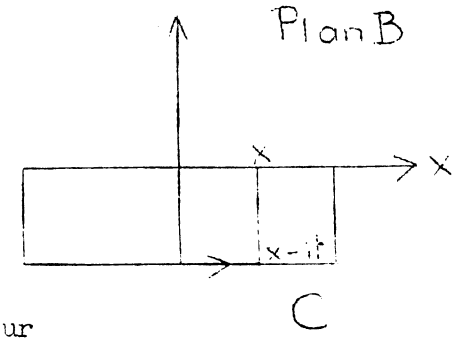
(On retrouve, en développant $\varphi(t)$, le résultat $E(X^2) = m^2 + m$).

LOI DE GAUSS

Soit x la variable réduite : $f(x) = \frac{1}{\sqrt{2\pi}}\, e^{-\frac{x^2}{2}}$

$$\varphi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{itx}\, e^{-\frac{x^2}{2}}\, dx = \frac{e^{-\frac{t^2}{2}}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{(x-it)^2}{2}}\, dx$$

soit une intégrale de la forme $\int_{-\infty}^{+\infty} e^{-\frac{z^2}{2}}\, dz$.



Intégrons sur le contour C :

$$\int_C e^{-\frac{z^2}{2}}\, dz = 0 \text{ (pas de pôle à l'intérieur de C)}$$

Si $|x| \to \infty$, les contributions des petits côtés tendent vers 0

Donc : $$\int_{-\infty}^{+\infty} e^{-\frac{(x - it)^2}{2}} dx = \int_{-\infty}^{+\infty} e^{-\frac{x^2}{2}} dx = \sqrt{2\pi}$$

et $$\boxed{\varphi(t) = e^{-\frac{t^2}{2}}}$$

ETUDE DE LA LOI DE POISSON

Considérons des points distribués au hasard sur une droite, et soit λ la plus petite distance entre 2 points consécutifs (on suppose qu'il n'y a pas de point d'accumulation).

On découpe l'intervalle ΔL sur lequel on compte les points en n intervalles égaux Δx tels que $\Delta x < \lambda$: $\Delta x = \frac{\Delta L}{n}$,

Soit g la densité des points sur la droite. Posons $m = g\Delta L$

La probabilité d'avoir 1 point sur Δx est : $g\Delta x$

———————— 0 ———————— est : $1 - g\Delta x$

1°/ Associons à chaque intervalle une variable aléatoire X prenant les valeurs

$X = 1$ s'il existe un point sur Δx prob. $= g\Delta x$

0 ———————— 0 ———————— prob. $= 1 - g\Delta x$

La fonction caractéristique de X est :

$$\varphi_X(t) = g\Delta x\, e^{it} + (1 - g\Delta x) = 1 + g\Delta x\,(e^{it} - 1)$$

$$g\Delta x = g\frac{\Delta L}{n} = \frac{m}{n}$$

Le nombre de points sur ΔL, c'est-à-dire sur n intervalles Δx, est :

$$k = \sum_{1}^{n} X_i \quad , \qquad \text{d'où :}$$

$$\varphi_k(t) = \left[\varphi_X(t)\right]^n = \left[1 + \frac{m(e^{it} - 1)}{n}\right]^n$$

Si $n \to \infty$ $\qquad \varphi_k(t) = e^{m(e^{it} - 1)} \longrightarrow$ LOI DE POISSON

$2^o/$ Cherchons maintenant la loi de probabilité des intervalles entre deux points consécutifs.

La probabilité d'avoir 0 point sur Δx est $1 - g\Delta x$;

La probabilité d'un intervalle ΔL, c'est-à-dire la probabilité d'avoir 0 point sur $\Delta L = n\Delta x$ est donc :

$$(1 - g\Delta x)^n = \left(1 - \frac{g\Delta L}{n}\right)^n \longrightarrow e^{-g\Delta L}$$

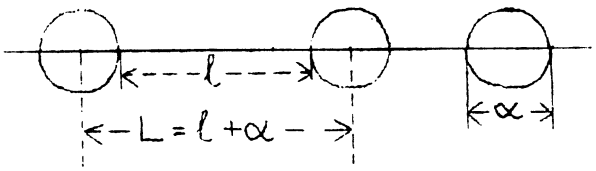
La loi de probabilité normalisée est :

$$\boxed{f(\Delta L) = g e^{-g\Delta L}} \qquad g = \frac{1}{\langle \Delta L \rangle}$$

$\langle \Delta L \rangle$ = distance moyenne entre 2 points.

Application

Traces de particules chargées dans une émulsion. On suppose que les centres de développement sont distribués au hasard le long de la trace, avec une densité g, et que tous les grains développés ont le même diamètre α .



La loi de probabilité (normalisée à 1) de l'intervalle L est :

$$f(L) = ge^{-gL}$$

La probabilité intégrale (d'observer un intervalle >L) est :

$$F(L) = \int_L^\infty f(\ell)\, d\ell = e^{-gL}$$

Le nombre d'intervalles >L par unité de longueur est :

$$N(L) = g\, F(L) = ge^{-gL}$$

On compte les "blobs" et les "gaps" (Voir PH Fowler et D.H. Perkins, Phil. Mag. 46,587, Juin 1955).

La densité des "blobs" est égale (± 1) au nombre d'intervalles visibles, c'est-à-dire L > α

$$B = ge^{-g\alpha}$$

D'autre part :

$$H = ge^{-gL} = ge^{-g\alpha}\, e^{-g\ell} = Be^{-g\ell}$$

$$L = \ell + \alpha$$

H est la densité des "gaps" de longueur $\geq \ell$.

Pour les traces de faible ionisation, le comptage des grains fournit une bonne approximation de g. Ces distributions sont bien vérifiées par l'expérience.

3°/ Dans le cas des PETITES SERIES, la LOI BINOMIALE tend vers la LOI DE POISSON.

La fonction caractéristique de la loi binômiale est :

$$\varphi_k(t) = (pe^{it} + q)^n = [1 + p(e^{it} - 1)]^n$$

Hypothèses :

n devient très grand, p devient très petit, mais de sorte que le produit np = m reste fini.

D'où : $\varphi_k(t) = \left[1 + \frac{m(e^{it} - 1)}{n}\right]^n \longrightarrow \boxed{e^{m(e^{it} - 1)}}$ (Loi de Poisson)

4°/ Si m devient grand, la LOI DE POISSON tend asymptotiquement vers la LOI DE GAUSS.

Passons à la variable réduite $\xi = \frac{k - m}{\sqrt{m}}$:

$$\varphi_\xi(t) = e^{-it\sqrt{m}} \; \varphi_k\left(\frac{t}{\sqrt{m}}\right)$$

Or, $$m(e^{it} - 1) = mit + m\frac{(it)^2}{2!} + m\frac{(it)^3}{3!} + \ldots$$

$$\varphi_\xi(t) = e^{-it\sqrt{m}} \; e^{\left[it\sqrt{m} + \frac{(it)^2}{2!} + \frac{1}{\sqrt{m}}\frac{(it)^3}{3!} + \ldots\right]}$$

$$= e^{\left[-\frac{t^2}{2} + \frac{1}{\sqrt{m}}\frac{(it)^3}{3!} + \frac{1}{m}\frac{(it)^4}{4!} + \ldots\right]}$$

Donc, si m devient grand,

$$\boxed{\varphi_\xi(t) \to e^{-\frac{t^2}{2}}}$$

Fonction caractéristique de la loi de Gauss

LOI DE GAUSS ou LOI DES GRANDS NOMBRES

Considérons n variables indépendantes $X_1 \ldots X_n$, supposées centrées et normées, suivant la même loi de probabilité (de Moivre) :

$$Z = X_1 + X_2 + \ldots + X_n$$

$$\varphi_X(t) = 1 + \frac{(it)^2}{2!} + \ldots$$

Posons : $$\psi_X(t) = \text{Log}\, \varphi_X(t) = \text{Log}(1 + \lambda) = \lambda - \frac{\lambda^2}{2} + \frac{\lambda^3}{3} + \ldots$$

(2ème fonction caractéristique)

Donc, $\psi_X(t)$ peut se mettre sous la forme générale :

$$\psi_X(t) = -\frac{t^2}{2}\,[1 + \epsilon(t)]$$

$$\psi_Z(t) = n\,\psi_X(t) \quad \text{et} \quad \psi_{\frac{Z}{\sqrt{n}}}(t) = -\frac{t^2}{2}\left[1 + \epsilon\left(\frac{t}{\sqrt{n}}\right)\right]$$

$$\epsilon\left(\frac{t}{\sqrt{n}}\right) \to 0 \text{ pour } n \to \infty \text{ si } t \text{ est borné}$$

Donc, $$\lim \psi(t) = -\frac{t^2}{2} \to \lim \varphi(t) = e^{-\frac{t^2}{2}}$$

fonction caractéristique de la Loi de Gauss.

Laplace généralise ce résultat dans son THEOREME SUR LA LOI DES ERREURS D'OBSERVATION : si les erreurs élémentaires sont indépendantes, petites et du même ordre de grandeur, et si leurs lois de probabilités, a priori différentes, obéissent à certaines conditions très générales de convergence, leur somme suit sensiblement la loi de Laplace-Gauss.

Ce théorème justifie, au moins particllement, l'optimisme habituel du physicien dans les calculs d'erreurs : même si leurs origines sont différentes, les causes d'erreurs sont assez nombreuses pour que le résultat puisse être considéré comme gaussien. On peut dire : tout fini par être gaussien !!.

Dans le cas particulier de la loi binômiale, on peut vérifier que $\varphi_\xi(t)$, avec

$$\xi = \frac{k - np}{\sqrt{npq}} = \frac{f_n - p}{\sqrt{\frac{pq}{n}}}, \quad \text{est de l'ordre de } e^{-\frac{t^2}{2}} \text{ pour n grand,}$$

c'est-à-dire que la loi binômiale tend asymptotiquement vers la loi de Gauss pour les grandes séries.

GRANDEURS ALEATOIRES A PLUSIEURS DIMENSIONS

VARIABLES INDEPENDANTES ET VARIABLES LIEES EN PROBABILITE

Sur chaque objet de la population, on mesure plusieurs caractères par exemple le poids et la taille d'un individu.

Autre exemple : un faisceau parallèle de particules traverse un écran : on détermine à la sortie de l'écran la déviation angulaire Θ et le déplacement latéral y de chaque trajectoire.

Limitons-nous pour le moment à 2 caracteres X et Y. On définit, comme dans le cas d'une seule variable, $E(X)$, $E(Y)$, σ_X, σ_Y.

Les deux variables X et Y, tout en étant soumises au hasard, peuvent avoir un lien de causalité : la connaissance de l'une réduit, dans une certaine mesure, l'indétermination de l'autre; on dit alors qu'elles sont liées en probabilité (liaison stochastique),

Considérons le cas de variables continues : la probabilité d'observer à la fois X entre x et x + dx et Y entre y et y + dy est égale à la probabilité d'observer X entre x et x + dx multipliée par la probabilité d'observer Y entre y et y + dy si l'on sait que X est compris entre x et x + dx, c'est-à-dire :

$$f(x,y)\,dx\,dy = \underbrace{a(x)\,dx}_{\text{probabilité marginale de x}} \times \underbrace{C_x(y)\,dy}_{\text{probabilité de y liée par x}}$$

$$a(x) = \int_{-\infty}^{+\infty} f(x,y)\,dy \qquad C_x(y) = \frac{f(x,y)}{\int f(x,y)\,dy}$$

De même :

$$f(x,y)dx\,dy = b(y)\,dy \times C_y(x)\,dx$$

Les variables X et Y sont <u>indépendantes</u> si la densité de probabilité est le produit des probabilités marginales :

$$f(x,y) = a(x)\,b(y)$$

c'est-à-dire si la loi liée est identique à la loi marginale.

Pour chaque valeur de x, on définit : une moyenne de y liée par x :

$$\langle y \rangle_x = \int y\, f(x,y)\,dy$$

un écart-type de y lié par x.

Le lieu de $\langle y \rangle_x$ est la COURBE DE REGRESSION de y en x. Mêmes définitions pour x fonction de y.

LE COEFFICIENT DE CORRELATION

a) Faisons d'abord l'hypothèse de l'indépendance des variables X et Y (supposées centrées et normées). Les lois marginales sont des lois de Gauss :

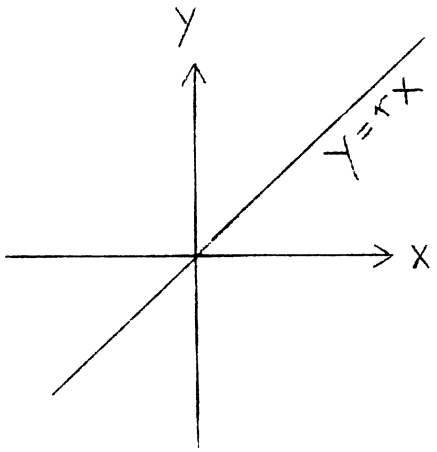
$$a(x) = \frac{1}{\sqrt{2\pi}}\, e^{-\frac{x^2}{2}} \qquad b(y) = \frac{1}{\sqrt{2\pi}}\, e^{-\frac{y^2}{2}}$$

La loi de probabilité de la variable aléatoire à 2 dimensions (X,Y) est donc :

$$f(x,y) = \frac{1}{2\pi} \; e^{-\frac{1}{2}(x^2 + y^2)}$$

Si les deux variables X et Y ne sont pas indépendantes, la somme des carrés $x^2 + y^2$ devient une forme quadratique $ax^2 + 2bxy + cy^2$ (un moyen simple d'obtenir des variables liées consiste à prendre deux combinaisons linéaires indépendantes des variables X et Y). Une telle forme quadratique peut toujours s'écrire $Ax^2 + (Bx - Cy)^2$ et on peut voir que la courbe de régression *) de y en x est une droite.

b) Cherchons donc à ajuster les observations (x_i, y_i) avec la droite $y = rx$ par la méthode des moindres carrés :



$$S = \frac{\sum_{i=1}^{n} (y_i - rx_i)^2}{n} \quad \text{doit être minimum,}$$

c'est-à-dire : $\frac{\partial S}{\partial r} = 0$

$$S = \frac{\sum y_i^2}{n} - 2r \frac{\sum x_i y_i}{n} + r^2 \frac{\sum x_i^2}{n}$$

$$= 1 - 2r \frac{\sum x_i y_i}{n} + r^2 \qquad \left(\frac{\sum x_i^2}{n} = \sigma_X^2 = 1, \text{ de même pour } y \right)$$

$$\frac{\partial S}{\partial r} = 0 \longrightarrow \boxed{r = \frac{\sum x_i y_i}{n}}$$

---

*) Origine du terme "régression". Ce terme provient d'une étude biométrique sur la corrélation entre les tailles des couples père-fils (Galton). Si la taille des pères, soit x, est supérieure à la moyenne de la race, il en est de même de la taille moyenne des fils, $\langle y \rangle_x$, mais dans une proportion moindre : la taille des fils régresse vers la taille de la race. Ce terme de régression est resté en statistique.

r est LE COEFFICIENT DE CORRELATION calculé à partir des observations. Le coefficient de corrélation théorique est : $\rho = E(XY)$.

Pour des variables non réduites :

$$\rho = \frac{E[X - E(X)][Y - E(Y)]}{\sigma_X \sigma_Y}$$

$y = \rho x$ est la moyenne de y à x donné : c'est l'équation de la droite de régression de y en x.

$S = 1 - \rho^2$ représente la variance de la variable Y liée par X.

La variable liée centrée et normée est donc $Y - \rho X / 1 - \rho^2$.

Les variables X et $Y - \rho X$ sont indépendantes : $E[X(Y - \rho X)] = 0$.

Loi marginale de X :

$$a(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$

Loi de Y liée par X :

$$C_x(y) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{1 - \rho^2}} e^{-\frac{(y - \rho x)^2}{2(1 - \rho^2)}}$$

D'ou :

$$f(x,y) = \frac{1}{2\pi\sqrt{1 - \rho^2}} e^{-\frac{1}{2} \frac{x^2 - 2\rho xy + y^2}{1 - \rho^2}}$$

$\rho = \pm 1$: corrélation parfaite, c'est-à-dire dépendance fonctionnelle

$\rho = 0$: corrélation nulle

Exemples

1. Déviation angulaire Θ et déplacement latéral y d'une trace à la sortie d'un écran d'épaisseur t.

(y et t mesurés en longueur de radiation)

Θ = angle projeté sur un plan.

Fermi a calculé la loi de probabilité de Θ et y :

$$F_t(\Theta,y) = \underbrace{\frac{\sqrt{3}}{2\pi}\,\frac{\omega^2}{t^2}}_{A}\; e^{-\omega^2\left[\frac{\Theta^2}{t} - \frac{3\Theta y}{t^2} + \frac{3y^2}{t^3}\right]}$$

où : $\omega = \dfrac{2\,p\beta c}{E_s}$ $\qquad E_s = \sqrt{4\pi \times 137\, m_e u^2} = 21$ MeV

$$E(\Theta) = 0 \qquad E(y) = 0$$

Le coefficient de l'exponentielle peut s'écrire :

$$a\Theta^2 + 2b\Theta y + cy^2 \qquad \text{avec } a = \frac{2\omega^2}{t} \quad b = -\frac{3\omega^2}{t^2} \quad c = \frac{6\omega^2}{t^3}$$

$$= \left(a - \frac{b^2}{c}\right)\Theta^2 + c\left(y + \frac{b}{c}\Theta\right)^2$$

$$= \left(c - \frac{b^2}{a}\right)y^2 + a\left(\Theta + \frac{b}{a}y\right)^2$$

D'où les lois marginales :

en Θ : $A\sqrt{\dfrac{2\pi}{c}}\; e^{-\frac{1}{2}\left(a - \frac{b^2}{c}\right)\Theta^2} = \dfrac{1}{\sqrt{2\pi}}\,\dfrac{\omega}{\sqrt{2t}}\; e^{-\frac{1}{2}\frac{\omega^2}{2t}\Theta^2}$

en y : $A\sqrt{\frac{2\pi}{a}}\, e^{-\frac{1}{2}\left(c - \frac{b^2}{a}\right) y^2} = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2}} \frac{\omega}{t^{3/2}}\, e^{-\frac{1}{2}\left(\frac{3}{2}\frac{\omega^2}{t^3}\right) y^2}$

D'où :

$$\sigma_\Theta = \frac{\sqrt{2t}}{\omega} \qquad \left(\sigma_\Theta^2 = \frac{1}{2}\left(\frac{Es}{p\beta c}\right)^2 t\right)$$

La linéarité en t résulte de l'additivité des variances.

$$\sigma_y = \sqrt{\frac{2}{3}}\, \frac{t^{3/2}}{\omega} \longrightarrow \sigma_y^2 = \frac{1}{3}\, t^2 \sigma_\Theta^2$$

Passons aux variables réduites $u = \frac{\Theta}{\sigma_\Theta}$ $v = \frac{y}{\sigma_y}$:

$$\left[\frac{2\omega^2}{t}\Theta^2 - \frac{6\omega^2}{t^2}\Theta y + \frac{6\omega^2}{t^3} y^2\right] = 4\left(u^2 - 2\frac{\sqrt{3}}{2} uv + v^2\right)$$

$$A = \frac{1}{2\pi}\sqrt{3}\frac{\omega^2}{t^2} = \frac{1}{2\pi}\,\frac{1}{2\,\sigma_\Theta \sigma_y}$$

La loi de probabilité peut s'écrire :

$$f(u,v) = \frac{1}{2\pi\sqrt{1-\rho^2}}\, e^{-\frac{1}{2}\frac{u^2 - 2\rho uv + v^2}{1-\rho^2}} \qquad \text{avec} \quad \boxed{\rho = \frac{\sqrt{3}}{2}}$$

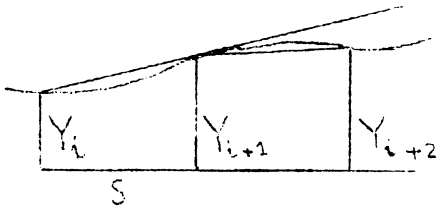
La droite de régression de Θ en y est :

$$\Theta = r\,\frac{\sigma_\Theta}{\sigma_y}\, y = \frac{3}{2t}\, y \qquad \text{(moyenne de } \Theta \text{ liée par y)}$$

2. Angles de diffusion entre cordes, Corrélation entre 2 angles successifs.

On mesure les flèches Y aux extrémités des cellules t.

On calcule les différences premières y et les différences secondes D.



L'angle entre 2 cordes successives est :

$$\omega_i = \frac{D_i}{t} = \frac{y_i + 1 - y_i}{t}$$

La différence entre ces y calculés est égale à celle entre les y de Fermi au second ordre près. D'où :

$$\sigma_\omega^2 = \frac{2}{t^2}\sigma_y^2 = \frac{2}{3}\sigma_\Theta^2$$

$$\boxed{\sigma_\omega = \sqrt{\frac{2}{3}}\,\sigma_\Theta}$$

Deux angles successifs entre cordes utilisent une partie commune de la trajectoire et ne sont donc pas indépendants.

Considérons une trace de longueur L grande devant la cellule t :

$$\Sigma\,\omega_i \not\equiv \Sigma\,\Theta_i$$

D'où :

$$\frac{1}{n}\left(\Sigma\,\omega_i\right)^2 = \frac{1}{n}\left(\Sigma\,\Theta_i\right)^2$$

Remarquons que $\langle \omega_i\, \omega_{i+1} \rangle \neq 0$, mais :

$$\langle \omega_i\, \omega_{i+2} \rangle = 0 \ \ldots \text{ et } \langle \Theta_i\, \Theta_{i+1} \rangle = 0$$

$$\langle \omega^2 \rangle + 2\langle \omega_i\, \omega_{i+1} \rangle = \langle \Theta^2 \rangle$$

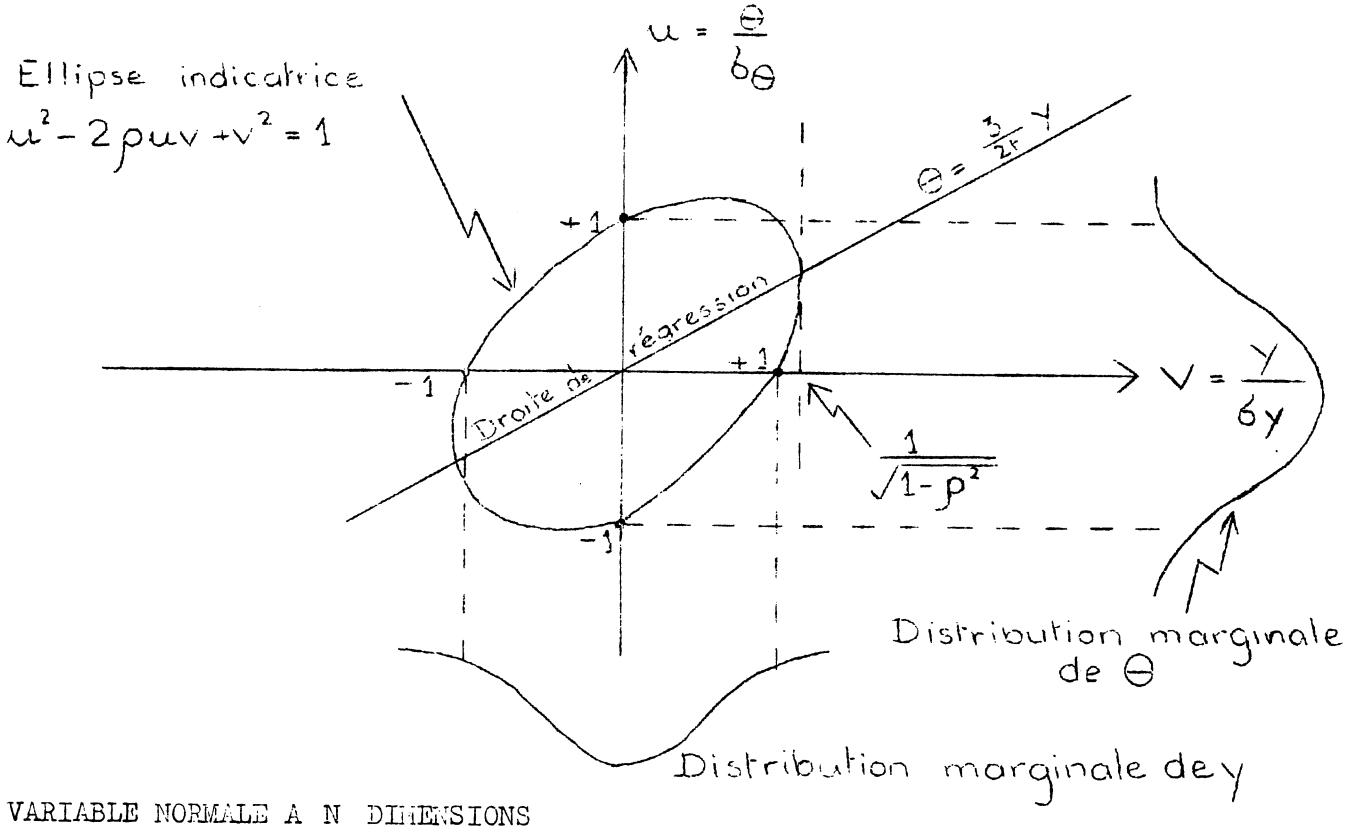
soit :

$$2 \langle \omega_i \, \omega_{i+1} \rangle = \sigma_\Theta^2 - \sigma_\omega^2 = \frac{1}{3} \sigma_\Theta^2$$

$$\boxed{\langle \omega_i \, \omega_{i+1} \rangle = \frac{1}{6} \sigma_\Theta^2}$$

D'où le coefficient de corrélation :

$$\rho = \frac{\langle \omega_i \, \omega_{i+1} \rangle}{\sigma_\omega^2} = \frac{1}{4}$$



VARIABLE NORMALE A N DIMENSIONS

Vecteur aléatoire $X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}$

$$M = E(X) = \begin{pmatrix} E(X_1) \\ \vdots \\ E(X_N) \end{pmatrix} = \begin{pmatrix} m_1 \\ \\ m_N \end{pmatrix}$$

Supposons les variables $X_1 \ldots X_N$ centrées. Si elles sont indépendantes, la loi de probabilité est le produit de N lois de Gauss :

$$f(x_1, x_2, \ldots x_N) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_1} e^{-\frac{1}{2}\frac{x_1^2}{\sigma_1^2}} \times \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_2} e^{-\frac{1}{2}\frac{x_2^2}{\sigma_2^2}}$$

$$\times \ldots\ldots \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_N} e^{-\frac{1}{2}\frac{x_N^2}{\sigma_N^2}} = \frac{1}{(2\pi)^{N/2}} \frac{1}{\sigma_1\sigma_2\ldots\sigma_N} e^{-\frac{1}{2}\left[\frac{x_1^2}{\sigma_1^2} + \frac{x_2^2}{\sigma_2^2} + \ldots + \frac{x_N^2}{\sigma_N^2}\right]}$$

La forme quadratique [ ] peut s'écrire : $X^T G' X$ *)

$$\text{avec} \quad G' = \begin{pmatrix} \frac{1}{\sigma_1^2} & & \\ & \frac{1}{\sigma_2^2} & \\ & & \ddots \; \frac{1}{\sigma_N^2} \end{pmatrix} = V'^{-1}$$

$$V' = \begin{pmatrix} \sigma_1^2 & & \\ & \sigma_2^2 & \\ & & \ddots \; \sigma_N^2 \end{pmatrix} = E(XX^T)$$

$$\frac{1}{\sigma_1\sigma_2\ldots\sigma_N} = \sqrt{\det G'} = \frac{1}{\sqrt{\det V'}}$$

N variables indépendantes :

$$f(x_1, x_2, \ldots x_N) = \frac{1}{(2\pi)^{N/2}} \frac{1}{\sqrt{\det V'}} e^{-\frac{1}{2} X^T G' X} \qquad V' = E(XX^T) \qquad G' = V'^{-1}$$

---

*) T indique l'opération transposition : $X^T = (X_1 \ldots X_n) \ldots$

On peut toujours passer de N variables quelconques Y_i aux variables indépendantes X par une transformation orthogonale C : $(C^T C = 1)$

$$\left.\begin{array}{l} X = CY \\ X^T = Y^T C^T \end{array}\right\} \rightarrow X^T G' X \rightarrow Y^T G\, Y \text{ avec} \qquad G = C^T G' C$$

$$V'G' = 1 \rightarrow \underbrace{C^T V' C}_{V}\, C^T G' C = 1 \rightarrow VG = 1$$

$$V = C^T V' C = E[\, C^T X\, X^T C] = E(YY^T)$$

D'autre part : det V' = det V, D'où :

LOI DE GAUSS A N VARIABLES

$$f(y_1 \ldots y_N) = \frac{1}{(2\pi)^{N/2}} \frac{1}{\sqrt{\det V}}\, e^{-\frac{1}{2} Y^T G Y} \qquad Y^T G Y = H(y_1 \ldots y_N)$$

$$V = E(YY^T) = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 & \rho\sigma_1\sigma_3 \ldots \\ \rho\sigma_1\sigma_2 & \sigma_2^2 & \ldots\ldots\ldots \\ \ldots\ldots\ldots & & \\ \ldots\ldots\ldots & & \end{pmatrix}$$

MATRICE DES VARIANCES (ou des covariances)

$G = V^{-1}$ est la MATRICE DES POIDS

Démonstration par la fonction caractéristique

La fonction caractéristique est définie par :

$$\varphi(t_1, t_2 \ldots t_N) = E\left(e^{i(\, t_1 X_1 + t_2 X_2 + \ldots + t_N X_N)}\right) = E\, e^{i\vec{t}\,.\,\vec{X}}$$

$\vec{t}$ et $\vec{X}$ vecteurs d'un espace à N dimensions

Dans le cas d'une loi normale, φ est toujours de la forme :

$$\varphi = e^{-\frac{1}{2} K(t_1 \ldots t_N)}$$

K étant une forme quadratique en $t_1 \ldots t_N$ qui peut s'écrire

$$K = t^T V t$$

a) Nature de V. Développons l'exponentielle dans les 2 expressions de φ:

$$\varphi = E[1 + i\vec{t},\vec{X} - \frac{1}{2} (\vec{t} \cdot \vec{X})^2 + \ldots] \qquad E(\vec{X}) = 0 \quad \text{(variables centrées)}$$

$$= 1 - \frac{1}{2} E(t_1^2 X_1^2 + t_2^2 X_2^2 + \ldots + 2 t_1 t_2 X_1 X_2 + \ldots)$$

$$= 1 - \frac{1}{2} (\sigma_1^2 t_1^2 + \sigma_2^2 t_2^2 + \ldots + 2 t_1 t_2 \sigma_1 \sigma_2 \rho_{12} + \ldots)$$

(ou encore : $\varphi = 1 - \frac{1}{2} \sum_{ij} t_i t_j E(X_i X_j)$)

D'autre part :

$$\varphi = 1 - \frac{1}{2} K(t_1 \ldots t_N) + \ldots$$

Identifions les termes quadratiques :

$$K = E(\vec{t} \cdot \vec{X})^2 = t^T V t$$

avec $\boxed{V_{ij} = E(X_i X_j)}$ MATRICE DES COVARIANCES

b) La densité de probabilité est de la forme :

$$f(\vec{X}) = A\, e^{-\frac{1}{2} H(x_1 \ldots x_N)} \qquad H = X^T G X$$

La relation entre densité de probabilité et fonction caractéristique s'écrit alors :

$$\int e^{i\vec{t}\cdot\vec{X}} A\, e^{-\frac{1}{2} X^T G X}\, d\vec{X} = e^{-\frac{1}{2} t^T V t} \qquad (1)$$

Par une substitution orthogonale C ($C^T C = 1$), nous pouvons rendre les n variables X_i indépendantes, c'est-à-dire réduire la forme quadratique H à ses axes principaux, ou encore "diagonaliser la matrice G" : $\boxed{X = CY}$,

d'où : $X^T G X \rightarrow Y^T \underbrace{C^T G C} Y = Y^T G' Y$ $\qquad G' = \begin{pmatrix} \alpha_1 & & \\ & \alpha_2 & \\ & & \ddots \\ & & & \alpha_N \end{pmatrix}$

($\alpha_i = \frac{1}{\sigma_i^2}$ pour les nouvelles variables)

D'autre part :

$$\vec{t}\cdot\vec{X} = t^T X = t^T C Y = u^T Y = \vec{u}\cdot\vec{Y}$$

avec : $u^T = t^T C \rightarrow u^T C^T = t^T$ et $\boxed{t = Cu}$

La relation (1) devient :

$$\int e^{i\vec{u}\cdot\vec{Y}} A\, e^{-\frac{1}{2} Y^T G' Y}\, d\vec{Y} = e^{-\frac{1}{2} u^T V' u} \qquad V' = C^T V C$$

Le jacobien d'une transformation orthogonale est égal à 1.

Il y a décomposition en un produit de termes :

$$\int e^{iu_k y_k} e^{-\frac{1}{2}\alpha_k y_k^2} dy_k = \sqrt{\frac{2\pi}{\alpha_k}}\, e^{-\frac{1}{2}\frac{u_k^2}{\alpha_k}}$$

Donc :

$$\int e^{i\vec{u}\cdot\vec{Y}} \frac{\sqrt{\alpha_1\alpha_2\ldots\alpha_N}}{(2\pi)^{N/2}} e^{-\frac{1}{2}Y^T G' Y} d\vec{Y} = e^{-\frac{1}{2}u^T G'^{-1} u}$$

donc : $V' = G'^{-1}$ soit : $C^T V C\, C^T G C = 1 \rightarrow \boxed{G = V^{-1}}$

D'autre part :

$$\alpha_1\alpha_2\ldots\alpha_N = \det G' = \det G = \frac{1}{\det V}$$

D'où :

$$\boxed{f(\vec{X}) = \frac{1}{(2\pi)^{N/2}} \frac{1}{\sqrt{\det V}} e^{-\frac{1}{2}X^T V^{-1} X}}$$

(voir Cramer, p. 118)

FONCTION D'UN VECTEUR ALEATOIRE NORMAL

"PROPAGATION" DE LA MATRICE DES VARIANCES

1°/ Fonction linéaire :

Soit U = AX où X est un vecteur aléatoire normal, A une matrice non aléatoire.

$$E(X) = M \qquad E(U) = AM$$

$$V_U = E\{[U - E(U)]\,[U - E(U)]^T\} = E\{A[X - M]\,[X - M]^T A^T\} = AE[(X - M)(X - M)^T]A^T$$

donc $\boxed{V_U = A\, V_X A^T}$

2°/ Fonction quelconque

$U = U(X)$, c'est-à-dire : $u_1 = f_1(x_1 \ldots x_n)$

$u_2 = f_2(x_1, x_2 \ldots x_n)$

$\ldots\ldots\ldots\ldots\ldots$

$u_k = f_n(x_1, x_2 \ldots x_n)$

$$\left(\frac{\partial u}{\partial x}\right)_{ij} = \frac{\partial f_i}{\partial x_j}$$

Développons autour de la valeur moyenne $E(X) = M\ (m_1, m_2 \ldots m_n)$, en nous limitant aux termes du 1er ordre :

$$U(X) = U(M) + \frac{\partial U}{\partial X}\ (X - M)$$

(c'est-à-dire qu'au premier ordre : $E[U(X)] = U[E(X)]$)

$$\boxed{V_U = \left(\frac{\partial U}{\partial X}\right) V_X \left(\frac{\partial U}{\partial X}\right)^T}$$

Dans le cas particulier d'une fonction de n variables indépendantes, $u = f(x_1 \ldots x_n)$, on retrouve la relation classique :

$$\boxed{\sigma_u^2 = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i}\right)^2 \sigma_i^2}$$

LA LOI POLYNOMIALE

Au lieu de l'alternative : réalisation de l'événement A - non réalisation de A ou réalisation de l'événement contraire B, nous avons maintenant N possibilités. Par exemple, on fait n tirages indépendants dans une urne contenant N espèces différentes de boules (en remettant la boule dans l'urne après chaque tirage) : les nombres observées sont $n_1, n_2 \ldots n_N$, les probabilités sont données par la composition de l'urne.

Un autre cas est celui de la comparaison d'un histogramme expérimental avec une loi théorique : on dispose de n mesures que l'on répartit entre N catégories (exemple d'un histogramme de masse d'un système de 2 particules).

Etudions d'abord le cas simple où il n'existe que 3 possibilités, donc 2 variables algébriquement indépendantes :

			Variables auxiliaires	
Catégories	Probabilité	Tirages	X	Y
①	p_1	n_1	1	0
②	p_2	n_2	0	1
③	p_3	n_3	0	0
	$\Sigma p_i = 1$	$\Sigma n_i = 1$		

La probabilité du "tirage" (n_1, n_2, n_3) si l'on fait n épreuves successives est donnée par la loi polynômiale :

$$P_{n_1, n_2, n_3} = \frac{n!}{n_1! n_2! n_3!} p_1^{n_1} p_2^{n_2} p_3^{n_3}$$

avec $n_1 + n_2 + n_3 = n$ donné

$p_1 + p_2 + p_3 = 1$

$1^{o}/$ On affecte chaque tirage i de deux variables aléatoires X et Y prenant les valeurs 1 ou 0 :

$X_i \nearrow 1$ probabilité p_1 ; $X_i \searrow 0$ probabilité $q_1 = 1-p_1 = p_2 + p_3$

$Y_i \nearrow 1$ probabilité p_2 ; $Y_i \searrow 0$ probabilité $q_2 = 1-p_2 = p_1+p_3$

$$E(X_i) = p_1 \qquad E(Y_i) = p_2$$

$$n_1 = \sum X_i \qquad \text{d'où :} \quad E(n_1) = np_1$$

$$\sigma^2_{n_1} = E(n_1 - np_1)^2 = E\left(\sum_i \xi_i\right)^2 = np_1 q_1 \qquad \left(\xi_i = X_i - p_1\right)$$

De même : $E(n_2) = np_2$ $\qquad \sigma^2_{n_2} = E(n_2 - np_2)^2 = np_2 q_2$

On peut choisir les 2 variables réduites :

$$\frac{n_1 - np_1}{\sqrt{np_1 q_1}} \quad \text{et} \quad \frac{n_2 - np_2}{\sqrt{np_2 q_2}}$$

(on peut choisir deux variables quelconques parmi les 3 variables n_1, n_2, n_3 liées par $n_1 + n_2 + n_3 = n$)

Coefficient de corrélation

$$n_1 - np_1 = \sum \xi_i \qquad \xi = X - p$$
$$n_2 - np_2 = \sum \eta_j \qquad \eta = Y - p$$

(variables centrées)

$$E[(n_1 - np_1)(n_2 - np_2)] = \sum_{ij} E(\xi_i \eta_j)$$

or les ξ et η provenant de tirages différents sont indépendants :

$$E(\xi_i \eta_j) = 0 \text{ pour } i \neq j$$

d'où : $$E[(n_1 - np_1)(n_2 - np_2)] = n\, E(X-p_1)(Y-p_2)$$

$$\rho = \frac{E[(n_1 - np_1)(n_2 - np_2)]}{\sqrt{np_1 q_1}\ \sqrt{np_2 q_2}} = \frac{E(X-p_1)(Y-p_2)}{\sqrt{p_1 q_1\ p_2 q_2}} \quad \text{(indépendant de n)}$$

$$E(X-p_1)(Y-p_2) = E(XY - p_1 Y - p_2 X + p_1 p_2) = -p_1 p_2$$

(on voit directement que $E(XY) = 0$, d'après la définition même de l'espérance mathématique)

d'où : $$\boxed{\rho = -\sqrt{\frac{p_1 p_2}{q_1 q_2}}}$$

2°/ On montre, comme dans le cas d'une seule variable, que, pour n grand, la loi polynômiale tend vers une loi de Gauss.

Avec les variables réduites

$$\zeta_1 = \frac{n_1 - np_1}{\sqrt{np_1 q_1}} \qquad \zeta_2 = \frac{n_2 - np_2}{\sqrt{np_2 q_2}}$$

cette loi de Gauss est :

$$f(\zeta_1, \zeta_2)\, d\zeta_1\, d\zeta_2 = \frac{1}{2\pi} \frac{1}{\sqrt{1-\rho^2}} e^{-\frac{1}{2} \frac{\zeta_1^2 - 2\rho\, \zeta_1 \zeta_2 + \zeta_2^2}{1-\rho^2}} d\zeta_1\, d\zeta_2$$

$$1-\rho^2 = 1 - \frac{p_1 p_2}{q_1 q_2} = \frac{(1-p_1)(1-p_2) - p_1 p_2}{q_1 q_2} = \frac{p_3}{q_1 q_2}$$

Par raison de symétrie, on préfère aux variables $\zeta_1 \zeta_2$ les 3 variables x_1, x_2, x_3 liées algébriquement par la relation $x_1 + x_2 + x_3 = 0$:

$$x_1 = \frac{n_1 - np_1}{\sqrt{n}} \quad x_2 = \frac{n_2 - np_2}{\sqrt{n}} \quad x_3 = \frac{n_3 - np_3}{\sqrt{n}}$$

D'où :

$$\frac{\zeta_1^2 - 2\rho\,\zeta_1\zeta_2 + \zeta_2^2}{1-\rho^2} = \left[\frac{x_1^2}{p_1 q_1} + 2\sqrt{\frac{p_1 p_2}{q_1 q_2}}\,\frac{x_1 x_2}{\sqrt{p_1 q_1 p_2 q_2}} + \frac{x_2^2}{p_2 q_2}\right] \times \frac{q_1 q_2}{p_3}$$

$$= \frac{q_2}{p_1 p_3} x_1^2 + \frac{2x_1 x_2}{p_3} + \frac{q_1}{p_2 p_3} x_2^2$$

$$= \left(\frac{1}{p_1} + \frac{1}{p_3}\right) x_1^2 + \frac{2x_1 x_2}{p_3} + \left(\frac{1}{p_2} + \frac{1}{p_3}\right) x_2^2$$

$$= \frac{x_1^2}{p_1} + \frac{x_2^2}{p_2} + \frac{x_3^2}{p_3} \qquad x_3^2 = (x_1 + x_2)^2$$

D'autre part :

$$d\zeta_1\, d\zeta_2 \times \frac{1}{\sqrt{1-\rho^2}} = \frac{dx_1\, dx_2}{\sqrt{p_1 q_1 p_2 q_2}} \times \sqrt{\frac{q_1 q_2}{p_3}} = \frac{dx_1\, dx_2}{\sqrt{p_1 p_2 p_3}}$$

D'où :

$$f(x_1, x_2, x_3) = \frac{1}{2\pi} \frac{1}{\sqrt{p_1 p_2 p_3}} e^{-\frac{1}{2}\left[\frac{x_1^2}{p_1} + \frac{x_2^2}{p_2} + \frac{x_3^2}{p_3}\right]} \delta(x_1 + x_2 + x_3)$$

Cette expression appelle quelques remarques : en apparence, c'est une loi de Gauss à 3 dimensions sans corrélations. En réalité, cette loi est DEGENEREE dans le plan $x_1 + x_2 + x_3 = 0$, et les deux variables algébriquement indépendantes, x_1 et x_2 par exemple, ne sont plus indépendantes en probabilité. Mais la symétrie de la loi à 3 variables la rend plus maniable dans les applications.

Plus généralement, la loi polynômiale à N dimensions (N catégories) tend vers la loi de Gauss :

$$f(x_1, \ldots x_N) = \frac{1}{(2\pi)^{\frac{N-1}{2}}} \frac{1}{\sqrt{\Pi\, p_i}} e^{-\frac{1}{2}\sum_i \frac{x_i^2}{p_i}} \delta\left(\sum x_i = 0\right)$$

avec $$x_i = \frac{n_i - np_i}{\sqrt{n}}$$

Le nombre de DEGRES DE LIBERTE, c'est-à-dire de variables algébriquement indépendantes, est $N-1$.

II. DES PROBABILITES A L'EXPERIENCE CONCRETE

Tests d'hypothèses et estimation statistique

La Statistique mathématique a pour objet d'extraire l'information apportée par les observations expérimentales, à l'aide du calcul des probabilités.

On peut distinguer deux approches successives :

1°/ On veut, par une mesure, confirmer ou infirmer une prévision théorique : c'est un TEST D'HYPOTHESE.

2°/ Si le test est défavorable, ou s'il n'existe pas d'hypothèse a priori, c'est l'expérience seule qui peut fournir une information : d'où le problème de L'ESTIMATION STATISTIQUE. Un cas fréquent, auquel nous nous limiterons ici, est celui de l'estimation paramétrique : la loi de probabilité dépend de un ou plusieurs paramètres inconnus, l'expérience peut nous informer sur ces paramètres.

Comment exprimer l'information fournie par l'expérience ?

Exemple : On détermine l'énergie d'une particule par une mesure effectuée sur sa trajectoire. On sait que la méthode de mesure conduit à une incertitude exprimée par l'écart-type σ_E. On connaît donc la loi de probabilité (supposée gaussienne) de la mesure E autour de la valeur vraie E_0 .

Inversement, on veut estimer E_0 par la mesure E : peut-on parler d'une probabilité de E_0 (donnée par la loi de Gauss d'écart-type σ_E centrée sur E)? Ceci n'a de sens que si E_0 est également une variable aléatoire; c'est le cas si la particule fait partie d'un faisceau, l'énergie des particules de ce faisceau étant distribuée selon la loi g(E). C'est une absurdité si E_0 doit être considérée comme une variable certaine.

Le problème apparaît encore mieux sur une loi dissymétrique comme la loi de Poisson. La probabilité d'observer n événements (n petit), si u est le nombre espéré, a pour expression $P_n = e^{-u} \frac{u^n}{n!}$. Peut-on, inversement, si l'on a effectivement observé n, considérer $P(u) = e^{-u} \frac{u^n}{n!}$ comme la loi de probabilité de u ? On pourrait être tenté de le faire en remarquant que :

$$\int_0^\infty P(u)\, du = \frac{1}{n!} \int_0^\infty e^{-u} u^n\, du = \frac{\Gamma(n+1)}{n!} = 1$$

normalisation semblable à $\sum_n P_n = 1$

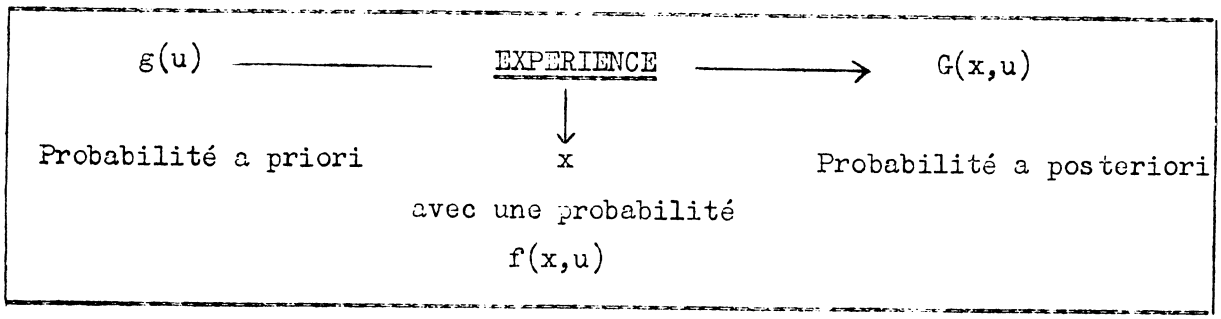
Ici encore, il faudrait que u soit une variable aléatoire.

On voit donc apparaître 2 cas possibles :

a) La grandeur u que l'on veut estimer possède une loi de probabilité A PRIORI $g(u)$.

La loi de probabilité de la mesure x dépend de u, soit $f(x,u)$.

Alors l'information tirée de l'expérience change la loi de probabilité A PRIORI $g(u)$ en une loi A POSTERIORI $G(x,u)$.



La probabilité de u, si l'expérience a donné x, est égale à la probabilité que l'expérience faite corresponde à la valeur u ($g(u)$) multipliée par la probabilité d'observer x sachant que l'on a u; soit :

$$G(x,u) = \frac{g(u)\, f(x,u)}{\int g(u)\, f(x,u)\, du}$$

Un cas particulier simple est celui où u est, a priori, également probable (dans un certain intervalle). Alors $G(x,u) = f(x,u)$.

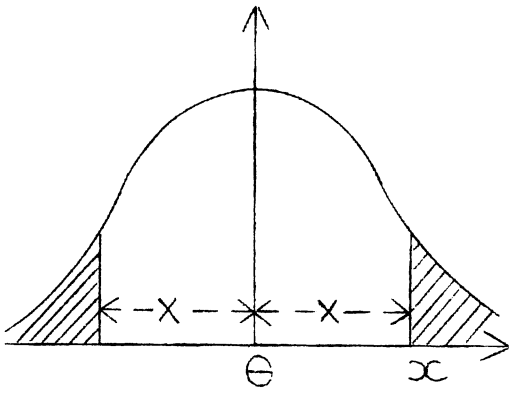
Reprenons l'exemple de la loi de Poisson. D'une infinité d'expériences correspondant chacune à une valeur de u supposé distribué uniformément, on extrait toutes les expériences pour lesquelles le résultat de la mesure est n. $P_n(u)$ est la loi de probabilité a posteriori de u si l'on a observé n. La valeur moyenne de u pour cette classe d'expériences est :

$$\langle u \rangle = \int_0^\infty u\, P_n(u)\, du = \int_0^\infty e^{-u}\, \frac{u^{n+1}}{n!}\, du = \frac{\Gamma(n+2)}{n!} = n+1$$

En raison de la dissymétrie de la loi, cette valeur moyenne de u n'est pas égale au nombre n observé.

b) En général, la grandeur u que l'on veut estimer est une grandeur inconnue, mais CERTAINE (Exemple : détermination par l'expérience de la masse d'une particule).

On affecte alors une probabilité à l'expérience elle-même, considérée comme une EPREUVE ALEATOIRE. La mesure fournit un INTERVALLE ALEATOIRE (intervalle de confiance) ayant une probabilité donnée de contenir la vraie valeur u.



LOI DE GAUSS (Loi symétrique)

1°/ Test d'hypothèse

Une valeur x déterminée par l'expérience appartient-elle à la distribution de valeur centrale Θ et de dispersion σ ? (Exemple : un angle de diffusion).

σ peut être connu a priori (théorie)
estimé expérimentalement

$= \sqrt{Npq}$ dans le cas limite d'une loi binômiale

$= \sqrt{N}$ dans le cas limite d'une loi de Poisson.

La probabilité pour que, dans l'hypothèse (Θ,σ), l'expérience donne le résultat x ou un résultat moins bon (c'est-à-dire plus grand que x si $x > \Theta$, ou inférieur à x si $x < \Theta$) est :

$$P = \int_x^{+\infty} \frac{1}{\sqrt{2\pi}\,\sigma}\, e^{-\frac{(x-\Theta)^2}{2\sigma^2}}\, dx$$

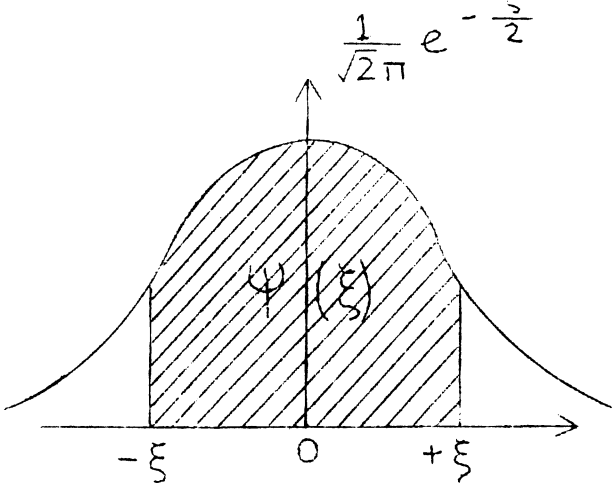
Soit $\xi = \frac{X-\Theta}{\sigma}$: les tables donnent $\psi(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\xi}^{+\xi} e^{-\frac{\xi^2}{2}}\, d\xi$

d'où $P = \frac{1-\psi(\xi)}{2}$

Pour $X - \Theta = 2\sigma$, $\psi = 0.95$ et $P = 2.5\ \%$.

L'hypothèse est acceptée ou rejetée avec un certain SEUIL DE PROBABILITE.

ξ	$\psi(\xi)$
0.5	0.38
1.0	0.68
1.5	0.87
2.0	0.95
2.6	0.99



On peut encore exprimer le test d'hypothèse sous la forme suivante :

La probabilité pour que, dans l'hypothèse (Θ,σ), l'expérience fournisse un résultat x dans un intervalle $(\Theta-X, \Theta+X)$ centré sur Θ est :

$$P = \int_{\Theta - X}^{\Theta + X} = \psi(\xi)$$

Exemple : P = 95 % dans l'intervalle $AB(\Theta - 2\sigma, \Theta + 2\sigma)$.

L'hypothèse est acceptée si le résultat x est dans cet intervalle, rejetée s'il est en dehors.

Risques : - rejeter à tort l'hypothèse (5 %)
- accepter l'hypothèse alors que x appartient en réalité à une distribution de valeur centrale $\Theta' \neq \Theta$ (probabilité de l'intervalle AB pour la loi de Gauss centrée sur Θ').

2°/ Estimation

L'hypothèse est rejetée, ou bien il n'y a pas d'hypothèse. La meilleure estimation de Θ est évidemment x.

Généralement, on ne peut parler de la "probabilité de Θ". On définit alors un intervalle (Θ_1, Θ_2), dit INTERVALLE DE CONFIANCE (fiducial limits) de la manière suivante :

Il est de moins en moins probable que l'expérience donne le résultat x quand la valeur supposée de Θ s'écarte de x. Donc :

Si $\Theta < x$, les valeurs supérieures à x deviennent peu probables.

Soit $\Theta = \Theta_1$:

$$P(\Theta_1) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_x^{+\infty} e^{-\frac{(x-\Theta_1)}{2\sigma^2}} dx = \frac{1 - \psi(\xi_1)}{2}$$

Probabilité de trouver un résultat $\geqslant x$ si la valeur centrale est Θ_1 .

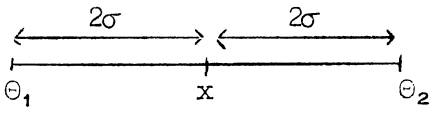
Si $\Theta > x$, les valeurs inférieures à x deviennent peu probables.

Soit $\Theta = \Theta_2$:

$$P'(\Theta_2) = \frac{1}{\sqrt{2\pi}\,\sigma} \int_{-\infty}^{x} e^{-\frac{(x-\Theta_2)}{2\sigma^2}} dx = \frac{1 - \psi(\xi_2)}{2}$$

Probabilité de trouver un résultat $\leqslant x$ si la valeur centrale est Θ_2 .

Exemple : P = P' = 2.5 % : il y a une probabilité 95 % pour que l'intervalle symétrique $(x - 2\sigma,\ x + 2\sigma)$ contienne la vraie valeur centrale Θ.



La probabilité est attachée, non à Θ, mais à l'intervalle, c'est-à-dire à l'expérience.

REMARQUE - TEST DE LA MOYENNE D'UN ECHANTILLON

Un échantillon de n observations $x_1 \ldots x_n$ provient-il de la distribution de valeur centrale Θ et de dispersion σ ?

On peut, comme ci-dessus, comparer avec Θ la moyenne des x_i, en prenant pour écart-type $\sigma/\sqrt{n}$. Mais, si n est petit ($n < 30$), la loi de

probabilité à utiliser n'est plus la loi de Gauss, mais la LOI DE STUDENT-FISHER qui en dérive pour les petits échantillons, et qui dépend de n. C'est cette même loi qui doit être utilisée pour la comparaison des moyennes de 2 échantillons.

LOI DE POISSON (loi dissymétrique) $P_n = e^{-u} \frac{u^n}{n!}$

1°/ Test d'hypothèse

Le nombre moyen attendu étant u, on observe n. n est-il compatible avec u ?

Si u et n sont suffisamment grands, la distribution est sensiblement gaussienne, et on peut raisonner comme précédemment avec $\sigma = \sqrt{u}$.

Sinon, on dira que, dans l'hypothèse u, la probabilité d'obtenir le résultat u ou un résultat moins bon est :

$$\text{Si } n > u \qquad P = \sum_{n}^{\infty} e^{-u} \frac{u^k}{k!} = 1 - \sum_{o}^{n-1} e^{-u} \frac{u^k}{k!}$$

$$\text{Si } n < u \qquad P' = \sum_{o}^{n} e^{-u} \frac{u^k}{k!}$$

Remarque

On peut simplifier le calcul de P et P' en utilisant les tables de la fonction Γ incomplète.

$$\text{Posons : } \Phi_N(u) = \frac{\int_o^u e^{-x} x^N dx}{\int_o^\infty e^{-x} x^N dx} = \frac{1}{N!} \int_o^u e^{-x} x^N dx$$

En intégrant par parties, on obtient :

$$\Phi_N(u) = - e^{-u} \frac{u^N}{N!} + \Phi_{N-1}(u)$$

On calcule de même $\Phi_{N-1}(u)$ et la suite jusqu'à $\Phi_0(u) = \int_0^u e^{-x}dx = 1 - e^{-u}$.

D'où : $$\boxed{\Phi_N(u) = 1 - \sum_0^N e^{-u} \frac{u^k}{k!}}$$

$\underline{n > u}$ $\qquad P = \Phi_{n-1}(u)$

$\underline{n < u}$ $\qquad P' = 1 - \Phi_n(u)$

2°/ Estimation (Fisher, Regener)

Le raisonnement est le même que celui fait dans le cas d'une distribution gaussienne.

Il est de moins en moins probable d'observer n si la valeur théorique supposée u s'écarte de n.

Si $\underline{u < n}$, les valeurs $\geqslant n$ deviennent peu probables.

Soit $u = u_1$:

$$P(u_1) = \sum_n^\infty e^{-u_1} \frac{u_1^k}{k!} = \Phi_{n-1}(u_1)$$

Probabilité de trouver n ou plus si la valeur attendue est u_1 .

Si $\underline{u > n}$, les valeurs $\leqslant n$ deviennent peu probables.

Soit $u = u_2$:

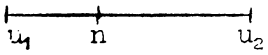
$$P'(u_2) = \sum_0^n e^{-u_2} \frac{u_2^k}{k!} = 1 - \Phi_n(u_2) \quad *)$$

Ici encore, on fait correspondre aux probabilités $P(u_1)$ et $P'(u_2)$ un INTERVALLE DE CONFIANCE (u_1, u_2). La probabilité que cet intervalle contienne la valeur u est $p = 1 - P(u_1) - P'(u_2)$.

Exemple : $P(u_1) = P'(u_2) = 5\ \%$, soit $p = 90\ \%$.

Dans l'approximation gaussienne, $\psi(\xi) = 0.90 \rightarrow \xi = 1{,}645$, c'est-à-dire que l'intervalle de confiance est : $n \pm 1{,}645\sqrt{n}$.

	LIMITES DE CONFIANCE (90 %)			
	POISSON		LOI NORMALE	
n	u_1	u_2	u_1	u_2
0	0	3	-	0
1	0.05	4.74	-	2.65
2	0.35	6.30	-	4.32
3	0.82	7.75	0.15	5.85
4	1.37	9.15	0.71	7.29
6	2.61	11.84	1.97	10.03
10	5.43	16.96	4.80	15.20
20	13.26	29.06	12.64	27.36
50	38.96	63.28	38.37	61.63



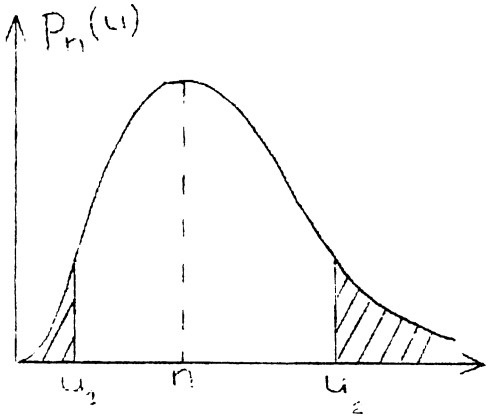
(D'après Regener)

---

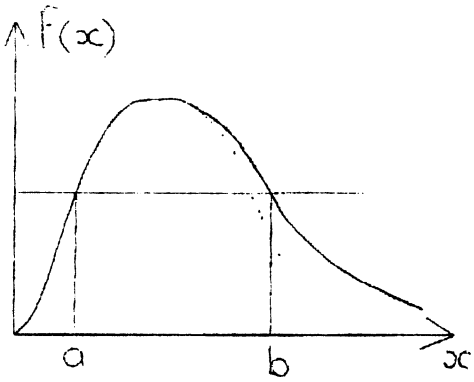
*) En utilisant la probabilité "inverse" (u considérée comme une variable aléatoire a priori équiprobable), on aurait écrit :

$$P(u_1) = \int_0^{u_1} e^{-u} \frac{u^n}{n!}\, du = \Phi_n(u_1) \text{ au lieu de } \Phi_{n-1}(u_1)$$

$$P'(u_2) = \int_{u_2}^{\infty} e^{-u} \frac{u^n}{n!}\, du = 1 - \Phi_n(u_2)$$



7863/p/mh



REMARQUE - CHOIX DE L'INTERVALLE DE CONFIANCE

Ce choix est arbitraire, puisqu'il existe un nombre infini d'intervalles correspondant à une probabilité donnée. Cependant, on a intérêt à choisir le plus petit de ces intervalles.

Soit f(x) une loi de probabilité continue. La probabilité attachée à un intervalle (a,b) est :

$$P = \int_a^b f(x)dx \ .$$

Faisons varier l'intervalle à probabilité constante : $f(b)db - f(a)da = 0$. L'intervalle (a-b) est minimum pour $da - db = 0$. D'où $f(a) = f(b)$. Pour une loi symétrique comme la loi de Gauss, l'intervalle symétrique est le meilleur.

LOI NORMALE MULTIDIMENSIONNELLE

LOI DE χ^2

Soit un élément aléatoire constitué par les N caractères $X_1, X_2, \ldots X_N$. L'ensemble des valeurs $x_1, x_2 \ldots x_N$ obtenues par l'expérience est-il compatible avec la population définie par les valeurs centrales $m_1, \ldots m_N$ et les écarts-types $\sigma_1 \ldots \sigma_N$?

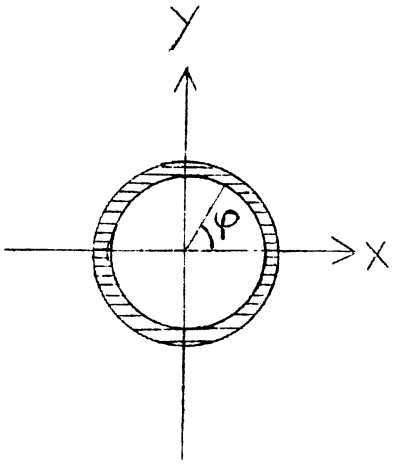
La loi de probabilité du vecteur aléatoire X est :

$$f(x_1 \ldots x_N) = \frac{1}{(2\pi)^{N/2}} \frac{1}{\sqrt{\det V}} \, e^{-\frac{1}{2}(X-M)^T V^{-1} (X-M)}$$

$(X-M)^T V^{-1} (X-M) = H(x_1 \ldots x_N)$ V = matrice des variances

Cette loi est difficilement maniable. On la remplace par une loi globale de l'écart entre le point expérimental $(x_1 \ldots x_N)$ et le "point central" $M(m_1, \ldots m_N)$.

Considérons l'exemple simple de 2 variables indépendantes x et y, supposées centrées et normées.



$$f(x,y)dx\,dy = \frac{1}{2\pi} e^{-\frac{1}{2}(x^2+y^2)} dx\,dy$$

En coordonnées polaires : $r^2 = x^2 + y^2$, $dx\,dy = rdrd\varphi$

D'où, après intégration sur φ :

$$f(r)dr = e^{-\frac{r^2}{2}} rdr \qquad r^2 = \left(\frac{x_1 - m_1}{\sigma_1}\right)^2 + \left(\frac{x_2 - m_2}{\sigma_2}\right)^2$$

$$E(r^2) = 2$$

Si les 2 variables x et y sont liées en probabilité :

$$f(x,y)dx\,dy = \frac{1}{2\pi\sqrt{1-\rho^2}} e^{-\frac{1}{2}\frac{x^2 - 2\rho xy + y^2}{1-\rho^2}} dx\,dy$$

On pose encore :

$$r^2 = \frac{x^2 - 2\rho xy + y^2}{1-\rho^2}$$

d'où :

$$f(r)dr = e^{-\frac{r^2}{2}} rdr$$

On vérifie que l'on a toujours $E(r^2) = 2$.

$E(r^2)$ est le nombre de variables algébriquement indépendantes, c'est-à-dire le nombre de dimensions du VECTEUR ALEATOIRE $\vec{X}$, ou encore le nombre de DEGRES DE LIBERTE.

VARIABLE χ^2

Dans le cas général, on pose :

$$\chi^2 = (X - M)^T V^{-1} (X - M)$$

c'est-à-dire, s'il s'agit de N variables indépendantes

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{x_i - m_i}{\sigma_i} \right)^2 \qquad \text{d'où} \quad E(\chi^2) = N$$

$\chi^2 = H(x_1, x_2, \ldots x_N) = C^{te}$ est l'équation d'un "ellipsoïde" de l'espace à N dimensions. La probabilité d'avoir χ compris entre χ et $\chi + d\chi$ est proportionnelle à $e^{-\frac{1}{2}\chi^2}$ (c'est-à-dire à $f(x_1, \ldots x_N)$) et au volume compris entre les "ellipsoïdes" correspondant à χ et $\chi + d\chi$ ($d\chi$ provenant de $dx_1, dx_2, \ldots dx_N$). Le volume d'un "ellipsoïde" à N dimensions est proportionnel à χ^N, donc la différentielle fait intervenir χ^{N-1} .

La loi de probabilité normalisée est donc :

$$\frac{e^{-\frac{\chi^2}{2}} \chi^{N-1} \, d\chi}{\int_0^\infty e^{-\frac{\chi^2}{2}} \chi^{N-1} \, d\chi}$$

LOI DE χ^2
(Karl PEARSON)

Propriétés de la loi de χ^2

a) Moyenne et écart-type

Posons $\frac{\chi^2}{2} = v$ $\qquad$ $\frac{N}{2} = h$

La loi de χ^2 prend alors la forme :

$$\frac{e^{-v}\, v^{h-1}\, dv}{\Gamma(h)}$$

$$E(v) = \frac{1}{\Gamma(h)} \int_0^\infty e^{-v}\, v^h\, dv = \frac{\Gamma(h+1)}{\Gamma(h)} = h \qquad \text{d'où :} \qquad \boxed{E(\chi^2) = N}$$

$$E(v^2) = \frac{1}{\Gamma(h)} \int_0^\infty e^{-v}\, v^{h+1}\, dv = \frac{\Gamma(h+2)}{\Gamma(h)} = h(h+1) \quad \text{et ainsi de suite}$$

$$\sigma^2_{\chi^2} = 4\,\sigma^2_v = 4\left[E(v^2) - \left\{E(v)\right\}^2\right] = 4h \qquad \boxed{\sigma^2_{\chi^2} = 2N}$$

b) <u>Loi limite</u>

La variable réduite est : $\xi = \dfrac{\chi^2 - E(\chi^2)}{\sigma_{\chi^2}} = \dfrac{v-h}{\sqrt{h}}$

On connaît la fonction caractéristique de v puisqu'on connaît tous ses moments.

$$\varphi_v(t) = 1 + it\,h + \frac{(it)^2}{2!}\, h(h+1) + \ldots = \frac{1}{(1-it)^h}$$

$$\varphi_{v-h}(t) = \frac{e^{-iht}}{(1-it)^h}$$

$$\psi = \operatorname{Log} \varphi_{v-h}(t) = h\left[-it - \operatorname{Log}(1-it)\right] = h\left[\frac{(it)^2}{2} + \frac{(it)^3}{3!} + \ldots\right]$$

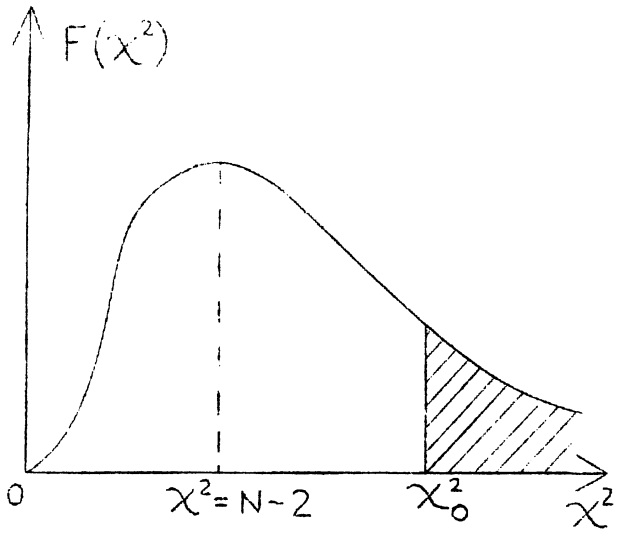
$$\psi_\xi = \frac{(it)^2}{2} + \frac{(it)^3}{3!}\,\frac{1}{\sqrt{h}} + \frac{(it)^4}{4!}\,\frac{1}{h} + \ldots$$

Si $N \to \infty$, $\phi \to -\frac{t^2}{2}$: la loi limite de la loi de χ^2 est une loi de Gauss.

Si le nombre de dimensions est grand, la variable $\frac{\chi^2 - N}{\sqrt{2N}}$ suit la loi normale (s'applique pratiquement pour $N \geq 30$).

TEST D'HYPOTHESE

La loi de χ^2 fournit un test de compatibilité de l'ensemble des valeurs $(x_1 \ldots x_N)$ avec la population définie par les valeurs centrales $(m_1 \ldots m_N)$ et les dispersions $(\sigma_1, \ldots \sigma_N)$. On calcule $\chi^2 \to \chi_0^2$. La probabilité pour que le résultat de l'expérience soit ce qu'il est ou pire est :



$$P(\chi^2 \geq \chi_0^2) = \int_{\chi_0^2}^{\infty} F(\chi^2)\, d\chi^2$$

et s'exprime à l'aide de la fonction Γ incomplète :

$$P(\chi^2 \geq \chi_0^2) = \frac{\int_0^V e^{-v}\, v^{h-1}\, dv}{\Gamma(h)} \qquad \text{avec} \qquad V = \frac{\chi_0^2}{2}$$

On choisit un SEUIL DE PROBABILITE, par exemple P = 5 %, d'où χ_0^2 pour un nombre donné ν de degrés de liberté :

Si χ^2 observé $< \chi_0^2(\nu)$ l'hypothèse est acceptée

Si χ^2 observé $> \chi_0^2(\nu)$ l'hypothèse est rejetée

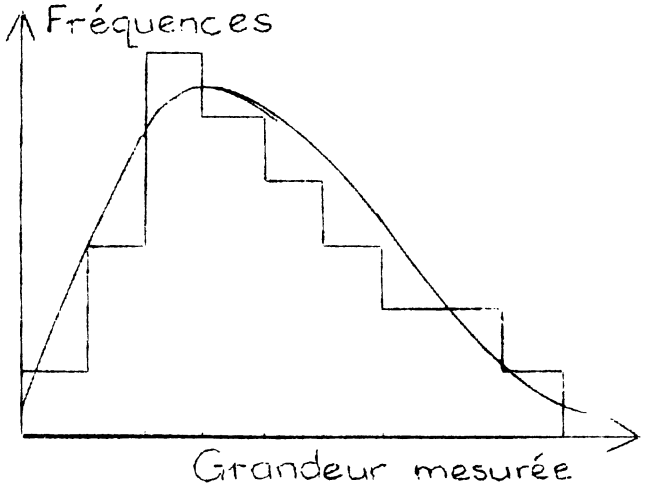
Extrait de la table de χ^2

ν	χ^2_0		
	P = 10 %	5 %	1 %
1	2.7	3.8	6.6
2	4.6	6.0	9.2
3	6.2	7.8	11.3
4	7.8	9.5	13.3
5	9.2	11.1	15.1
10	16.0	18.3	23.2
15	22.3	25.0	30.6
20	28.4	31.4	37.6
25	34.4	37.6	44.3
30	40.3	43.8	50.9

L'accord est certainement satisfaisant si $\chi^2_0 < \nu$. Cependant, il convient de se méfier d'un χ^2 trop petit, puisque $E(\chi^2) = \nu$ et que la densité de probabilité maximum est obtenue pour $\chi^2 = \nu - 2$ (si le χ^2 observé est trop petit, les σ sont peut-être surestimés).

APPLICATION - COMPARAISON D'UNE LOI THEORIQUE ET D'UN HISTOGRAMME EXPERIMENTAL

Les n valeurs mesurées sont réparties en N classes : $n_1, n_2 \ldots n_N$. Il n'est pas nécessaire que les bandes soient de largeurs égales. On aura avantage, au contraire, à fabriquer des classes à probabilités égales. Il faut que le nombre d'observations dans chaque classe soit suffisamment grand (≥ 30) pour que le test χ^2 soit correct, c'est-à-dire pour que les fluctuations dans chaque classe soient gaussiennes.



Pour chaque classe, on détermine, d'après la loi théorique, les probabilités p_i, d'où les nombres attendus np_i .

On forme :

$$\chi^2 = \sum_{i=1} \frac{(n_i - np_i)^2}{np_i}$$

Les n_i ne sont pas algébriquement indépendants : $\sum n_i = n$. La loi de χ^2 à utiliser est celle à $\nu = N - 1$ degrés de liberté.

Ce résultat est général. On peut former un χ^2 avec des variables entre lesquelles existent certaines relations algébriques : le nombre de degrés de liberté de la loi de χ^2 est égal au nombre de variables algébriquement indépendantes.

L'ESTIMATION PARAMETRIQUE

La loi de probabilité, de forme analytique connue, dépend d'un certain nombre de paramètres inconnus. Elle permet de tirer de l'expérience une information sur ces paramètres.

On dispose de n observations $x_1, x_2 \ldots x_n$. Soit $F(x_1, x_2 \ldots x_n, \Theta)dx_1 \ldots dx_n$ la loi de probabilité de l'échantillon, Θ étant le paramètre inconnu.

Si les observations sont indépendantes : $F(x_1, \ldots x_n, \Theta) = f(x_1, \Theta)\, f(x_2, \Theta) \ldots f(x_n, \Theta)$.

Exemple : détermination de la vie moyenne d'une particule instable à partir de n observations de temps de vol.

PRECISION DE L'ESTIMATION

Soit $t(x_1 \ldots x_n)$ une estimation de Θ. L'échantillon étant considéré comme un élément aléatoire dont la probabilité est donnée par F, l'estimation t est une variable aléatoire. La précision de l'estimation t faite par une méthode donnée est mesurée par $\sigma_t^2 = E(t - \Theta)^2$.

a) $$\int \ldots \int F(x_1 \ldots x_n, \Theta)dx_1 \ldots dx_n = 1$$

Supposons qu'on puisse dériver par rapport à Θ sous le signe $\int$:

$$\int \cdots \int \frac{\partial F}{\partial \Theta} \, dx_1 \ldots dx_N = 0 \quad \text{ou} \quad \int \cdots \int \frac{1}{F} \frac{\partial F}{\partial \Theta} F \, dx_1 \ldots dx_N = 0$$

$$\boxed{E\left[\frac{1}{F} \frac{\partial F}{\partial \Theta}\right] = E\left[\frac{\partial}{\partial \Theta} \operatorname{Log} F\right] = 0} \qquad (1)$$

b) Supposons l'estimation CORRECTE : $E(t) = \Theta$

(Si $E(t) = \Theta + B_n(\Theta)$, l'estimation est BIAISEE)

$$\int \cdots \int t(x_1 \ldots x_N) \; F(x_1 \ldots x_N, \Theta) \, dx_1 \ldots dx_N = \Theta$$

d'où, comme précédemment :

$$\int \cdots \int t(x_1 \ldots x_N) \frac{1}{F} \frac{\partial F}{\partial \Theta} \; F \, dx_1 \ldots dx_N = 1$$

soit :

$$E\left[t \frac{1}{F} \frac{\partial F}{\partial \Theta}\right] = 1$$

ce qu'on peut encore écrire, d'après (1) :

$$\boxed{E\left[(t-\Theta)\left(\frac{1}{F} \frac{\partial F}{\partial \Theta}\right)\right] = 1}$$

c) Nous pouvons maintenant calculer la variance $\sigma_t^2 = E(t-\Theta)^2$. Pour cela, considérons l'expression :

$$E\left[u(t-\Theta) + v \frac{1}{F} \frac{\partial F}{\partial \Theta} \right]^2 \geqslant 0$$

$$\rightarrow \quad u^2 E(t-\Theta)^2 + 2uv E\left[(t-\Theta) \frac{1}{F} \frac{\partial F}{\partial \Theta} \right] + v^2 E\left[\frac{1}{F} \frac{\partial F}{\partial \Theta} \right]^2 \geqslant 0$$

soit : $u^2\sigma_t^2 + 2uv + v^2 A \geqslant 0$

d'où : $\Delta = 1 - A\sigma_t^2 \leqslant 0$

$$\boxed{\sigma_t^2 \geqslant \frac{1}{E\left[\frac{1}{F} \frac{\partial F}{\partial \Theta} \right]^2}}$$

Pour toutes les méthodes possibles d'estimation de Θ, la précision a une limite qui ne dépend que de la loi de probabilité de l'échantillon.

La quantité $A = E\left[\frac{1}{F} \frac{\partial F}{\partial \Theta} \right]^2$ est appelée INDICE DE CAPACITE INFORMATIVE de la loi de probabilité.

En résumé : une loi de probabilité donnée possède une certaine capacité informative. L'information disponible est plus ou moins bien utilisée par la méthode d'estimation (analogie avec le 2ème principe de la thermodynamique).

Exemple : Loi de probabilité gaussienne, n observations indépendantes.

$$\frac{\partial}{\partial \Theta} \text{Log } F = n \frac{\partial}{\partial \Theta} \text{Log } f \quad \text{avec} \quad f = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{1}{2} \frac{(x-\Theta)^2}{\sigma^2}}$$

$$E\left[\frac{\partial}{\partial \Theta} \text{Log } f \right]^2 = E\left[\frac{x-\Theta}{\sigma^2} \right]^2 = \frac{1}{\sigma^2} \qquad A = \frac{n}{\sigma^2} \quad : \quad \text{A est d'autant}$$

plus grand que σ est plus petit et que n est plus grand. La meilleure estimation possible a une précision $\sigma_t = \sigma/\sqrt{n}$: c'est l'écart-type de la moyenne des n observations.

Remarques

1°/ On peut donner de A une autre expression plus facilement calculable :

$$\frac{\partial}{\partial\Theta} \text{Log } F = \frac{1}{F} \frac{\partial F}{\partial\Theta}$$

$$\frac{\partial^2}{\partial\Theta^2} \text{Log } F = -\frac{1}{F^2}\left(\frac{\partial F}{\partial\Theta}\right)^2 + \frac{1}{F}\frac{\partial^2 F}{\partial\Theta^2}$$

d'où :

$$\int\cdots\int \frac{\partial^2}{\partial\Theta^2} (\text{Log } F)\, F\, dx_1 \ldots dx_N = -\int\cdots\int \left(\frac{1}{F}\frac{\partial F}{\partial\Theta}\right)^2 F\, dx_1 \ldots dx_N$$

$$+ \underbrace{\int\cdots\int \frac{\partial^2 F}{\partial\Theta^2}\, dx_1 \ldots dx_N}_{= 0}$$

$$\boxed{A = E\left[\frac{1}{F}\frac{\partial F}{\partial\Theta}\right]^2 = E\left[-\frac{\partial^2}{\partial\Theta^2} \text{Log } F\right]}$$

2°/ $t - \Theta$ et $1/F\ \partial F/\partial\Theta$ sont 2 variables aléatoires d'espérance mathématique nulle et de variances σ_t^2 et A.

Le coefficient de corrélation entre ces 2 variables est :

$$\rho = \frac{E\left[\left(t-\Theta\right)\left(\frac{1}{F}\frac{\partial F}{\partial\Theta}\right)\right]}{\sigma_t A} = \frac{1}{\sigma_t A} \leq 1$$

Pour la meilleure estimation possible, $\rho = 1$, et les 2 variables dépendent fonctionnellement l'une de l'autre.

Ce qui a été dit pour un paramètre s'applique également au cas de plusieurs paramètres.

COMMENT FAIRE L'ESTIMATION ?

Il existe 2 méthodes qui, asymptotiquement, sont équivalentes, et fournissent alors toute l'information disponible.

1°/ MINIMUM DU χ^2

Cette méthode s'applique si la loi de probabilité de l'échantillon est gaussienne (ou asymptotiquement gaussienne). Elle fournit l'information maximum.

Exemple : l'élément aléatoire $X_1 \ldots X_N$ dépend d'un paramètre Θ. On forme :

$$\chi^2 = \sum_{i=1}^{N} \frac{\left[x_i - m_i(\Theta)\right]^2}{\sigma_i^2}$$

(dans le cas où il n'y a pas de corrélations entre les x_i)

La condition $\frac{d\chi^2}{d\Theta} = 0$ fournit l'estimation t de Θ. Ce χ^2 minimum suit une loi à $\nu = N-1$ degrés de liberté.

Si l'élément aléatoire $X_1, X_2 \ldots X_N$ dépend de k paramètres, on a k conditions $\frac{\partial\chi^2}{\partial\Theta_j} = 0$ $(j = 1, k)$ et le χ^2_m minimum suit une loi à $\nu = N-k$ degrés de liberté.

On peut donner une image géométrique de cette propriété : χ^2 représente le carré de la "distance", mesurée selon une métrique donnée par la loi de probabilité, du point $X(x_1 \ldots x_N)$ au point $M(m_1 \ldots m_N)$. (Tous les points de l'"ellipsoïde" $H(x_1 \ldots x_N) = C^{te}$ sont à la même "distance" de M). Si $m_1 \ldots m_N$ dépendent d'un paramètre Θ, le lieu de M est une courbe et le carré de la plus courte distance de χ à cette courbe suit une loi de χ^2 à $N-1$ dimensions.

Par exemple, si nous avons 3 variables indépendantes x_1, x_2, x_3, le carré de la distance de X à l'axe x_3 est $\chi^2 = x_1^2 + x_2^2$, qui suit une loi à 2 dimensions.

Si $m_1 \ldots m_N$ dépendent de 2 paramètres, le lieu de M est une surface, et le carré de la plus courte distance de X à cette surface suit une loi de χ^2 à $N-2$ dimensions, etc...

Le nombre ν de degrés de liberté de la loi de χ^2 est égal, de façon générale, au nombre de variables aléatoires indépendantes moins le nombre de paramètres inconnus (donc que l'on veut estimer) indépendants :

$$\nu = N_1 - C_1 - (N_2 - C_2)$$

N_1 = nombre de variables aléatoires (mesures),
C_1 = nombre de liaisons algébriques entre ces variables,
N_2 = nombre de paramètres inconnus,
C_2 = nombre de liaisons entre ces paramètres.

Exemples :

1°/ N mesures indépendantes X_i, valeurs centrales Θ_i connues (test d'hypothèse) : $\nu = N$.

2°/ N mesures indépendantes X_i, valeurs centrales inconnues : $\nu = 0$. L'estimation donne $\Theta_i = X_i$.

3°/ Comparaison d'un histogramme avec une loi connue a priori : $\nu = N - 1$.

4°/ "Fit" cinématique d'une réaction observée dans une chambre à bulles : sur chaque trajectoire, on mesure l'impulsion p et les angles Θ,φ. On dispose donc de N mesures indépendantes ($N_1 = N$, $C_1 = 0$) correspondant à $N_2 = N$ paramètres inconnus (impulsions et directions). Ces N paramètres sont liés par $C_2 = C$ relations algébriques, appelées "contraintes" (conservation de l'impulsion et de l'énergie). D'où : $\nu = N - (N - C) = C$.

La méthode du minimum de χ^2 est donc une METHODE DES MOINDRES CARRES pondérés par l'inverse des variances.

Exemple : estimation de la valeur centrale d'une série de n observations gaussiennes indépendantes.

La loi élémentaire de la variable x_i est :

$$f(x_i,\Theta) = \frac{1}{\sqrt{2\pi}\,\sigma_i}\, e^{-\frac{(x_i - \Theta)^2}{2\sigma_i^2}}$$

$$\chi^2 = \sum_i \frac{(x_i - \Theta)^2}{\sigma_i^2}$$

$$\frac{d\chi^2}{d\Theta} = 0 \rightarrow \sum_i \frac{x_i - \Theta}{\sigma_i^2} = 0 \qquad \text{d'où :}$$

$$\boxed{t = \frac{\sum_i \frac{x_i}{\sigma_i^2}}{\sum_i \frac{1}{\sigma_i^2}}}$$

(moyenne pondérée : si les σ_i^2 sont égaux, on retrouve $t = \frac{\sum x_i}{n}$

Puisque les x_i sont indépendants, on calcule directement :

$$\sigma_t^2 = \frac{1}{\sum_i \frac{1}{\sigma_i^2}} \qquad \text{soit :} \qquad \boxed{\frac{1}{\sigma_t^2} = \sum_i \frac{1}{\sigma_i^2}}$$

C'est le résultat que l'on obtient en calculant $\Lambda = E\left[- \frac{\partial^2}{\partial \Theta^2} \text{Log } F \right]$.
La méthode du minimum de χ^2 fournit donc toute l'information disponible.
Par contre, supposons Θ connu et tous les $\sigma_i^2 = \sigma^2$ inconnu. On ne peut estimer σ^2 par cette méthode.

2°/ <u>MAXIMUM DE VRAISEMBLANCE</u> (maximum of likelihood, Fisher)

L'estimation t de Θ est donnée par la condition :

$$F(x_1, x_2, \ldots x_N; \Theta) \text{ maximum}$$

soit : $$\frac{\partial F}{\partial \Theta} = 0$$

ou :

$$\boxed{\frac{1}{F} \frac{\partial F}{\partial \Theta} = \frac{\partial}{\partial \Theta} \text{Log } F = 0} \qquad (1)$$

On montre que cette méthode fournit asymptotiquement, c'est-à-dire si le nombre n d'observations est grand, toute l'information disponible :

$$\sigma_t^2 \xrightarrow[n \to \infty]{} \frac{1}{E\left[\frac{1}{F}\frac{\partial F}{\partial \Theta}\right]^2}$$

Si la loi de l'échantillon est gaussienne, on voit facilement qu'il y a identité entre les 2 méthodes.

Dans le cas de k paramètres $\Theta_1 \ldots \Theta_k$, la condition du maximum de F conduit à k équations du type (1).

Exemples :

- Estimation de la valeur centrale d'une série de n observations gaussiennes indépendantes : comme précédemment.

- Estimation de la variance σ^2 d'une série de n observations gaussiennes indépendantes :

$$F(x_1 \ldots x_n ; \Theta) = \frac{1}{(2\pi)^{n/2} (\sigma^2)^{n/2}} e^{-\frac{1}{2} \sum_i \frac{(x_i - m)^2}{\sigma^2}}$$

$$\text{Log } F = C^{te} - \frac{n}{2} \text{Log } \sigma^2 - \frac{1}{2} \sum \frac{(x_i - m)^2}{\sigma^2}$$

$$\frac{\partial}{\partial \sigma^2} \text{Log } F = -\frac{n}{2}\frac{1}{\sigma^2} + \frac{1}{2} \sum \frac{(x_i - m)^2}{\sigma^4} = 0$$

d'où :

$$\text{Estimation de } \sigma^2 = s^2 = \frac{\sum (x_i - m)^2}{n}$$

- Loi polynômiale : les p_i sont fonctions d'un paramètre Θ. On observe $n_1, n_2 \ldots n_N$ avec $\sum n_i = n$

a) Minimum de χ^2 : $\chi^2 = \sum_i \frac{[n_i - np_i(\Theta)]^2}{np_i(\Theta)}$ (N - 1 degrés de liberté)

$$\frac{\partial \chi^2}{\partial \Theta} = 0 \rightarrow \sum_i \left[np_i'(\Theta) - \frac{n_i^2}{n} \frac{p_i'(\Theta)}{[p_i(\Theta)]^2} \right] = 0$$

b) Maximum de vraisemblance :

$$F = P_{n_1, n_2, \ldots n_N} = \frac{n!}{n_1! \ldots n_N!} [p_1(\Theta)]^{n_1} \ldots [p_N(\Theta)]^{n_N}$$

$$\text{Log } F = C^{te} + \sum n_i \text{ Log } p_i(\Theta)$$

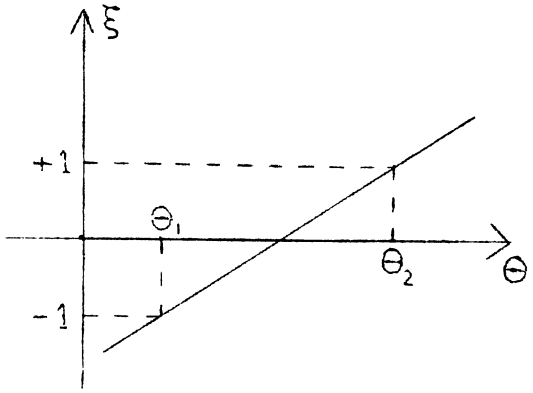
$$\frac{\partial}{\partial \Theta} \text{Log } F = 0 \rightarrow \sum_i n_i \frac{p_i'(\Theta)}{p_i(\Theta)} = 0 \quad , \quad \text{d'où t .}$$

On peut vérifier que les méthodes sont équivalentes au second ordre près (pour n grand). Mais la méthode du maximum de vraisemblance est d'un maniement plus facile.

- Loi de Poisson : on peut vérifier que les deux méthodes conduisent à la même équation pour t.

Calcul pratique de t On peut calculer t :

- par approximations successives
- par une méthode graphique



Considérons la variable :

$$\xi = \frac{\frac{\partial}{\partial \Theta} \text{Log } F}{\sqrt{E\left[\frac{\partial}{\partial \Theta} \text{Log } F\right]^2}} \text{ (Bartlett)}$$

C'est une variable centrée et normée, asymptotiquement gaussienne. On construit ξ fonction du paramètre Θ. Le graphique permet de déterminer l'estimation t du maximum de vraisemblance et l'intervalle de confiance (Θ_1, Θ_2).

APPLICATION - DETERMINATION DE LA VIE MOYENNE τ D'UNE PARTICULE INSTABLE (Bartlett)

La désintégration n'est détectée que si elle a lieu pendant un certain temps T, dit TEMPS POTENTIEL. On suppose que la probabilité d'observation est constante dans T, elle est nulle à l'extérieur de l'intervalle T.

La loi de probabilité élémentaire de l'instant t de la désintégration est :

$$f(t)dt = \frac{e^{-\frac{t}{\tau}} \frac{dt}{\tau}}{\int_0^T e^{-\frac{t}{\tau}} \frac{dt}{\tau}} = \frac{e^{-\frac{t}{\tau}} dt}{\tau\left[1 - e^{-\frac{T}{\tau}}\right]}$$

(Le zéro des temps est arbitraire, pourvu qu'il soit le même pour t et T). L'échantillon est constitué de n observations $t_1, t_2 \ldots t_n$ auxquelles correspondent les temps potentiels $T_1 \ldots T_n$.

Il est commode de prendre comme paramètre $\lambda = \frac{1}{\tau}$. La loi de l'échantillon est donc :

$$F(t_1 \ldots t_n ; \lambda) = f(t_1, \lambda)\, f(t_2, \lambda) \ldots f(t_n, \lambda) \text{ avec :}$$

$$f(t_i, \lambda) = \frac{\lambda\, e^{-\lambda t_i}}{1 - e^{-\lambda T_i}}$$

$$\text{Log } F = \sum_i \left[\text{Log } \lambda - \lambda t_i - \text{Log}\left(1 - e^{-\lambda T_i}\right) \right]$$

$$\frac{\partial}{\partial \lambda} \text{Log } F = \sum_i \left[\frac{1}{\lambda} - t_i - \frac{T_i\, e^{-\lambda T_i}}{1 - e^{-\lambda T_i}} \right]$$

L'estimation de τ est donnée par l'équation :

$$\tau = \frac{1}{\lambda} = \frac{1}{n} \sum_i \left[t_i - \frac{T_i \, e^{-\lambda T_i}}{1 - e^{-\lambda T_i}} \right]$$

Si $T_i \to \infty$, on retrouve $\tau = \frac{\sum t_i}{n}$

Calcul de σ_λ^2

$$\frac{\partial^2}{\partial \lambda^2} \text{Log } F = \sum_i \left[- \frac{1}{\lambda^2} + \frac{T_i^2 \, e^{-\lambda T_i}}{\left(1 - e^{-\lambda T_i}\right)^2} \right]$$

expression indépendante de la variable aléatoire t. Donc :

$$E\left[- \frac{\partial^2}{\partial \lambda^2} \text{Log } F \right] = \frac{1}{\lambda^2} \sum_i \left[1 - \frac{\lambda^2 T_i^2 \, e^{-\lambda T_i}}{\left(1 - e^{-\lambda T_i}\right)^2} \right]$$

On forme la variable de Bartlett :

$$\xi = \frac{\sum_i \left[\lambda t_i + \frac{\lambda T_i \, e^{-\lambda T_i}}{1 - e^{-\lambda T_i}} \right] - n}{\sqrt{\sum_i \left[1 - \frac{(\lambda T_i)^2 \, e^{-\lambda T_i}}{\left(1 - e^{-\lambda T_i}\right)^2} \right]}}$$

et on détermine λ et σ_λ sur le graphique $\xi(\lambda)$, d'où l'estimation de τ et l'intervalle de confiance (τ_1, τ_2).

ESTIMATION PARAMETRIQUE PAR METHODE DES MOINDRES CARRES (FITS)

L'estimation paramétrique par moindres carrés ne constitue qu'un petit domaine du champ de l'estimation paramétrique. Nous la considérerons cependant assez longuement ici car c'est la méthode de base qu'utilisent les grands programmes de chambres à bulles du type THRESH ou GRIND.

Les grands calculateurs effectuant les opérations sont bien adaptés aux calculs matriciels. Les considérations qui suivent ont pour ambition de faire comprendre la méthode générale utilisée qui consiste à rechercher le minimum du χ^2 du problème (moindres carrés). Pour réaliser cette opération, on travaille par approximations successives en linéarisant les équations et on répète le processus autant de fois que nécessaire (iteration).

Nous ne ferons pas, pour notre part, intervenir l'iteration et les formules qui seront déduites doivent être considérées comme valables à chaque stade des processus iteratifs.

La méthode d'exposition sera très progressive afin de permettre une acclimatation lente aux notations très condensées utilisées.

a) Cas où il y a indépendance statistique entre les mesures et où on veut estimer des paramètres à partir des grandeurs mesurées → ESTIMATION PARAMETRIQUE SANS CORRELATIONS NI CONTRAINTES.

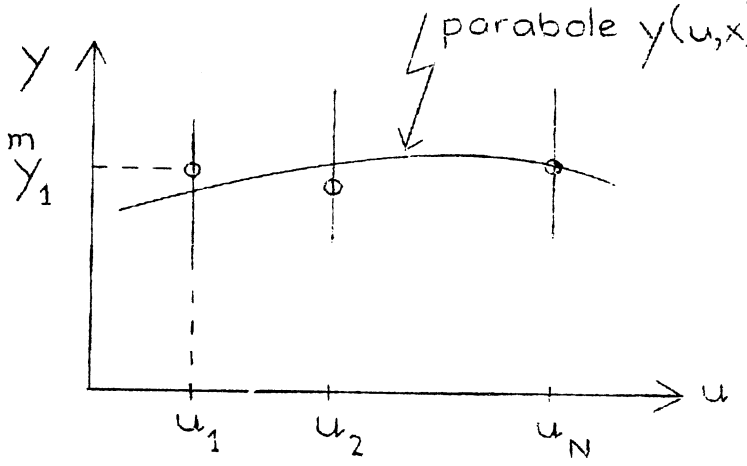
Ce genre de problème se présente quand on veut faire passer une courbe de forme connue par des points expérimentaux soumis à erreurs. On connaît donc la forme de l'équation algébrique de la fonction à adapter et on veut, au moyen des mesures, estimer les paramètres la définissant.

Par exemple, considérons, comme introduction à la méthode générale, le problème de faire passer une parabole

$$y = x_0 + x_1 u + x_2 u^2$$

par les points $(\overset{m}{y}_1, u_1), \ldots, (\overset{m}{y}_N, u_N)$ où u_N sont des quantités fixes et $\overset{m}{y}_N$ sont les résultats de mesure.

Quelles sont les meilleures valeurs des paramètres x_0, x_1 et x_2 ?



La méthode des moindres carrés nous dit de former la quantité

$$m = \sum_i \left(\frac{{}^{m}y_i - y_i}{\sigma_i} \right)^2$$

et de la rendre minimum par rapport aux 3 paramètres x_0, x_1 et x_2.

σ_i est l'erreur sur ${}^{m}y_i$ (écart-type)

Il vient donc :

$$\left.\begin{aligned}
x_0 \sum \frac{1}{\sigma_i^2} + x_1 \sum \frac{u_i}{\sigma_i^2} + x_2 \sum \frac{u_i^2}{\sigma_i^2} &= \sum \frac{{}^{m}y_i}{\sigma_i^2} \\
x_0 \sum \frac{u_i}{\sigma_i^2} + x_1 \sum \frac{u_i^2}{\sigma_i^2} + x_2 \sum \frac{u_i^3}{\sigma_i^2} &= \sum \frac{{}^{m}y_i u_i}{\sigma_i^2} \\
x_0 \sum \frac{u_i^2}{\sigma_i^2} + x_1 \sum \frac{u_i^3}{\sigma_i^2} + x_2 \sum \frac{u_i^4}{\sigma_i^2} &= \sum \frac{{}^{m}y_i u_i^2}{\sigma_i^2}
\end{aligned}\right\}$$ Système d'équations dites "Equations normales"

d'où l'on peut déduire x_0 et x_1, x_2 par la méthode classique de résolution d'un système d'équations linéaires.

On voit s'introduire naturellement le formalisme matriciel pour résoudre le problème simple que nous nous étions posé. Ceci devient encore plus évident quand on se propose de calculer les variances des x.

Etudions donc le cas général d'un ensemble ${}^{m}y_j$ de mesures d'une fonction $y(u_1 \ldots u_N, x_1 \ldots x_N)$, où :

- u_j = $j^{ème}$ point de mesure, fixé avec $j = 1, \ldots, N$
- x_i = $i^{ème}$ paramètre à évaluer, avec $i = 1, \ldots, n$
- ${}^{m}y_i$ = résultat de la mesure au point u_j.

Posons :

$$\Delta y_j = y_j - \overset{m}{y}_j \qquad \Delta x_i = x_i - (x_i)_o$$

où $(x_i)_o$ est une valeur approchée de x_i .

Dans ces conditions, il faut rendre minimum

$$m = \sum_1^N \left[\frac{1}{\sigma_j^2} (\Delta y_j)^2 \right] \rightarrow \frac{\partial m}{\partial x_i} \equiv 0$$

qui exprime que la courbe $y(u,x)$ passe au plus près des points expérimentaux $(\overset{m}{y},u)$, compte-tenu des latitudes permises autour de ces points exprimées par les variances σ_j^2 attachées aux mesures $\overset{m}{y}_j$.

On a donc :

$$\frac{\partial m}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\sum_1^N \frac{(\Delta y_j)^2}{\sigma_j^2} \right) = 0 \qquad \text{pour } i = 1, \ldots, n$$

En développant le 1er membre autour de $(x_i)_o$, il vient :

$$\sum_1^N \frac{1}{\sigma_j^2} (\Delta y_j) \left(\frac{\partial \Delta y_j}{\partial x_i} \right)_o + \frac{1}{2} \sum_k \Delta x_k \left(\frac{\partial^2 m}{\partial x_i \partial x_k} \right)_o$$

mais :

$$\frac{\partial^2 m}{\partial x_i \partial x_k} = \frac{\partial}{\partial x_i} \left(\frac{\partial m}{\partial x_k} \right) \sim \frac{\partial}{\partial x_i} \left(\frac{\partial \Sigma \Delta y_j^2}{\partial x_k} \right) \sim \left(\frac{\partial \Sigma \Delta y_j}{\partial x_i} \right) \cdot \left(\frac{\partial \Sigma \Delta y_j}{\partial x_k} \right) + 2 (\Sigma \Delta y_j) \frac{\partial^2 (\Sigma \Delta y_j)}{\partial x_i \partial x_k}$$

et comme les Δy sont petits par hypothèses $(\overset{m}{y} \simeq y)$, on négligera le dernier terme. On peut finalement écrire, avec

$$H_{k\ell} = \sum_{1}^{N} \frac{\partial(\Delta y_j)}{\partial x_k} \cdot \frac{1}{\sigma_j^2} \cdot \frac{\partial(\Delta y_j)}{\partial x_\ell} \quad \text{(matrice symétrique)}$$

$$K_\ell = \sum_{1}^{N} \frac{\Delta y_j}{\sigma_j^2} \cdot \frac{\partial(\Delta y_j)}{\partial x_\ell} \qquad k, \ell = 1, \ldots, n$$

les équations normales sous la forme :

$$\Delta x_k = - H^{-1}_{k\ell} K_\ell$$

La détermination de Δx_i est non biaisée.

Soit Δx_i^* le complément exact à $(x_i)_o = \tilde{x}_i$, valeur approchée de x_i, pour obtenir la valeur exacte x_i. On a, d'après les équations normales

$$\langle \Delta x_i \rangle \left(\sum_{1}^{N} \frac{1}{\sigma_j^2} \left(\frac{\partial \Delta y_j}{\partial x_i} \right) \left(\frac{\partial \Delta y_j}{\partial x_k} \right) \right) = \left(\sum_{1}^{N} \left(y_j - \overset{m}{y}_j \right) \frac{\partial \Delta y_j}{\partial x_k} \frac{1}{\sigma_j^2} \right)$$

mais :

$$y_j - \overset{m}{y}_j = \Delta x_i^* \left(\frac{\partial \Delta y_j}{\partial x_i} \right)$$

donc :

$$\langle \Delta x_i \rangle = \Delta x_i^* \qquad \text{cqfd.}$$

On peut évaluer les variances sur x_i (ou Δx_i)

$$\Delta x_i = - H^{-1}_{ik} \sum_{1}^{N} \left(\frac{1}{\sigma_j^2} \Delta y_j \frac{\partial \Delta y_j}{\partial x_k} \right)$$

et comme $\langle \Delta y_j \rangle = 0$ puisque $\langle \overset{m}{y}_j \rangle = y_j$ et que $y_j = \overset{m}{y}_j + \Delta y_j$

$$\Delta x_i - \langle \Delta x_i \rangle = - H^{-1}_{ik} \sum_1^N \frac{1}{\sigma_j^2} \left(y_j - \overset{m}{y_j} \right) \frac{\partial \Delta y_j}{\partial x_k}$$

$$\langle (\Delta x_i - \langle \Delta x_i \rangle)(\Delta x_\ell - \langle \Delta x_\ell \rangle) \rangle = + H^{-1}_{ik} H^{-1}_{\ell m} \sum_1^N \langle (\Delta y_j)^2 \rangle \frac{\partial \Delta y_j}{\partial x_k} \cdot \frac{\partial \Delta y_j}{\partial x_m} \cdot \frac{1}{\sigma_j^4} = H^{-1}_{i\ell}$$

puisque $\langle \Delta y_j^2 \rangle = \sigma_j^2$

Donc, la matrice H que nous avons introduite plus haut est en fait la matrice des poids. En repassant aux notations G, on a donc :

$$\underset{y}{G_m} = \begin{pmatrix} 1/\sigma_1^2 & & \\ & \ddots & \\ & & 1/\sigma_N^2 \end{pmatrix}$$

$$\Sigma \frac{\partial \Delta y_j}{\partial x_i} \cdot \frac{\partial \Delta y_j}{\partial x_k} \frac{1}{\sigma_j^2} = (H)_{ik} = (G_x)_{ik}$$

En posant :

$$\frac{\partial \Delta y_j}{\partial x_i} = \frac{\partial y_j}{\partial x_i} = A_{ji}$$

$$G_x = A^T \underset{y}{G_m} A \qquad \rightarrow \qquad G_x^{-1} = \left(A^T \underset{y}{G_m} A \right)^{-1}$$

Remarque

Cette formule est un cas particulier d'une formule de même forme plus générale, la simplification intervenant ici étant la diagonalité de la matrice $\underset{y}{G_m}$, ce qui n'est pas apparent dans notre notation.

On peut aussi chercher à calculer la matrice des covariances attachées aux y_j, mais le calcul sera fait de façon générale au paragraphe suivant.

b) Généralisation au cas où il y a des corrélations entre les mesures et où on veut estimer des paramètres à partir des grandeurs mesurées → ESTIMATION PARAMETRIQUE AVEC CORRELATIONS ET SANS CONTRAINTES.

Les grandeurs mesurées sont alors $y_1(x_1 \ldots x_n)$, $y_2(x_1 \ldots x_n)$ où les x_i représentent toujours les paramètres à estimer à partir des mesures des y_j soit $\overset{m}{y}_j$.

En notant comme précédemment Y le vecteur des y et ΔY le vecteur correction à apporter au vecteur $\overset{m}{Y}$ pour aboutir au vecteur vrai Y satisfaisant exactement aux équations fonctionnelles du problème, la probabilité d'avoir l'échantillon $\overset{m}{y}_1, \overset{m}{y}_2, \ldots \overset{m}{y}_N$, soit $\overset{m}{Y}$ est

$$f(\overset{m}{y}_1, \ldots, \overset{m}{y}_N) \simeq \exp\left\{-\frac{1}{2}(Y-\overset{m}{Y})^T \underset{Y}{V_m^{-1}} (Y-\overset{m}{Y})\right\} = \exp\left\{-\frac{1}{2}(\Delta Y)^T \underset{Y}{G_m} \Delta Y\right\}$$

où : $\underset{Y}{V_m} = \underset{Y}{G_m^{-1}}$ est la matrice de covariances des $\overset{m}{Y}$.

La solution des moindres carrés est celle du maximum de vraissemblance coïncidant avec celle du minimum de χ^2, c'est-à-dire celle qui rend

$$M = (\Delta Y)^T \underset{Y}{G_m} (\Delta Y) = \text{MINIMUM par rapport aux paramètres à estimer}$$

soit :

$$\frac{\partial M}{\partial x_1} = \frac{\partial M}{\partial x_2} = \ldots = \frac{\partial M}{\partial x_n} = 0 \quad \text{ou encore } \partial M/\partial X = \begin{vmatrix} \partial M/\partial x_1 \\ \vdots \\ \partial M/\partial x_n \end{vmatrix} = 0$$

Pour dériver M, on se guide sur ce que l'on fait sur une forme quadratique algébrique en remarquant que $\underset{Y}{G_m}$ n'est pas fonction des x_i .

$$\frac{\partial M}{\partial X} = 2(\Delta Y)^T \underset{Y}{G_m} \left(\frac{\partial \Delta Y}{\partial X}\right) = 0$$

soit $\tilde{X}$ une valeur approchée de X, on peut écrire :

$$\begin{cases} Y(X) = Y(\tilde{X}) + \dfrac{\partial}{\partial \tilde{X}} (Y(X))\, \Delta X \\ X \quad = \tilde{X} + \Delta X \end{cases}$$

ou encore avec

$$A = \frac{\partial Y}{\partial \tilde{X}} = \frac{\partial Y}{\partial \Delta X}$$

$$Y = \tilde{Y} + A\,\Delta X \qquad \text{avec} \qquad \tilde{Y} = Y(\tilde{X})$$

Exploitons maintenant les conditions de moindres carrés, $\frac{\partial M}{\partial X} = 0$

→

$$0 = 2(Y - \overset{m}{Y})^T \underset{Y}{G_m} \frac{\partial}{\partial X} (Y - \overset{m}{Y}) = 2(Y - \overset{m}{Y})^T \underset{Y}{G_m} \frac{\partial Y}{\partial \Delta X}$$

soit :

$$\overset{m}{Y}{}^T \underset{Y}{G_m} \underbrace{\frac{\partial Y}{\partial \Delta X}}_{A} = Y^T \underset{Y}{G_m} \underbrace{\frac{\partial Y}{\partial \Delta X}}_{A} = (\tilde{Y} + A\,\Delta X)^T \underset{Y}{G_m} \frac{\partial Y}{\partial \Delta X}$$

$$\Delta X^T (A^T \underset{Y}{G_m} A) = (\overset{m}{Y} - \tilde{Y})^T \underset{Y}{G_m} A$$

$$\boxed{\Delta X = (A^T \underset{Y}{G_m} A)^{-1} A^T \underset{Y}{G_m} (\overset{m}{Y} - \tilde{Y})}$$

équation normale qui définit ΔX → ENSEMBLE DES EQUATIONS NORMALES DU PROBLEME des moindres carrés considéré.

On peut calculer $G_{\Delta X}^{-1} = G_X^{-1}$ matrice d'erreurs sur les x_j et leurs corrélations. On a :

$$G_{\Delta X}^{-1} = G_X^{-1} = \left(\frac{\partial X}{\partial Y}\right)_m G_{m\,Y}^{-1} \left(\frac{\partial X}{\partial Y}\right)_m^T = \left(\frac{\partial \Delta X}{\partial Y}\right)_m G_{m\,Y}^{-1} \left(\frac{\partial \Delta X}{\partial Y}\right)_m^T$$

$$= \left[\left(A^T G_{m\,Y} A\right)^{-1} A^T G_{m\,Y}\right] G_{m\,Y}^{-1} \left[\left(A^T G_{m\,Y} A\right)^{-1} A^T G_{m\,Y}\right]^T$$

$$= \left(A^T G_{m\,Y} A\right)^{-1} \left(A^T G_{m\,Y} A\right) \left(A^T G_{m\,Y} A\right)^{-1}$$

$$\boxed{G_X^{-1} = G_{\Delta X}^{-1} = \left(A^T G_{m\,Y} A\right)^{-1}} \qquad \text{avec } A = \frac{\partial Y}{\partial \Delta X}$$

On retrouve bien la même expression que précédemment, mais ici $G_{m\,Y}$ n'est plus supposée diagonale.

Remarque

Il ne faut pas, dans la formule ci-dessus, effectuer l'inversion par la règle $(BCD)^{-1} = D^{-1} C^{-1} B^{-1}$, car A et A^T ne sont pas, en général, des matrices carrées.

On peut en déduire G_Y^{-1}.

Remarquons que $\left(\frac{\partial Y}{\partial Y}\right)_m = \left(\frac{\partial Y}{\partial X}\right) \cdot \left(\frac{\partial X}{\partial Y}\right)_m = \left(\frac{\partial Y}{\partial X}\right) \left(A^T G_{m\,Y} A\right)^{-1} A^T G_{m\,Y}$

et donc :

$$G_Y^{-1} = \left(\frac{\partial Y}{\partial Y}\right)_m G_{m\,Y}^{-1} \left(\frac{\partial Y}{\partial Y}\right)_m^T$$

$$= A \left(A^T G_{m\,Y} A\right)^{-1} A^T G_{m\,Y} G_{m\,Y}^{-1} \left(A \left(A^T G_{m\,Y} A\right)^{-1} A^T G_{m\,Y}\right)^T$$

$$= A \left(A^T \underset{Y}{G_m} A \right)^{-1} A^T \underbrace{\underset{Y}{G_m} \underset{Y}{G_m^{-1}}}_{1} \underset{Y}{G_m} A \left(A \underset{Y}{G_m} A^T \right)^{-1} A^T$$

$$= A \left(A^T \underset{Y}{G_m} A \right)^{-1} \underbrace{\left(A^T \underset{Y}{G_m} A \right) \left(A \underset{Y}{G_m} A^T \right)}_{1} \left(A \underset{Y}{G_m} A^T \right)^{-1} A^T$$

→

$$\boxed{A \left(A^T \underset{Y}{G_m} A \right)^{-1} A^T = A \, G_X^{-1} A^T = G_Y^{-1}}$$

c) Exemple simple d'application

Fit d'une parabole sur des points expérimentaux dans le cas où il y a indépendance des points entre eux.

Soit $y = x_1 u + x_2 u^2 + x_0$ l'équation de cette parabole.

Définissons aussi :

$\overset{m}{y_j}$ les n ordonnées mesurées chacune avec une erreur σ_j (σ_j^2 = variance) avec indépendance des σ entre eux et égalité de tous les σ.

u_j les n abscisses correspondantes considérées comme des données.

x_i avec i = 0,1,2, les 3 parametres à optimiser.

On a :

$$y = \begin{pmatrix} y_1 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{pmatrix} \qquad x = \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_{1\,1} \\ x_{1\,2} \\ x_{1\,3} \end{pmatrix}$$

soit :

$y = Ax$ avec A matrice (non carrée) d'élément $A_{ij} = \dfrac{\partial y_i}{\partial x_j}$

Par conséquent :

$$A = \begin{pmatrix} 1 & u_1 & u_1^2 \\ 1 & u_2 & u_2^2 \\ \cdots & \cdots & \cdots \end{pmatrix} \quad \text{et} \quad A^T = \begin{pmatrix} 1 & 1 & \cdots \\ u_1 & u_2 & \cdots \\ u_1^2 & u_2^2 & \cdots \end{pmatrix}$$

a) Calculons :

$$G_\alpha^{-1} = \left(A^T \underset{y}{G_m} A \right)^{-1}$$

$$G_\alpha = \begin{pmatrix} 1 & 1 & \cdots \\ u_1 & u_2 & \cdots \\ u_1^2 & u_2^2 & \cdots \end{pmatrix} \begin{pmatrix} 1/\sigma_1^2 & & \\ & \cdot & \\ & & 1/\sigma_n^2 \end{pmatrix} \begin{pmatrix} 1 & u_1 & u_1^2 \\ 1 & u_2 & u_2^2 \\ \cdots & \cdots & \cdots \end{pmatrix}$$

$$= \begin{pmatrix} \sum_1^n 1/\sigma_j^2 & \sum_1^n u_j/\sigma_j^2 & \sum_1^n u_j^2/\sigma_j^2 \\ \sum_1^n u_j/\sigma_j^2 & \sum_1^n u_j^2/\sigma_j^2 & \sum_1^n u_j^3/\sigma_j^2 \\ \sum_1^n u_j^2/\sigma_j^2 & \sum_1^n u_j^3/\sigma_j^2 & \sum_1^n u_j^4/\sigma_j^2 \end{pmatrix} = \frac{1}{\sigma^2} \begin{pmatrix} \Sigma & S_1 & S_2 \\ S_1 & S_2 & S_3 \\ S_2 & S_3 & S_4 \end{pmatrix} = \frac{(G'_x)}{\sigma^2}$$

ou :

$$\begin{cases} S_1 = \sum_1^n u_j \ \ldots \ S_4 = \sum_1^n u_j^4 \\ \sigma_1^2 = \ \ldots \ = \sigma_n^2 = \sigma^2 \\ \Sigma = n \end{cases}$$

En inversant cette matrice :

$$G_x^{-1} = \frac{\sigma^2}{\det (G'_x)} \begin{pmatrix} \begin{vmatrix} S_2 & S_3 \\ S_3 & S_4 \end{vmatrix} & - \begin{vmatrix} S_1 & S_3 \\ S_2 & S_4 \end{vmatrix} & \begin{vmatrix} S_1 & S_2 \\ S_2 & S_3 \end{vmatrix} \\ \begin{vmatrix} S_1 & S_2 \\ S_3 & S_4 \end{vmatrix} & \begin{vmatrix} \Sigma & S_2 \\ S_2 & S_4 \end{vmatrix} & - \begin{vmatrix} \Sigma & S_1 \\ S_2 & S_3 \end{vmatrix} \\ \begin{vmatrix} S_1 & S_2 \\ S_2 & S_3 \end{vmatrix} & \begin{vmatrix} \Sigma & S_1 \\ S_2 & S_3 \end{vmatrix} & \begin{vmatrix} \Sigma & S_1 \\ S_1 & S_2 \end{vmatrix} \end{pmatrix}$$

ERREURS ET CORRELATIONS SUR x_0, x_1 et x_2 .

b) Calculons ensuite $A^T G_m \overset{m}{y}$ pour calculer α à partir de la formule de la page 68, avec $\tilde{y} \overset{y}{=} 0$. On a :

$$A^T G_m \overset{m}{y} = \begin{pmatrix} 1 & 1 & \cdots \\ u_1 & u_2 & \cdots \\ u_1^2 & u_2^2 & \cdots \end{pmatrix} \begin{pmatrix} 1/\sigma_1^2 & & \\ & \cdot & \\ & & 1/\sigma_n^2 \end{pmatrix} \begin{pmatrix} \overset{m}{y_1} \\ \overset{m}{y_2} \\ \cdot \end{pmatrix}$$

$$= \begin{pmatrix} \sum_1^n \overset{m}{y_j}/\sigma_j^2 \\ \sum_1^n \overset{m}{y_j}\, u_j/\sigma_j^2 \\ \sum_1^n \overset{m}{y_j}\, u_j^2/\sigma_j^2 \end{pmatrix} = \begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}$$

et :

$$x_0 = (x)_{11} = \left\{ s_1 \begin{vmatrix} S_2 & S_3 \\ S_3 & S_4 \end{vmatrix} - s_2 \begin{vmatrix} S_1 & S_3 \\ S_2 & S_4 \end{vmatrix} + s_3 \begin{vmatrix} S_1 & S_2 \\ S_2 & S_3 \end{vmatrix} \right\} \frac{1}{D_0}$$

$$= \frac{1}{D_0} \begin{vmatrix} s_1 & S_1 & S_2 \\ s_2 & S_2 & S_3 \\ s_3 & S_3 & S_4 \end{vmatrix} = \frac{D_1}{D_0}$$

avec $D_0 = \det(G'_x)$.

De même :

$x_1 = (x)_{12} = \frac{D_2}{D_0} = \frac{1}{D_0} \begin{vmatrix} \Sigma & s_1 & s_2 \\ s_1 & s_2 & s_3 \\ s_2 & s_3 & s_4 \end{vmatrix}$	$\sigma^2_{x_1} = \left(G_x^{-1}\right)_{22} = \sigma^2 \frac{\begin{vmatrix} \Sigma & s_2 \\ s_2 & s_4 \end{vmatrix}}{D_0}$
$x_2 = (x)_{13} = \frac{D_3}{D_0} = \frac{1}{D_0} \begin{vmatrix} \Sigma & s_1 & s_1 \\ s_1 & s_2 & s_2 \\ s_2 & s_3 & s_3 \end{vmatrix}$	$\sigma^2_{x_2} = \left(G_\alpha^{-1}\right)_{33} = \sigma^2 \frac{\begin{vmatrix} \Sigma & s_1 \\ s_1 & s_2 \end{vmatrix}}{D_0}$
$x_0 = (x_0)_{11} = \frac{D_1}{D_0} = \frac{1}{D_0} \begin{vmatrix} s_1 & s_1 & s_2 \\ s_2 & s_2 & s_3 \\ s_3 & s_3 & s_4 \end{vmatrix}$	$\sigma^2_{x_0} = \left(G_\alpha^{-1}\right)_{11} = \sigma^2 \frac{\begin{vmatrix} s_2 & s_3 \\ s_3 & s_4 \end{vmatrix}}{D_0}$

c) Par

$$G_Y^{-1} = A\, G_X^{-1}\, A^T$$ on peut évaluer les erreurs aux points $1,\ldots,n$.

Vue la complexité de G_a^{-1} (même dans le cas simple traité ici!) nous ne ferons pas le calcul explicitement, nous en laisserons le soin à un programme IBM par exemple.

d) Il est plus intéressant de revenir aux équations normales du problème, soit :

$$\frac{\partial}{\partial x_0}\left\{\sum_1^n\left(y_j^m - x_0 - x_1 x_j - x_2 u_j^2\right)\right\} = -2\left\{\sum_1^n\left(y_j^m - x_0 - x_1 u_j - x_2 u_j^2\right)\right\} = 0$$

$$\frac{\partial}{\partial x_1}\left\{\sum_1^n\left(y_j^m - x_0 - x_1 x_j - x_2 u_j^2\right)\right\} = -2\left\{\sum_1^n u_j\left(y_j^m - x_0 - x_1 u_j - x_2 u_j^2\right)\right\} = 0$$

$$\frac{\partial}{\partial x_2}\left\{\sum_1^n\left(y_j^m - x_0 - x_1 x_j - x_2 u_j^2\right)\right\} = -2\left\{\sum_1^n u_j^2\left(y_j^m - x_0 - x_1 u_j - x_2 u_j^2\right)\right\} = 0$$

La valeur calculée par ces équations de y_j est $\overset{c}{y}_j = x_0 + x_1 u_j + x_2 u_j^2$.

Calculons :

$$Y_j = \overset{m}{y}_j - \overset{c}{y}_j = \overset{m}{y}_j - x_0 - x_1 u_j - x_2 u_j^2$$

$$Y_j^2 = \left(\overset{m}{y}_j - \overset{c}{y}_j\right)^2 = \overset{m}{y}_j^2 - 2\,\overset{m}{y}_j\left(x_0 + x_1 u_j + x_2 u_j^2\right) + \left(x_0 + x_1 u_j + x_2 u_j^2\right)^2$$

et en sommant sur j

$$\sum_1^n Y_j^2 = \sum_1^n \overset{m}{y}_j^2 + \sum_1^n\left\{\left(x_0 + x_1 u_j + x_2 u_j^2\right)\underbrace{\left(x_0 + x_1 u_j + x_2 u_j^2 - 2\,\overset{m}{y}_j\right)}\right\}$$

$-\overset{m}{y}_j$ en fonction des équations normales.

$$= \sum_1^n \overset{m}{y}_j^2 - \sum_1^n\left(x_0 + x_1 u_j + x_2 u_j^2\right)\overset{m}{y}_j$$

Donc :

$$\sum_1^n \left({}^m y_j - {}^c y_j \right)^2 = \sum_1^n {}^m y_j^2 - x_0 \sum_1^n {}^m y_j - x_1 \sum u_j \, {}^m y_j - x_2 \sum u_j^2 \, {}^m y_j$$

A partir de cette somme, on peut évaluer la variance S^2 de l'échantillon des y_j par

$$S^2 = \frac{1}{n-3} \sum_1^n \left({}^m y_j - {}^c y_j \right)^2$$

où le 3 tient compte du fait qu'il y a 3 contraintes linéaires entre les y_j du fait des équations normales. Donc :

$$S^2 = \text{estimation de la variance sur } y = \frac{1}{n-3} \left(\sum_1^n {}^m y_j^2 - \alpha_0 \sum_1^n {}^m y_j - \alpha_1 \sum_1^n x_j {}^m y_j - \alpha_2 \sum_1^n x_j^2 {}^m y_j \right)$$

En outre comme on a vu que $E({}^c x) = x \to {}^c y$ coïncide en moyenne avec $\langle y \rangle$ et par suite

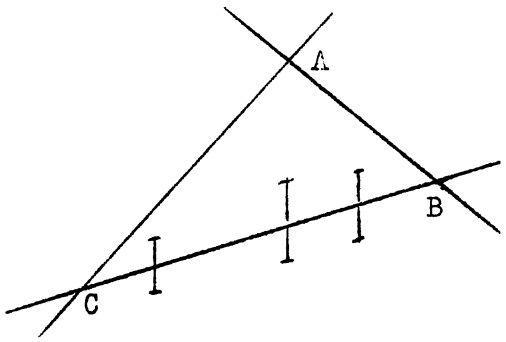
$\sum_1^n \left({}^m y_j - {}^c y_j \right)^2$ est une variable χ^2_{n-3} au facteur $\sigma^2_{y_j}$ pris, et :

$$\text{variance sur } S^2 = \text{variance} \left\{ \frac{\sigma^2}{n-3} \chi^2_{n-3} \right\} = \frac{\sigma^4}{(n-3)^2} \text{ variance} \left(\chi^2_{n-3} \right) = \frac{2\sigma^4}{n-3}$$

c) Cas où il y a des liaisons algébriques entres les grandeurs à estimer → ESTIMATION PARAMETRIQUE AVEC CORRELATIONS ET AVEC CONTRAINTES

Dans ce qui précède, nous avons considéré des variables aléatoires qui n'étaient pas forcément statistiquement indépendantes, c'est-à-dire que les diverses estimations faites n'étaient pas indépendantes entre elles et que toute modification apportée à une de ces estimations (par exemple au cours d'itérations du processus d'estimation) rejaillissait obligatoirement sur d'autres estimations.

Pour préciser ce fait, et en vue de considérations futures, prenons l'exemple simple de l'estimation des 3 angles d'un triangle. Pour ce faire, nous mesurons des points sur les côtés du triangle et par ces points nous faisons passer, par exemple, les 3 droites de moindres carrés.



En opérant ainsi puisque BC est commune aux angles $\hat{C}$ et $\hat{B}$, toute modification de la droite de moindres carrés "CB" modifie à la fois ces 2 angles. L'estimation de l'angle $\hat{B}$ n'est pas statistiquement indépendante de celle de $\hat{C}$. Il y a corrélation statistique entre l'estimation de $\hat{B}$ soit $\hat{B}^*$ et celle de $\hat{C}$ soit $\hat{C}^*$.

Maintenant, il est bien connu que pour tout triangle (notamment celui construit à partir des estimations $\hat{A}^*$, $\hat{B}^*$, $\hat{C}^*$), on doit avoir :

$$\hat{A} + \hat{B} + \hat{C} = 2\pi$$

Si on veut respecter cette relation dans notre estimation, il faut trouver la solution des moindres carrés avec une condition (contrainte) algébrique supplémentaire complètement indépendante de la méthode d'estimation et des liaisons statistiques qui peuvent exister en son sein.

Nous aurons donc à résoudre, en ce cas, un problème algébrique de minimum (celui contenant la partie statistique du problème) lié par des contraintes algébriques (celles-ci contenant les conditions physiques du problème). Pour ce faire, il existe une méthode algébrique classique, celle des MULTIPLICATEURS DE LAGRANGE que nous rappellerons ici.

Soit $\Phi(u_1 \ldots u_n)$ une fonction 2 fois différentiables et des fonctions $F_1(u_1 \ldots u_n)$, $F_2(u_1 \ldots u_n)$ jouissant des mêmes propriétés. Il faut trouver :

$$\Phi(u_1 \ldots u_n) = \text{MINIMUM} \qquad \text{(contient le moindre carré)}$$

en même temps que

$$F_j(u_1 \ldots u_n) = 0 \qquad \text{(contient les contraintes algébriques)}$$

On forme alors :

$$\Psi(u_1 \ldots u_n) = \Phi(u_1 \ldots u_n) - \sum_1^m k_j F_j(u_1 \ldots u_n) = 0$$

On a le minimum de Φ pour

$$\begin{cases} \dfrac{\partial \Psi}{\partial u_1} = \ldots = \dfrac{\partial \Psi}{\partial u_n} = 0 \quad \rightarrow \quad n \text{ équations} \\ \text{avec} \\ F_j(u_1, \ldots, u_n) = 0 \quad \rightarrow \quad m \text{ équations} \end{cases}$$

soit m+n équations pour calculer les n variables u et les m variables k.

1°) Expression de la condition de minimum lié dans le cas où toutes les grandeurs sont mesurées et sont d'autre part liées par des contraintes algébriques.

La condition des moindres carrés s'écrit toujours :

$$M = (\Delta Y)^T \underset{Y}{G_m} \Delta Y = \text{MINIMUM}$$

Il faut y adjoindre les contraintes qui lient les variables contenues dans M, soit :

$$F_j(y_1 \ldots y_N) = 0 = F(Y)$$

Celles-ci ne sont pas forcément linéaires et si on connaît une valeur approchée $\tilde{Y}$ de Y, on pout écrire :

$$\tilde{Y} = \overset{m}{Y} + \tilde{\Delta Y} \qquad Y = \overset{m}{Y} + \Delta Y \rightarrow Y - \tilde{Y} = \Delta Y - \tilde{\Delta Y}$$

$$F(Y) = F(\tilde{Y}) + \frac{\partial F}{\partial \tilde{Y}} (\Delta Y - \tilde{\Delta Y}) = 0 = F(\tilde{Y}) + B\Delta Y - B\tilde{\Delta Y}$$

soit :

$$B\Delta Y + R = 0 \quad \text{avec} \quad \begin{cases} B = \dfrac{\partial F}{\partial \tilde{Y}} = \underset{m}{\dfrac{\partial F}{\partial Y}} \\ R = F(\tilde{Y}) - B\tilde{\Delta Y} \end{cases}$$

On a donc pour le minimum lié :

$$\begin{cases} M = (\Delta Y)^T \underset{Y}{G_m} \Delta Y = \text{MINIMUM} \\ B\Delta Y + R = 0 \end{cases}$$

La méthode des multiplicateurs de Lagrange, conduit à former :

$$M' = (\Delta Y)^T \underset{Y}{G_m} \Delta Y + 2\, k^T (B\Delta Y + R)$$

et à minimiser. Donc :

$$\frac{\partial M'}{\partial(\Delta Y)} = 0 = 2(\Delta Y)^T \underset{Y}{G_m} + 2\, k^T B \qquad \text{(k est supposé constant dans cette méthode)}$$

soit :

$$\boxed{\Delta Y = - \underset{Y}{G_m^{-1}}\, B^T k} \qquad \text{(N équations)}$$

et :

$$\left(B \underset{Y}{G_m^{-1}}\, B^T \right) k = R = G_B^{-1} k$$

$$\boxed{k = G_B R} \qquad (j = 1 \ldots m \rightarrow m \text{ équations})$$

On peut en déduire la matrice de covariances sur les Y.

On a :

$$G_Y^{-1} = \left(\frac{\partial Y}{\partial \overline{m}} \right) \underset{Y}{G_m^{-1}} \left(\frac{\partial Y}{\partial \overline{m}} \right)^T$$

Or,

$$\frac{\partial Y}{\partial Y}_m = \mathbb{1} + \frac{\partial \Delta Y}{\partial Y}_m = \mathbb{1} - G_{m\,Y}^{-1} B^T \frac{\partial k}{\partial Y}_m = \mathbb{1} - G_{m\,Y}^{-1} B^T G_B^{-1} \frac{\partial R}{\partial Y}_m$$

$$= \mathbb{1} - G_{m\,Y}^{-1} B^T G_B^{-1} \frac{\partial F}{\partial Y}_m$$

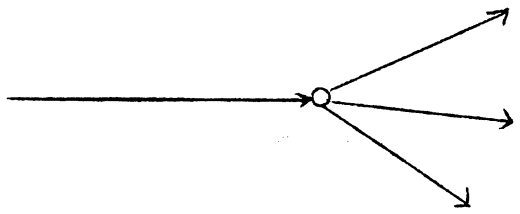
soit :

$$\boxed{G_{Y}^{-1} = G_{m\,Y}^{-1} - \left(G_{m\,Y}^{-1} B^T\right) G_B^{-1} \left(B\, G_{m\,Y}^{-1}\right)}$$

terme introduit par le minimum lié
(contraintes algébriques)

Un exemple simple de contraintes algébriques

Soit n traces d'une interaction, c'est-à-dire la particule initiale (plus la particule cible) plus n - 1 traces sortantes.



On veut traiter la cinématique de cette interaction ayant mesuré pour chaque particule :

- son impulsion (grandeur et direction)
- sa masse (en fait c'est une donnée)

Les contraintes algébriques sont celles de :

- la conservation de l'impulsion
- la conservation de l'énergie

soit :

$$\sum_1^n \vec{P}_i = 0 \qquad M_T = \sum_1^n U_i \quad \text{où} \quad M_T = \text{masse de la cible}$$
$$U_i = (P_i^2 + M_i^2)^{1/2}$$

donc 4 équations de contraintes.

Les grandeurs mesurées sont $1/P_i$ déduites de la mesure de courbure (grandeur additive) avec une erreur $\sigma^2\ 1/P_i$.

φ_i, λ_i angles d'orientations (azimut et dip) des impulsions avec les erreurs $\sigma^2_{\varphi_i}$ et $\sigma^2_{\lambda_i}$.

On a donc :

$$\overset{m}{y}_{1i} = \frac{1}{P_i} \qquad \overset{m}{y}_{2i} = \lambda_i \qquad \overset{m}{y}_{3i} = \varphi_i \qquad \rightarrow \qquad \overset{m}{y} = \begin{vmatrix} 1/P_i \\ \lambda_i \\ \varphi_i \end{vmatrix}$$

Reécrivons les contraintes algébriques en fonction de ces nouvelles variables, en projetant $\vec{P}$ sur les axes de référence dans lesquels φ et λ sont définis. Il vient :

$$\left.\begin{aligned} F_1 &= \sum_1^n \left(P_X\right)_i = \sum_i P_i \cos\lambda_i \cos\varphi_i = 0 \\ F_2 &= \sum_1^n \left(P_Y\right)_i = \sum_i P_i \cos\lambda_i \operatorname{Sin}\varphi_i = 0 \\ F_3 &= \sum_1^n \left(P_Z\right)_i = \sum_i P_i \operatorname{Sin}\lambda_i = 0 \end{aligned}\right\} \text{ conservation de l'impulsion}$$

$$\left.\begin{aligned} F_4 &= -M_T + \sum_i \left(P_i^2 + M_i^2\right)^{1/2} = 0 \end{aligned}\right\} \text{ conservation de l'énergie}$$

1°/ Il faut alors évaluer la matrice $B = \frac{\partial F}{\partial y}_m$. Pour la trace i, il vient :

$$(B)_i = \begin{pmatrix} -P_i^2 \cos\lambda_i \cos\varphi_i & -P_i \operatorname{Sin}\lambda_i \cos\varphi_i & -P_i \cos\lambda_i \operatorname{Sin}\varphi_i \\ -P_i^2 \cos\lambda \operatorname{Sin}\varphi_i & -P_i \operatorname{Sin}\lambda_i \operatorname{Sin}\varphi_i & +P_i \cos\lambda_i \cos\varphi_i \\ -P_i^2 \operatorname{Sin}\lambda_i & P_i \cos\lambda_i & 0 \\ +P_i^3/U_i & 0 & 0 \end{pmatrix}$$

de B, on passe à G_B par

$$G_B = (B\ G^{-1}\ B^T)^{-1}$$

avec :

$$G_{m\ Y}^{-1} = \begin{pmatrix} \sigma^2_{\frac{1}{P}} & \sigma^2_{\frac{1}{P},\lambda} & \sigma^2_{\frac{1}{P},\varphi} \\ \sigma^2_{\frac{1}{P},\lambda} & \sigma^2_{\lambda} & \sigma^2_{\lambda\varphi} \\ \sigma^2_{\frac{1}{P},\varphi} & \sigma_{\lambda\varphi} & \sigma^2_{\varphi} \end{pmatrix}$$

où σ^2_{xy} représentent les covariances entre x et y qui sont déduites des mesures et de la méthode d'estimation utilisée.

2°/ La première évaluation de R se fait avec $\Delta\tilde{Y} = 0$. Dans ces conditions :

$$R^o = F(\tilde{Y}) - B\Delta\tilde{Y} \rightarrow R = F(\tilde{Y}) = F(\overset{m}{Y} + \Delta\tilde{Y}) = F(\overset{m}{Y})$$

3°/ Les multiplicateurs de Lagrange sont dans ce cas :

$$k \rightarrow k^c = G_B\ R^o = G_B\ F(\overset{m}{Y})$$

4°/ La première évaluation des ΔY s'en déduit immédiatement par :

$$(\Delta Y)^o = -\ G_{m\ Y}^{-1}\ B^T\ k^o$$

donc :

$$Y^o = \overset{m}{Y} + \Delta Y^o$$

et :

$$G_{Y^o}^{-1} = G_{m\ Y}^{-1} - G_{m\ Y}^{-1}\ B^T\ G_B^{-1}\ B\ G_{m\ Y}^{-1}$$

2°/ Cas général avec contraintes algébriques et paramètres à estimer indirectement à partir des grandeurs mesurées.

Les mesures de $y_j(x_1 \ldots x_n)$ seront notées $\overset{m}{y}_j$. Les x sont les paramètres à estimer à partir des y.

Les contraintes algébriques sont de la forme $F_k(y_1 \ldots y_N) = 0$.

On a donc, sous forme implicite

$$\Phi_k(x_1 \ldots x_n ;\ y_1 \ldots y_N) = \Phi = \Phi\ (X,Y)$$

Ces fonctions ne sont pas forcément linéaires. On supposera que l'on connaît des valeurs approchées $\tilde{X}$ et $\tilde{Y}$ de X et Y. Dans ces conditions :

$$\Phi = \Phi(\tilde{X}, \overset{m}{Y} + \Delta\tilde{Y}) + \frac{\partial\Phi}{\partial\tilde{X}}\ \Delta\tilde{X} + \frac{\partial\Phi}{\partial\tilde{Y}}\ (\Delta Y - \Delta\tilde{Y}) = 0$$

avec :

$$Y = \overset{m}{Y} + \Delta Y \qquad \tilde{Y} = \overset{m}{Y} + \Delta\tilde{Y} \qquad X = \tilde{X} + \Delta\tilde{X}$$

soit :

$$A\,\Delta X + B\,\Delta Y + R = 0 \quad \text{avec} \quad \begin{cases} A = \partial\Phi/\partial X \\ B = \partial\Phi/\partial\tilde{Y} = \partial\Phi/\partial\overset{m}{Y} \\ R = \Phi(\tilde{X},\tilde{Y}) - B\,\Delta\tilde{Y} \end{cases}$$

La condition des moindres carrés s'écrit toujours :

$$M = (\Delta Y)^T\ \underset{Y}{G_m}\ \Delta Y = \text{MINIMUM}$$

a) La méthode des multiplicateurs de Lagrange conduit à minimiser

$$M' = (\Delta Y)^T\ \underset{Y}{G_m}\ \Delta Y + 2\,k^T(A\,\Delta X + B\,\Delta Y + R) = \text{minimum}$$

Considérons d'abord les données partielles de M' par rapport à Δy, à $\Delta X = C^{te}$, qui expriment les conditions de minimum lié pour M; il vient :

$$\frac{\partial M'}{\partial \Delta Y} = 0 = 2(\Delta Y)^T \underset{Y}{G_m} + 2\, k^T B$$

soit :

$$\boxed{\Delta Y = - \underset{Y}{G_m^{-1}}\, B^T k} \qquad \boxed{k = G_B(A\,\Delta X + R)} \; ; G_B = B \underset{Y}{G_m^{-1}}\, B^T$$

b) Portant ces expressions dans M', il vient :

$$M' = (A\,\Delta X + R)^T G_B\, (A\,\Delta X + R)$$

car,

$$M' = \left[\underset{Y}{G_m^{-1}}\, B^T G_B^{-1}(A\,\Delta X + R)\right]^T \underset{Y}{G_m} \left[\underset{Y}{G_m^{-1}}\, B^T G_B^{-1}\, (A\,\Delta X + R)\right]$$

$$= (A\,\Delta X + R)^T \underbrace{(G_B)^T}_{G_B} \underbrace{B \underset{Y}{G_m^{-1}} \underset{Y}{G_m} \underset{Y}{G_m^{-1}} B^T}_{G_B^{-1}} G_B (A\,\Delta X + R)$$

Si nous évaluons maintenant les dérivées partielles de M' par rapport à ΔX, à $\Delta Y = C^{te}$, on obtient :

$$\frac{\partial M'}{\partial \Delta X} = 0 = 2(A\,\Delta X + R)^T G_B A \rightarrow (\Delta X)^T (A^T G_B A) = - R^T G_B A$$

soit :

$$\boxed{\Delta X = - \left(A^T G_B A\right)^{-1} A^T G_B R}$$

c) On peut en déduire les matrices de covariances pour lesX et les Y.

On a :

$$G_{\Delta X}^{-1} = G_X^{-1} = \left(\frac{\partial \Delta X}{\partial Y} \right) \; G_Y^{-1} \left(\frac{\partial \Delta X}{\partial Y} \right)^T$$

or,

$$\frac{\partial \Delta X}{\partial Y} = - \left(A^T G_B A \right)^{-1} A^T G_B \frac{\partial R}{\partial Y} = - \left(A^T G_B A \right)^{-1} A^T G_B \frac{\partial R}{\partial \Delta \tilde{Y}}$$

$$= - \left(A^T G_B A \right)^{-1} A^T G_B B$$

Donc :

$$G_X^{-1} = G_{\Delta X}^{-1} = \left(\left(A^T G_B A \right)^{-1} A^T G_B B \right) G_Y \left(\left(A^T G_B A \right)^{-1} A^T G_B B \right)^T$$

$$= \left(A^T G_B A \right)^{-1} A^T G_B \underbrace{B \, G_Y \, B^T}_{G_B^{-1}} G_B A \left(A^T G_B A \right)^{-1}$$

$$= \left(A^T G_B A \right)^{-1} \left(A^T G_B A \right) \left(A^T G_B A \right)^{-1}$$

→

$$\boxed{G_X^{-1} = \left(A^T G_B A \right)^{-1}}$$

Et :

$$G_Y^{-1} = \left(\frac{\partial Y}{\partial \underset{\sim}{m}}\right) G_{mY}^{-1} \left(\frac{\partial Y}{\partial \underset{\sim}{m}}\right)^T \text{ avec } \frac{\partial Y}{\partial \underset{\sim}{m}} = \mathbb{1} - G_{mY}^{-1} B^T \frac{\partial k}{\partial \underset{\sim}{m}}$$

$$= \mathbb{1} - G_{mY}^{-1} B^T G_B (B - A(K^{-1}) A^T G_B B)$$

avec :

$$K^{-1} = \left(A^T G_B A\right)^{-1} = (K^{-1})^T$$

Donc :

$$G_{mY}^{-1} = \left[\mathbb{1} - G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B - G_{mY}^{-1} B^T G_B B\right] G_{mY}^{-1} \left[\mathbb{1} - B^T G_B A K^{-1} A^T G_B B G_{mY}^{-1} - B^T G_B B G_{mY}^{-1}\right]$$

$$= G_{mY}^{-1} - G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B G_{mY}^{-1} - G_{mY}^{-1} B^T G_B B G_{mY}^{-1}$$

$$+ G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B B G_{mY}^{-1} - G_{mY}^{-1} B^T G_B B G_{mY}^{-1} + G_{mY}^{-1} B^T G_B B G_{mY}^{-1}$$

$$- G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B G_{mY}^{-1} + G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B A K^{-1} A^T G_B B G_{mY}^{-1}$$

$$+ G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B B G_{mY}^{-1}$$

$$\boxed{G_Y^{-1} = G_{mY}^{-1} - G_{mY}^{-1} B^T G_B B G_{mY}^{-1} + G_{mY}^{-1} B^T G_B A (A^T G_B A)^{-1} A^T G_B B G_{mY}^{-1}}$$

car,

$$G_{mY}^{-1} B^T G_B A K^{-1} \underbrace{A^T G_B A}_{K} K^{-1} A^T G_B B G_{mY}^{-1} = G_{mY}^{-1} B^T G_B A K^{-1} A^T G_B B G_{mY}^{-1}$$

La comparaison entre le cas des liaisons sans détermination de paramètres et celui où il y a en outre des paramètres, est faite dans le tableau ci-après.

CONTRAINTES SEULES

contraintes $F_j(y_1 \ldots y_n) = 0$

$y_i = q^{\text{té}}$ mesurée $\rightarrow y_i^m$

A calculer $R = F(\tilde{Y}) - B\,\Delta\tilde{Y}$

$$B = \frac{\partial F}{\partial \tilde{Y}} = \frac{\partial F}{\partial \Delta\tilde{Y}} \qquad \Delta\tilde{Y} = Y - \tilde{Y}$$

$$B\Delta Y + R = 0$$

condition des moindres carrés

A calculer $M = (\Delta Y)^T \underset{Y}{G_m}(\Delta Y) + 2\,k^T(B\,\Delta Y + R)$

$$G_B = \left(B\ \underset{Y}{G_m^{-1}}\ B^T\right)^{-1}$$

$$\frac{\partial M}{\partial \Delta Y} = 0 \rightarrow \Delta Y = -\ \underset{Y}{G_m^{-1}}\ B^T k$$

$$k = G_B R$$

matrice d'erreurs sur les grandeurs mesurées

$$G_Y^{-1} = \underset{Y}{G_m^{-1}} - \underset{Y}{G_m^{-1}}\ B^T\ G_B^{-1}\ B\ \underset{Y}{G_m^{-1}}$$

7863/p/mh

CONTRAINTES + PARAMETRES A ESTIMER

contraintes $F_j(y_1 \ldots y_n ; x_1 \ldots x_m) = 0$

$y_i = q^{\text{té}}$ mesurée $\rightarrow y_i^m$

x_j = paramètres non mesurés à estimer

$R = F(\tilde{Y},\tilde{X}) - B\,\Delta\tilde{Y}$

$$B = \frac{\partial F}{\partial \Delta\tilde{Y}} = \frac{\partial F}{\partial \tilde{Y}} \qquad \Delta\tilde{Y} = Y - \tilde{Y} \qquad A = \frac{\partial F}{\partial \tilde{X}} = \frac{\partial F}{\partial \Delta\tilde{X}}$$

$$A\Delta X + B\Delta Y + R = 0$$

condition des moindres carrés

$$M = (\Delta Y)^T \underset{Y}{G_m}(\Delta Y) + 2\,k^T(A\,\Delta X + B\,\Delta Y + R)$$

$$G_B = \left(B\ \underset{Y}{G_m^{-1}}\ B^T\right)^{-1}$$

$$\frac{\partial M}{\partial \Delta Y} = 0 \rightarrow \Delta Y = -\ \underset{Y}{G_m^{-1}}\ B^T k$$

$$k = G_B(A\,\Delta X + R)$$

→ Détermination des paramètres

$$\frac{\partial M}{\partial \Delta X} = 0 \rightarrow \Delta X = -\ (A^T G_B A)^{-1}\ A^T G_B R$$

$$G_X^{-1} = (A^T G_B A)^{-1}$$

matrice d'erreurs sur les grandeurs mesurées

$$G_Y^{-1} = \underset{Y}{G_m^{-1}} - \underset{Y}{G_m^{-1}}\ B^T G_B\ B\ \underset{Y}{G_m^{-1}}$$

$$+\ \underset{Y}{G_m^{-1}}\ B^T G_B(A(A^T G_B A)^{-1} A^T)\ G_B\ B\ \underset{Y}{G_m^{-1}}$$

REFERENCES *)

1) G. Darmois, Calcul des Probabilités, Centre de Documentation Universitaire, Paris (1959).

2) H. Cramer, Mathematical Methods of Statistics, Princeton University Press, Princeton (1954).

3) R.A. Fisher, Statistical Methods for Research Workers, Oliver and Boyd, Edinburgh (1959).

4) J. Orear, Notes on Statistics for Physicists, UCRL-8417 (1958).

5) V.H. Regener, Phys. Rev. 84, 161 (1951).

6) M.S. Bartlett, Phil. Mag. 44, 249 (1953).

7) R. Böck, Applications of a Generalised Method of Least Squares for Kinematical Analysis in Bubble Chambers, CERN 60-30 (1960).

8) R. Böck, Kinematic Analysis of Bubble Chamber Events : FIT, an IBM 709 Programme Imposing Momentum and Energy Conservation on Measurements of Complete Events, CERN 61-29 (1961).

9) D. Hudson, Lectures on Elementary Statistics and Probability, CERN 63-29 (1963).

10) D. Hudson, Statistics Lectures II : Maximum Likelihood and Least Squares; to be published as a CERN report (1964).

*) Il y a beaucoup plus de références sur les sujets statistiques dans 10).

KINEMATICAL ANALYSIS OF BUBBLE CHAMBER PICTURES

B. Ronne,
Track Chamber Division, CERN

I. INTRODUCTION

There are many different systems used in the treatment of bubble chamber pictures. Every big laboratory has its own system. In all of them the scanning and measurement has to be followed by geometrical reconstruction and kinematical calculations. Big computers are always used in the last two steps.

We will not try to make any comparison between different systems but only describe in some detail how the analysis is performed at CERN, especially by the group working with a heavy liquid chamber as detector.

Many examples in later Chapters will be taken from one special experiment concerning the properties of negative cascade-hyperons, and we will therefore concentrate somewhat on describing this experiment.

II. TREATMENT OF BUBBLE CHAMBER PICTURES

The three corresponding rolls with different views of the same events are examined visually and all events fulfilling special criteria are written down. The criteria of Ξ^- are mainly:

1) that a Λ (or V^0) comes from a kink of a negative track,
2) that the transverse momentum of the decay particles are about the same and oppositely directed,
3) that the transverse momentum is not obviously much greater than what is possible. The maximum transverse momentum ($\sim$ 140 MeV/c) is equal to the momentum of the particles in the Ξ^- rest system.

An event fulfilling the above criteria and where further a K^+ or a K^0 is associated with the production point of the Ξ^-, is noted as a signed Ξ^-. Those events without the K signature are noted as unsigned. In Fig. 4 we see one event which fulfils the criteria of signed Ξ^-.

Photographs are taken of all interesting events and short descriptions of the events are given on scanning sheets.

Before an event can be measured it has to be carefully prepared. The preparation of events is needed because the treatment of measured data is performed by a computer, and this must know for instance which tracks stop and which belong to a special interaction.

In our case the preparation includes labelling of vertices, tracks, stopping points, decay points and intermediate points of tracks. As this experiment is performed in heavy liquid, we often have a particle which is scattered a few degrees at one point. If one assumes that the particle loses only a small amount of energy in this single scattering, it may be worth while to measure the track after the interaction point also, to receive a more accurate value for the momentum of the particle. This is especially true if the particles stops in the chamber. Multiple scattering may further have as a result, a track which looks partly straight and partly curved. The geometry programme, which is described below, can only accept a track which has the same curvature along its entire length. Other tracks have to be divided in several pieces, with the help of intermediate points and each piece is treated separately by the geometry programme.

The measurements are made on a digitized projector, which gives the output coordinates (precision a few microns on the film) on a tape. This can be treated by the following chain of programmes which are described below.

REAP → THRESH → JOIN → GRIND

III. GEOMETRICAL RECONSTRUCTION

The data from the measuring machines are first sent through a programme named REAP. Some types of measuring errors and errors in labelling of tracks and vertices are now detected. REAP further prepares the data to be in a suitable order for the following programmes.

The geometrical reconstruction of tracks is made in THRESH. A detailed description of THRESH is given by Cnops (THRESH Manual) and Moorhead (CERN 60-33). The input tape from REAP contains measured coordinates of fiducial marks and of points along the tracks and also information which makes it possible to identify the event and recognize different types of tracks and vertices. This is needed later in GRIND.

Before the reconstruction of a track can start, one has to provide THRESH with some general information needed for all events in an experiment, e.g. coordinates of cameras and fiducial marks, refractive index of the media between the cameras and the back glass of the chamber, path length in each media, tolerances for the measured coordinates of fiducial marks, tolerances on the error of a reconstructed point etc.

A reference system is fixed. The z direction is chosen to be parallel to the uniform magnetic field. The cameras are positioned around the z axis. The plane $z = 0$ is defined to be in the back of the front glass. The apparent position (x_o, y_o) in the $z = 0$ plane of the fiducial marks, as seen from the cameras, can be calculated from the general information above. The coordinates (x_m, y_m) measured on the film can further be transformed through intermediate media to the plane $z = 0$. This transformation is described by the following equations:

$$\begin{cases} x_o = \alpha_1 + \alpha_2 x_m + \alpha_3 y_m \\ y_o = \alpha_4 + \alpha_5 x_m + \alpha_6 y_m \end{cases} \qquad (1)$$

The six constants α_i can be evaluated by the method of least squares (Chapter IV.2), if at least four fiducial marks have been measured. A set of α values is calculated for each view.

The number of measured fiducial marks needed can be reduced if one includes some additional conditions, i.e. that the coordinate systems are orthogonal and that the magnification in the x and y directions is the same.

The coordinates of all measured bubbles can now be transformed to the reference plane z = 0.

A light ray, which passes from a point inside the chamber to a point on the film, may in the chamber be described by the following two equations:

$$\begin{cases} x = F_x z + G_x \\ y = F_y z + G_y \end{cases} \qquad (2)$$

where F_x, F_y, G_x and G_y can be calculated (Moorhead, CERN 60-33). The line Eq. (2) is called a reconstruction line and can be derived for each measured point.

The position inside the chamber of a bubble, measured in at least two views, is identical with the intersection point of the corresponding reconstruction lines, where the intersection point is defined to be that point which is closest to the two lines. It is then easy to find the true coordinates of such bubbles.

A track is, however, measured at about 5-10 arbitrarily chosen points, and the measured points are normally not the same for different views. At the first reconstruction of a track, one uses the following method.

The two best views, according to the following criteria, are picked out. The first view is chosen to be the one on which the track is most nearly seen as an orthogonal projection. We then calculate the angle between the tangent to the track at the initial point and the line joining the camera corresponding to the first view with each one of the other cameras. The second view is chosen to be the one for which the corresponding camera gives the greatest angle. All points in space corresponding to the measurements in the first view are reconstructed. Before one can find the points in space, one must, however, have the reconstruction lines from exactly the same points in the second view. These lines are not available, but it is possible to interpolate between reconstruction lines of near positioned points until one finds

a missing line. This will intersect the corresponding line from the first view in the true space position of the bubble.

After all points in one view have been reconstructed, one determines a first approximation to a helix, which can describe the motion of the particle inside the chamber. The helix is described by the following equations:

$$\begin{cases} x' = \rho(\cos\Theta - 1) \\ y' = \rho \sin\Theta \\ z' = \rho\,\Theta\,\mathrm{tg}\,\alpha \end{cases} \qquad (3)$$

The origin is at the starting point of the track, the z direction, as before, along the magnetic field and the y direction along the tangent of the projection of the track in the z = 0 plane. ρ is the projected curvature in the same plane. α is the dip angle of the track and Θ is the angle between the x and x′ directions.

The parameters of the helix derived above are used as starting values in a final least squares fit, where the reconstruction lines for all measurements in all views are included. The last fit is an iterative process, and the parameters converge normally (in about 97% of the tracks) to the best fit solution.

For each track THRESH gives curvature, dip angle and azimuth angle.. It is preferable to use curvature instead of momentum because the first variable is more normally distributed than the second one, and the method of least squares is based on the assumption that the variables are normally distributed.

The angles of a track are given for one or both endpoints, while the momentum is given for a meanpoint. At a later stage, when one has assumed a mass for the particle, one can make an energy-loss correction and thus find the momentum at other points of the track.

THRESH also gives errors in the derived quantities. The uncertainty of track variables is mainly due to uncertainties of the measuring device and contributions from Coulomb scattering.

The uncertainty of coordinates from the measuring machine is assumed to be known. This constant error is propagated through all the space reconstruction and in the best fit solution it gives the corresponding uncertainties of the derived quantities.

The uncertainties due to Coulomb scattering depend on the mass of the particle. THRESH is mass independent and the multiple scattering errors are therefore included at a later stage.

All parts of a track which has been measured in several pieces are treated as separate tracks in THRESH. One has to combine the information from these pieces to one track. This is done in JOIN.

IV. KINEMATICAL CALCULATIONS

1) Constraint equations

A signed Ξ^- may look as in Fig. 4.

The possible hypotheses for the interpretation of an event have to be tested by kinematic calculations, which are made in GRIND. A V^o may, for example, be due to the decay of a K^o, Λ or $\bar{\Lambda}$, or it may be a two-prong star from the interaction of a neutral particle. Often there is more than one possible origin for the neutral particle and all hypotheses have then to be tested for each origin. The V^o's in Fig. 4 may, for example, have either A or R as origin. A V^- may be due to the decay of a Ξ^-, Σ^-, K^-, π^- or μ^-, or it may be a scattering of a negative particle.

The basis of testing different hypotheses is that the four momentum and energy equations have to be fulfilled at the decay of a particle. If we have less than four unknown quantities in these equations the system is overdetermined, and the possibility to satisfy all equations give a test of how good the hypothesis is. The test is in general performed by the method of least squares, which is described below. All measured quantities are fitted to give the best solution and the probability that the hypothesis is correct is also given.

For the Λ decay we can write the four energy and momentum equations in the following way:

$$\begin{cases} f_1 = P_\Lambda \cos\lambda_\Lambda \cos\varphi_\Lambda - P_p \cos\lambda_p \cos\varphi_p - P_\pi \cos\lambda_\pi \cos\varphi_\pi = 0 \\ f_2 = P_\Lambda \cos\lambda_\Lambda \sin\varphi_\Lambda - P_p \cos\lambda_p \sin\varphi_p - P_\pi \cos\lambda_\pi \sin\varphi_\pi = 0 \\ f_3 = P_\Lambda \sin\lambda_\Lambda - P_p \sin\lambda_p - P_\pi \sin\lambda_\pi = 0 \\ f_4 = \sqrt{P_\Lambda^2 + M_\Lambda^2} - \sqrt{P_p^2 + M_p^2} - \sqrt{P_\pi^2 + M_\pi^2} = 0 \end{cases} \qquad (4)$$

where P_i, λ_i, and φ_i are the momentum, dip angle and azimuth angle of particle i.

If we assume that all three parameters of the proton and the pion are known and further that the lambda comes from a given vertex, we have only one unknown quantity, P_Λ. In this case the event is subject to three constraints, and we talk about a 3 C-fit.

We may treat the mass of the decaying particle as unknown and have then a 2 C-fit.

Assuming the production point of the V^0 to be unknown, there are three missing variables (P_Λ, λ_Λ and φ_Λ) in the equations above, and we have still a 1 C-fit to find out if the Λ hypothesis for the V^0 is correct.

For the Ξ^- decay we have equations corresponding to Eq. (4) if we take the fitted lambda as measured. In the best case we have no unknown quantities and thus a 4 C-fit. Mostly, however, the Ξ^- track is straight and therefore the momentum of the Ξ^- is missing. We have then a 3 C-fit with the Ξ^- mass known and a 2 C-fit if the mass is calculated.

In the examples above we have only tracks from one vertex, which are subject to a fit. These types of fits are called 1-vertex fits. Once all hypotheses have been tested by 1-vertex fits, one may go a step further and, for example, combine the four equations from the lambda decay and the four from the Ξ^- decay to a 2-vertices fit with eight equations, which in the best case gives a 7 C-fit (P_Λ unknown).

2) The method of least squares

A description of different ways of using the method of least squares in kinematical analysis of bubble chamber events is given by R. Böck (CERN 60-30 and 61-29) and Berge et al. (UCRL-9097).

We denote the measured variables by m_i, i=1,2 ... I, and the unknowns by x_j, j=1,2 ... J. The superscript 0 refers to unfitted quantities. The constraint equations are written $f_k(x,m)$, k=1,2 ... K. The error matrix of the measured variables is called G_m^{-1}, where the element $(G_m^{-1})_{ii}$ is the variance of the element m_i and $(G_m^{-1})_{ij}$ the covariance of elements m_i and m_j. The inverse, G_m, of an error matrix is called a weighting matrix.

The method of least squares is based on the assumption of normally distributed variables and states that the best set of variables is that for which the function

$$\chi^2 = \sum_{j=1}^{J} \sum_{i=1}^{I} (m_i - m_i^0)\ (G_m)_{ij}\ (m_j - m_j^0) \qquad (5)$$

has a minimum, and where the variables fulfil the equations:

$$f_k(x,m) = 0 \quad k = 1,2 \ldots K\ . \qquad (6)$$

Assuming uncorrelated variables $[(G_m^{-1})_{ij} = 0$ for $i \neq j]$ we find that Eq. (5) is reduced to the well-known expression

$$\chi^2 = \sum_{i} \frac{(m_i - m_i^0)^2}{(G_m^{-1})_{ii}} \qquad (5')$$

i.e. one has to minimize the sum of the weighted squares of the deviations between fitted and measured quantities.

The least squares solution may be found in one of the following two ways.

2.1) The elimination method

The J unknowns x_j are eliminated from the constraint equations, and we get a new set of K- J equations

$$f_k(m) = 0 \qquad k = 1,2 \ldots K-J \qquad (7)$$

There are two possibilities to go on.

One may use the equation (7) to eliminate K- J of the measured variables from the function $\chi^2(m)$. The equations

$$\frac{d\chi^2(m)}{dm_i} = 0 \qquad i = 1,2 \ldots I-K+J \tag{8}$$

may then be solved to give the solution for the remaining I- K+ J variables and so on.

The other and better method is to introduce the Lagrangian multipliers α_k, k = 1,2 ... K-J. The problem is then reduced to finding the minimum value of

$$\chi^2(m,\alpha) = \sum_{j=1}^{I}\sum_{i=1}^{I} (m_i - m_i^0)\,(G_m)_{ij}\,(m_j - m_j^0) + 2\sum_{k=1}^{K-J}\alpha_k f_k(m). \tag{9}$$

In the first step we assume that the measured variables are uncorrelated. The minimum of χ^2 is then found by solving the following system of equations:

$$\begin{cases} \dfrac{d\chi^2}{dm_i} = 2\left\{(m_i - m_i^0)\,(G_m)_{ii} + \displaystyle\sum_{k=1}^{K-J}\alpha_k f_{ki}(m)\right\} = 0 & i=1,2 \ldots I \quad (10) \\[2ex] \dfrac{d\chi^2}{d\alpha_k} = 2\,f_k(m) = 0 & k=1,2 \ldots K-J \quad (11) \end{cases}$$

where

$$f_{ki}(m) = \frac{df_k(m)}{dm_i}\,.$$

Equations (11) are just the constraint conditions.

As these are in general not linear, one has to repeat the calculations below to get a still better solution until some given criteria are satisfied. A superscript ν means that this value has been derived in the ν-th iteration.

Assume that we have passed the ν-th iterative step and have to go on at least one step more. From Eq. (10) we have:

$$m_i^{\nu+1} = m_i^0 - \sum_{k=1}^{K-J} (G_m)_{ii}^{-1} f_{ki}^{\nu}(m)\ \alpha_k^{\nu+1} \qquad i=1,2 \ldots I. \tag{12}$$

The constraint equations can be expanded in the following way:

$$f_k^{\nu}(m) + \sum_{i=1}^{I} f_{ki}^{\nu}(m)\ (m_i^{\nu+1} - m_i^{\nu}) = 0 \qquad k=1,2 \ldots K-J. \tag{13}$$

We can now eliminate $m_i^{\nu+1}$ from equations (12) and (13) and get:

$$R_j^{\nu} - \sum_{k=1}^{K-J} S_{jk}^{\nu}\ \alpha_k^{\nu+1} = 0 \qquad j=1,2 \ldots K-J \tag{14}$$

where

$$R_j^{\nu} = f_j^{\nu}(m) + \sum_{i=1}^{I} f_{ji}^{\nu}(m)\ (m_i^0 - m_i^{\nu}) \tag{15}$$

$$S_{jk}^{\nu} = \sum_{i=1}^{I} f_{ki}^{\nu}(m)\ (G_m)_{ii}^{-1}\ f_{ji}^{\nu}(m)\ . \tag{16}$$

Eq. (14) is a system of K- J linear equations from which the unknown variables, $\alpha_k^{\nu+1}$, k=1,2 ... K- J, can be solved.

The new set of $m_i^{\nu+1}$ values is then obtained from relation Eq. (12), and the iteration process can go on until some stopping criteria are fulfilled. The iteration process is started with the values $m_i = m_i^0$ and $\alpha_k = 0$.

The calculations are more simplified when matrix notations are used. We re-write the equations above in this way and extend them to be valid also for correlated measurements (G_m^{-1} is no longer a diagonal matrix).

$$\chi^2 = (m - m^o)^T G_m (m - m^o) + 2\alpha^T f \tag{9'}$$

where T means a transposed matrix

$$\frac{d\chi^2}{dm} = 2\left\{(m - m^o)^T G_m + \alpha^T f_m\right\} = 0 \tag{10'}$$

where $f_m = df(m)/dm$ is a $(K - J) \times I$ matrix

$$m^{\nu+1} = m^o - G_m^{-1} f_m^{\nu T} \alpha^{\nu+1} \tag{12'}$$

$$f^\nu + f_m^\nu (m^{\nu+1} - m^\nu) = 0 \tag{13'}$$

$$R - S\,\alpha^{\nu+1} = 0 \tag{14'}$$

with

$$R = f^\nu + f_m^\nu (m^o - m^\nu) \tag{15'}$$

$$S = f_m^\nu\, G_m^{-1}\, f_m^{\nu T} \tag{16'}$$

and we get

$$\alpha^{\nu+1} = S^{-1} R \,. \tag{17}$$

If Eq. (12') is introduced into Eq. (9') we find

$$\chi^2 = (\alpha^{\nu+1})^T R \tag{18}$$

2.2) A generalized method

The elimination method has the disadvantage that the constraint equations have to be modified in many ways, depending on which variables are missing. One can, however, make the fit in a more general way, so that the same system of constraint equations can be used in all cases.

We have to minimize the expression:

$$\chi^2(m,x,\alpha) = (m-m^0)^T G_m (m-m^0) + 2\alpha^T f(x,m) \tag{19}$$

which means that the following system of equations has to be solved:

$$\begin{cases} \dfrac{d\chi^2}{dm} = 2\left\{(m-m^0)^T G_m + \alpha^T f_m\right\} = 0 & (20) \\ \dfrac{d\chi^2}{dx} = 2\alpha^T f_x = 0 & (21) \\ \dfrac{d\chi^2}{d\alpha} = 2f(x,m) = 0 & (22) \end{cases}$$

where $f_x = df(x,m)/dx$.

The constraint equations can now be expanded in the following way

$$f^\nu + f_x^\nu (x^{\nu+1} - x^\nu) + f_m^\nu (m^{\nu+1} - m^\nu) = 0 \ . \tag{23}$$

Exactly in the same way as above Eqs. (12′ - 17) we obtain:

$$\alpha^{\nu+1} = S^{-1} \left[R + f_x^\nu (x^{\nu+1} - x^\nu)\right] \tag{24}$$

with R and S defined by Eq. (15′) and 16′).

We introduce this vector into Eq. (21) and find:

$$x^{\nu+1} = x^\nu - (f_x^{\nu\,T} S^{-1} f_x^\nu)^{-1} f_x^{\nu\,T} S^{-1} R \ . \tag{25}$$

The problem is then solved. From the new set of $x^{\nu+1}$ values we calculate $\alpha^{\nu+1}$, Eq. (24), and finally $m^{\nu+1}$, Eq. (12′).

As above, Eq. (18), we have

$$\chi^2 = (\alpha^{\nu+1})^T \left[R + f_x (x^{\nu+1} - x^\nu)\right] . \tag{26}$$

The iteration process has to go on until some test indicates that a received set of approximations is good enough. One may, for example, require that the difference in χ^2 between two consecutive iterations is smaller than a given value, or still better that the constraint equations and the derivates Eq. (20) and (21) are zero within some given limits.

2.3) Calculation of errors

From Eqs. (12'), (15'), (24) and (25) above, we see that $m^{\nu+1}$ and $x^{\nu+1}$ can be expressed as explicit functions of m^o. Let us linearize these equations and write:

$$m^{\nu+1} = g(m^o) \tag{27}$$

$$x^{\nu+1} = h(m^o) \ . \tag{28}$$

The error matrices are then obtained from the formulae:

$$G_{m^{\nu+1}}^{-1} = \frac{dg}{dm^o} \, G_m^{-1} \left(\frac{dg}{dm^o}\right)^T \tag{29}$$

$$G_{x^{\nu+1}}^{-1} = \frac{dh}{dm^o} \, G_m^{-1} \left(\frac{dh}{dm^o}\right)^T \tag{30}$$

and the correlation between measured and unmeasured variables from:

$$C_{(mx)^{\nu+1}} = \frac{dg}{dm^o} \, G_m^{-1} \left(\frac{dh}{dm^o}\right)^T \ . \tag{31}$$

The two derivatives needed above, dg/dm^o and dh/dm^o, are obtained in the following way:

$$\begin{aligned}
\frac{dg}{dm^o} &= 1 - G_m^{-1} \, f_m^T \, \frac{d\alpha}{dm^o} \\
&= 1 - G_m^{-1} \, f_m^T \, S^{-1} \left\{ \frac{dR}{dm^o} + f_x \, \frac{d(x^{\nu+1} - x^{\nu})}{dm^o} \right\} \\
&= 1 - G_m^{-1} \, f_m^T \, S^{-1} \left\{ \frac{dR}{dm^o} - f_x (f_x^T \, S^{-1} f_x)^{-1} \, f_x^T \, S^{-1} \, \frac{dR}{dm^o} \right\} \\
&= 1 - G_m^{-1} \, f_m^T \, S^{-1} \left\{ f_m - f_x (f_x^T \, S^{-1} \, f_x)^{-1} \, f_x^T \, S^{-1} \, f_m \right\}
\end{aligned} \tag{32}$$

$$\frac{dh}{dm^o} = (f_x^T \, S^{-1} \, f_x)^{-1} \, f_x^T \, S^{-1} \, f_m \tag{33}$$

After having introduced these expression into Eq. (29 - 31) and simplified the results we obtain:

$$G_m^{-1}{}_{\nu+1} = G_m^{-1} - G_m^{-1} f_m^T S^{-1} f_m G_m^{-1} + G_m^{-1} f_m^T S^{-1} f_x (f_x^T S^{-1} f_x)^{-1} f_x^T S^{-1} f_m G_m^{-1} \quad (34)$$

$$G_x^{-1}{}_{\nu+1} = (f_x^T S^{-1} f_x)^{-1} \quad (35)$$

$$C_{(mx)^{\nu+1}} = -G_m^{-1} f_m^T S^{-1} f_x (f_x^T S^{-1} f_x)^{-1} . \quad (36)$$

One can see from Eq. (34) that the errors of the measured quantities are reduced in the least squares solution and that there are correlations between fitted variables even when the measured quantities are uncorrelated. Some examples are given in Chapter IV.4 and .5.

3) The χ^2 test of a hypothesis

After an event has passed through the kinematical fitting programme, one has to decide if the tested hypothesis is correct or not. All measured variables are forced to fulfil the constraint equations. The magnitude of χ^2 is dependent on how big the differences between the fitted and the measured values are. One can convert the χ^2 value and the number of degrees of freedom ($n = K - J$ in our notations above) into a probability by using the theoretical χ^2 distribution. The latter is given by the formula:

$$f_n(\chi^2)\, d\chi^2 = \frac{(\chi^2)^{n/2-1}}{2^{n/2}\Gamma(n/2)} e^{-\chi^2/2}\, d\chi^2 \quad (37)$$

where Γ is the Gamma function.

A derivation of the χ^2 distribution is given by D. Hudson (Lectures on elementary statistics and probability, CERN 63-29).

Examples of χ^2 distributions for three different numbers of degrees of freedom are shown in Fig. 1.

The mean of a χ^2 distribution is at $\chi^2 = n$, and we have further

$$\int_0^\infty f_n(\chi^2)\, d\chi^2 = 1 \,. \tag{38}$$

The probability that the χ^2 is greater than or equal to a given value χ_0^2 is

$$P_n(\chi^2 \geq \chi_0^2) = \int_{\chi_0^2}^\infty f_n(\chi^2)\, d\chi^2 \,. \tag{39}$$

These probabilities can be found in most statistical tables. One example is given in Chapter V.3, (Table 3).

Assume that the least square method above, gives as result the value χ_0^2 when testing a hypothesis. We can conclude that the hypothesis gives a possible interpretation of the event if the derived probability (P_n) is greater than 5%. If the probability is between 5% and 1%, we find the hypothesis to be doubtful, and if P_n is less than 1% we conclude that this hypothesis is very improbable.

The two percentage limits above (5% and 1%) may be compared with the corresponding limits (2.0 and 2.6 standard deviations) for a normally distributed variable.

Before we can use the probability test we have to check that the χ^2 distribution obtained from the fit procedure agrees with the theoretically expected one. If the experimental χ^2 distribution has a mean value, which is too low (high) we may suspect that the errors of the input parameters are systematically too big (small).

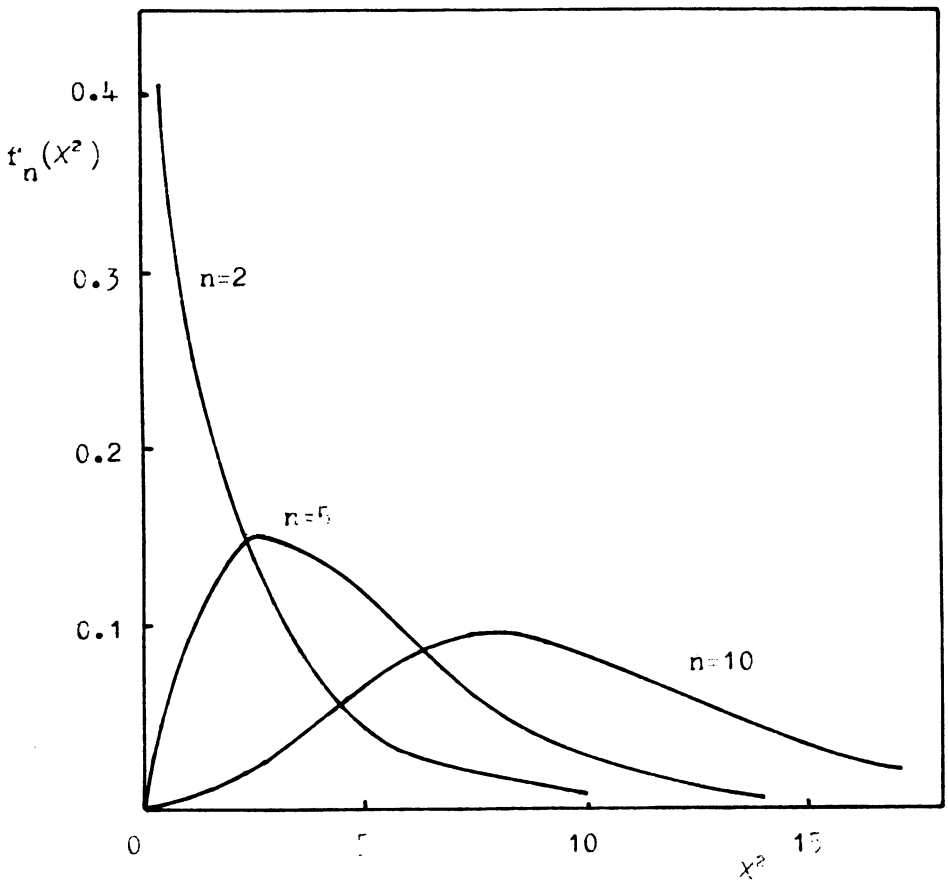


Fig. 1

χ^2 distributions for three different degrees of freedom

It is also possible to calibrate the errors assigned to each variable m_i. We know that

$$S(m_i) = \frac{m_i - m_i^o}{\sigma(m_i - m_i^o)} \qquad (40)$$

should be normally distributed with unit standard deviation and mean value zero. We can then correct the errors until $S(m_i)$ has the correct width. If the $S(m_i)$ distribution is very asymmetric, we conclude that the variable m_i is not normally distributed or that we have a systematic error in the measurement of m_i.

In Fig. 2 we give the experimental and theoretical χ^2 distribution for the 1-vertex Ξ^--fit with M_{Ξ^-} unknown, (see Chapter IV.1). The agreement between the two distributions seems to be good. A method to test the agreement by using probability paper is described in Appendix II.

4) Numerical example; fit of a Λ decay

We illustrate the practical use of the generalized method of least squares by testing the hypothesis that the event below (Fig. 3) is a decaying lambda

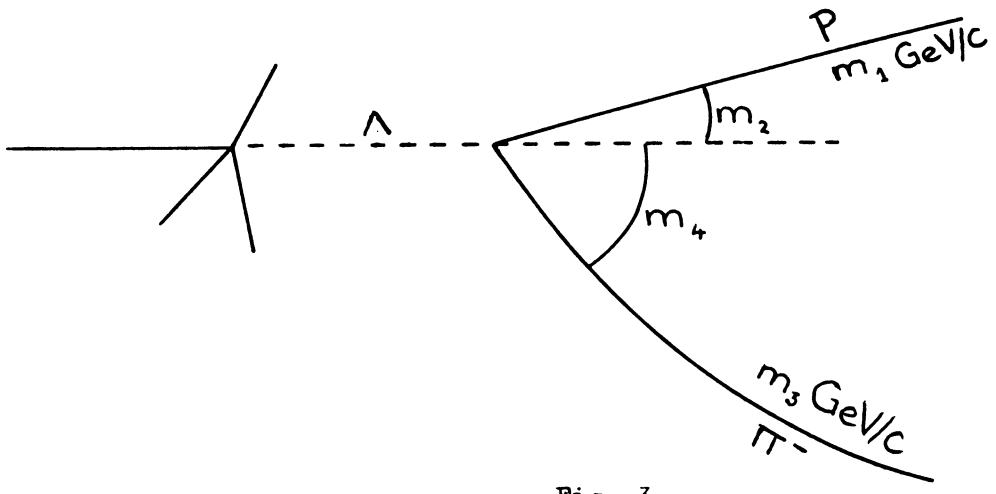


Fig. 3.

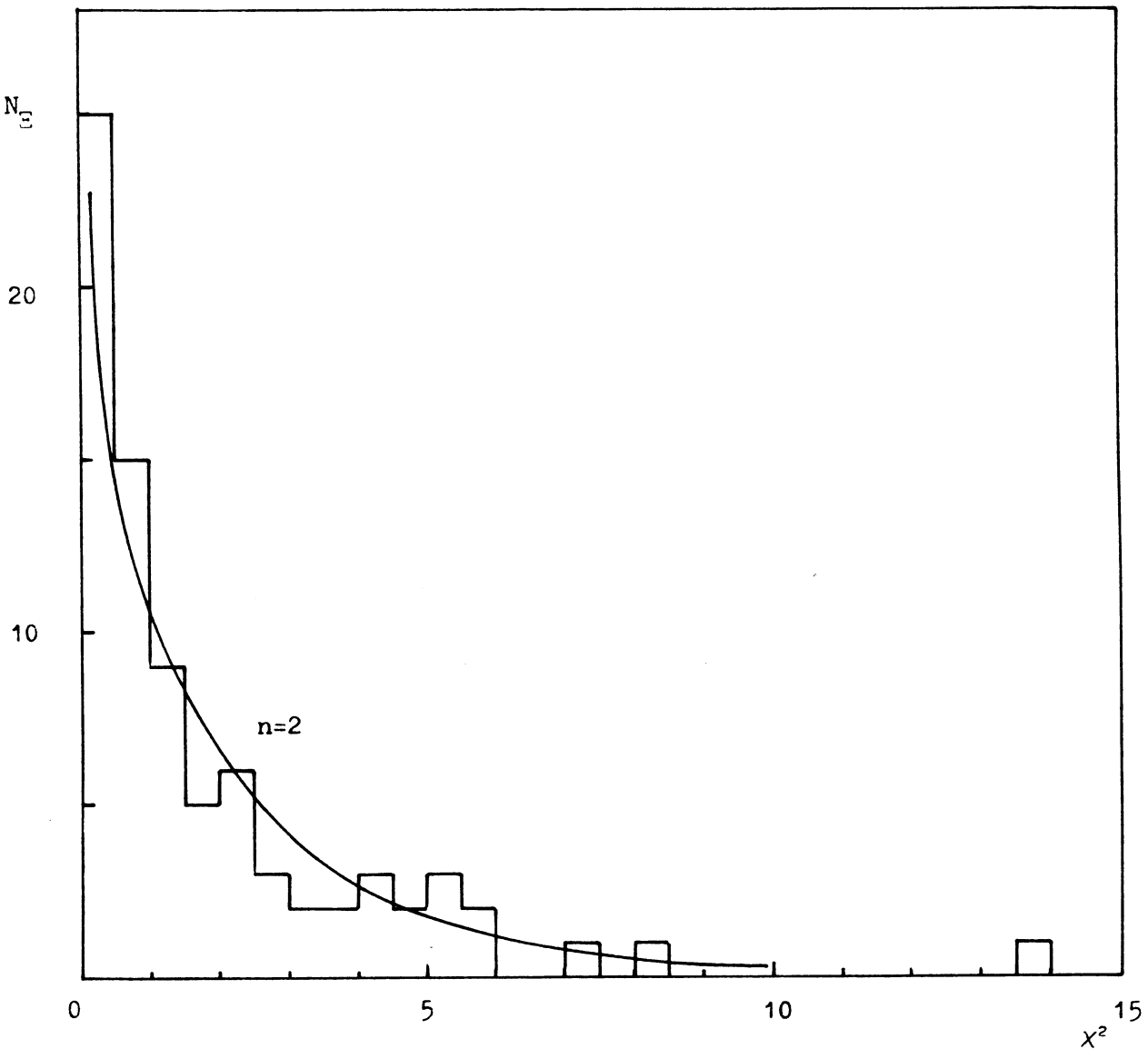


Fig. 2

Experimental and theoretical X^2 distribution for a 2 C-fit.

To make the calculations somewhat easier, we assume that the three tracks (Λ,P and π^-) are coplanar and further that the measured quantities are uncorrelated. The notation of the measured quantities (m_i) with errors (σ_i) is explained in the figure.

The numerical values are

$$\begin{aligned} m_1^0 &= 900 \pm 100 \text{ MeV/c} \\ m_2^0 &= 5^\circ.7 \pm 1^\circ.0 \\ m_3^0 &= 100 \pm 20 \text{ MeV/c} \\ m_4^0 &= 57^\circ.3 \pm 1^\circ.0 \ . \end{aligned}$$

The constraint equations can be written

$$\begin{aligned} f_1 &\equiv x - m_1 \cos m_2 - m_3 \cos m_4 = 0 \\ f_2 &\equiv m_1 - \sin m_2 - m_3 \sin m_4 = 0 \\ f_3 &\equiv \sqrt{x^2 + M_\Lambda^2} - \sqrt{m_1^2 + M_p^2} - \sqrt{m_3^2 + M_\pi^2} = 0 \end{aligned} \qquad (41)$$

where the only unknown quantity (x) is the momentum of the lambda.

We have three equations and one unknown, and thus a 2 C-fit.

The error matrix is

$$G_m^{-1} = \begin{bmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & 0 \\ 0 & 0 & \sigma_3^2 & 0 \\ 0 & 0 & 0 & \sigma_4^2 \end{bmatrix}$$

and the weighting matrix

$$G_m = \begin{bmatrix} \frac{1}{\sigma_1^2} & 0 & 0 & 0 \\ 0 & \frac{1}{\sigma_2^2} & 0 & 0 \\ 0 & 0 & \frac{1}{\sigma_3^2} & 0 \\ 0 & 0 & 0 & \frac{1}{\sigma_4^2} \end{bmatrix}$$

We have to minimize the expression

$$\chi^2(m,x,\alpha) = (m - m^0)^T G_m (m - m^0) + 2\alpha^T f(x,m) \qquad (19)$$

which can be written

$$\chi^2 = (m_1 - m_1^0 ; m_2 - m_2^0 ; m_3 - m_3^0 ; m_4 - m_4^0) \begin{bmatrix} \frac{1}{\sigma_1^2} & 0 & 0 & 0 \\ 0 & \frac{1}{\sigma_2^2} & 0 & 0 \\ 0 & 0 & \frac{1}{\sigma_3^2} & 0 \\ 0 & 0 & 0 & \frac{1}{\sigma_4^2} \end{bmatrix} \begin{bmatrix} m_1 - m_1^0 \\ m_2 - m_2^0 \\ m_3 - m_3^0 \\ m_4 - m_4^0 \end{bmatrix} +$$

$$+ 2(\alpha_1 ; \alpha_2 ; \alpha_3) \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} =$$

$$= \sum_{i=1}^{4} \frac{(m_i - m_i^0)^2}{\sigma_i^2} + 2 \sum_{j=1}^{3} \alpha_j f_j \, .$$

This is reduced to the first well-known term when the constraint equations are fulfilled.

The following system of equations has to be solved.

$$\begin{cases} \dfrac{d\chi^2}{dm_i} = 2 \left\{ \dfrac{m_i - m_i^0}{\sigma_i^2} + \displaystyle\sum_{j=1}^{3} \alpha_j \frac{df_j}{dm_i} \right\} = 0 \qquad i = 1,2,3,4 & (42) \\ \dfrac{d\chi^2}{dx} = 2 \displaystyle\sum_{j=1}^{3} \alpha_j \frac{df_j}{dx} = 0 & (43) \\ \dfrac{d\chi^2}{d\alpha_j} = 2 f_j = 0 \qquad j = 1,2,3 & (44) \end{cases}$$

We have thus eight equations and eight unknowns (α_1 α_2 α_3 m_1 m_2 m_3 m_4 and x).

The constraint equations can be expanded in the following way after we have passed the ν-th iterative step

$$f_j^\nu + \sum_{i=1}^{4} f_{ji}^\nu (m_i^{\nu+1} - m_i^\nu) + f_{x_j}^\nu (x^{\nu+1} - x^\nu) = 0 \qquad j = 1,2,3. \tag{45}$$

We have

$$\left\{ f_{ji}^\nu \right\} = \left\{ \frac{\partial f_j^\nu}{\partial m_i^\nu} \right\} \equiv \begin{bmatrix} -\cos m_2^\nu & + m_1^\nu \sin m_2^\nu & -\cos m_4^\nu & + m_3^\nu \sin m_4^\nu \\ +\sin m_2^\nu & + m_1^\nu \cos m_2^\nu & -\sin m_4^\nu & - m_3^\nu \cos m_4^\nu \\ -\dfrac{m_1^\nu}{\sqrt{m_1^{\nu 2} + M_p^2}} & 0 & -\dfrac{m_3^\nu}{\sqrt{m_3^{\nu 2} + M_\pi^2}} & 0 \end{bmatrix} \tag{46}$$

and

$$\left\{ f_{x_j}^\nu \right\} = \left\{ \frac{\partial f_j^\nu}{\partial x^\nu} \right\} \equiv \begin{bmatrix} 1 \\ 0 \\ \dfrac{x^\nu}{\sqrt{x^{\nu 2} + M_\Lambda^2}} \end{bmatrix} \tag{47}$$

We can re-write the constraint equations in a more suitable form.

$$\sum_{i=1}^{4} f_{ji}^\nu (m_i^{\nu+1} - m_i^0) + R_j + f_{x_j}^\nu (x^{\nu+1} - x^\nu) = 0 \qquad j = 1,2,3 \tag{48}$$

where

$$R_j = f_j^\nu - \sum_{i=1}^{4} f_{ji}^\nu (m_i^\nu - m_i^0) \tag{49}$$

Equation (42) can be written

$$m_i^{\nu+1} - m_i^0 = -\sigma_i^2 \sum_{j=1}^{3} \alpha_j^{\nu+1} f_{ji}^\nu \qquad i = 1,2,3,4 \ . \tag{42'}$$

We can now eliminate $m_i^{\nu+1}$ between Eqs (42') and (48).

$$\sum_{i=1}^{4} \sigma_i^2 f_{ji}^{\nu} \sum_{k=1}^{3} \alpha_k^{\nu+1} f_{ki}^{\nu} = R_j + f_{x_j}^{\nu} (x^{\nu+1} - x^{\nu}) \qquad j = 1,2,3. \tag{50}$$

After re-arranging the terms we have

$$\sum_{k=1}^{3} \alpha_k^{\nu+1} \sum_{i=1}^{4} f_{ji}^{\nu} f_{ki}^{\nu} \sigma_i^2 = R_j + f_{x_j}^{\nu} (x^{\nu+1} - x^{\nu}) \qquad j = 1,2,3 \tag{51}$$

or

$$\begin{cases} \alpha_1^{\nu+1} \sum_{i=1}^{4} f_{1i}^{\nu 2} \sigma_i^2 + \alpha_2^{\nu+1} \sum_{i=1}^{4} f_{1i}^{\nu} f_{2i}^{\nu} \sigma_i^2 + \alpha_3^{\nu+1} \sum_{i=1}^{4} f_{1i}^{\nu} f_{3i}^{\nu} \sigma_i^2 = R_1 + f_{x_1} (x^{\nu+1} - x^{\nu}) \\ \alpha_1^{\nu+1} \sum_{i=1}^{4} f_{2i}^{\nu} f_{1i}^{\nu} \sigma_i^2 + \alpha_2^{\nu+1} \sum_{i=1}^{4} f_{2i}^{\nu 2} \sigma_i^2 + \alpha_3^{\nu+1} \sum_{i=1}^{4} f_{2i}^{\nu} f_{3i}^{\nu} \sigma_i^2 = R_2 + f_{x_2}^{\nu} (x^{\nu+1} - x^{\nu}) \\ \alpha_1^{\nu+1} \sum_{i=1}^{4} f_{3i}^{\nu} f_{1i}^{\nu} \sigma_i^2 + \alpha_2^{\nu+1} \sum_{i=1}^{4} f_{3i}^{\nu} f_{2i}^{\nu} \sigma_i^2 + \alpha_3^{\nu+1} \sum_{i=1}^{4} f_{3i}^{\nu 2} \sigma_i^2 = R_3 + f_{x_3}^{\nu} (x^{\nu+1} - x^{\nu}) \end{cases} \tag{51'}$$

The three unknowns $(\alpha_i^{\nu+1})$ can be solved from this linear system of equations.

Eq. (51) is of course identical with the equations derived in Chapter IV.2.2.

$$\alpha^{\nu+1} = S^{-1} [R + f_x^{\nu} (x^{\nu+1} - x^{\nu})]. \tag{24}$$

We have namely

$$S = f_m^{\nu} \, G_m^{-1} \, f_m^{\nu\,T} =$$

$$= \begin{bmatrix} f_{11}^{\nu} & f_{12}^{\nu} & f_{13}^{\nu} & f_{14}^{\nu} \\ f_{21}^{\nu} & f_{22}^{\nu} & f_{23}^{\nu} & f_{24}^{\nu} \\ f_{31}^{\nu} & f_{32}^{\nu} & f_{33}^{\nu} & f_{34}^{\nu} \end{bmatrix} \begin{bmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & 0 \\ 0 & 0 & \sigma_3^2 & 0 \\ 0 & 0 & 0 & \sigma_4^3 \end{bmatrix} \begin{bmatrix} f_{11}^{\nu} & f_{21}^{\nu} & f_{31}^{\nu} \\ f_{12}^{\nu} & f_{22}^{\nu} & f_{32}^{\nu} \\ f_{13}^{\nu} & f_{23}^{\nu} & f_{33}^{\nu} \\ f_{14}^{\nu} & f_{24}^{\nu} & f_{34}^{\nu} \end{bmatrix} =$$

$$= \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix} \tag{52}$$

where

$$s_{jk} = \sum_{i=1}^{4} f_{ji}^{\nu} \, f_{ki}^{\nu} \, \sigma_i^2 \ . \tag{53}$$

The S matrix has to be inverted before we can solve $\alpha_i^{\nu+1}$. We have

$$S^{-1} = \frac{1}{|S|} \begin{bmatrix} S_{11} & S_{21} & S_{31} \\ S_{12} & S_{22} & S_{32} \\ S_{13} & S_{23} & S_{33} \end{bmatrix} \tag{54}$$

where $|S|$ is the determinant of the matrix S and S_{jk} is the co-factor of the element s_{jk}. (The co-factor S_{jk} is equal to $(-1)^{j+k}$ times that minor which is obtained when the j-th row and the k-th column are deleted.)

The solution of Eq. (51) is

$$\alpha_j^{\nu+1} = \frac{1}{|S|} \sum_{k=1}^{3} S_{kj} \left[R_k + f_{x_k}^{\nu} \left(x^{\nu+1} - x^{\nu} \right) \right] \qquad j = 1,2,3 \ . \tag{55}$$

$\alpha_j^{\nu+1}$ is eliminated from Eq. (43)

$$\sum_{j=1}^{3} f_{x_j}^{\nu} \sum_{k=1}^{3} S_{kj} \left[R_k + f_{x_k}(x^{\nu+1} - x^{\nu})\right] = 0 \qquad (43')$$

and $x^{\nu+1} - x^{\nu}$ can be solved

$$x^{\nu+1} - x^{\nu} = - \frac{\sum_{j=1}^{3} f_{x_j}^{\nu} \sum_{k=1}^{3} S_{kj} R_k}{\sum_{j=1}^{3} f_{x_j}^{\nu} \sum_{k=1}^{3} S_{kj} f_{x_k}^{\nu}} \qquad (56)$$

The solution Eq. (56) is of course also obtained from Eq. (25) after some matrix operations.

The χ^2 value can be calculated from Eq. (26)

$$\chi^2 = \sum_{j=1}^{3} \alpha_j^{\nu+1} \left[R_j + f_{x_j}(x^{\nu+1} - x^{\nu})\right] \qquad (26)$$

The numerical calculations are made in the following order:

(i) An approximate value of x is obtained by solving the first constraint equation (41).

(ii) The derivative matrices Eq. (46) and (47) are calculated. We have $\nu = 0$ in the first step.

(iii) The S matrix Eq. (52) is constructed and inverted.

(iv) The correction to the unknown variable is solved Eq. (56).

(v) The α vector Eq. (55) and the correction vector $(m_i^{\nu+1} - m_i^{o})$, Eq. (42') are evaluated.

(vi) χ^2 is calculated, Eq. (26).

(vii) A test is made to see if the derivatives Eqs. (42 - 44) are smaller than some given values. If this is not the case, we start again with (ii) above and now replace x^{ν} and m_i^{ν} with $x^{\nu+1}$ and $m_i^{\nu+1}$.

(viii) When the given stopping conditions are fulfilled we calculate the errors in the fitted quantities, Eqs. (34 - 36).

Results from calculations on the given example are given in Table 1.

Step	m_1 MeV/c	m_2 degrees	m_3 MeV/c	m_4 degrees	x MeV/c	f_1 MeV/c	f_2 MeV/c	f_3 MeV	χ^2
0	900.0	5.73	100.0	57.30	949.5	0.000	5.703	-6.974	-
1	812.7	5.37	89.9	57.16	857.9	0.090	5.321	-0.076	1.17
2	806.7	5.40	90.4	57.18	852.2	0.001	0.004	0.002	1.22
3	806.9	5.40	90.4	57.18	852.3	0.000	0.000	0.000	1.22

Table 1

We find that the constraint equations are well fulfilled already after two steps. The χ^2 value of the fit is lower than the mean value we expect to have (= 2 for a 2 C-fit) and we conclude that the tested event is in good agreement with the given hypothesis.

The error matrix of the fitted quantities derived after step 3 is (σ_i given in GeV/c and radians)

$$G_{m^3}^{-1} = \begin{bmatrix} 0.002360 & -0.000655 & -0.000353 & -0.000137 \\ -0.000655 & 0.000187 & 0.000105 & -0.000001 \\ -0.000353 & 0.000105 & 0.000063 & -0.000033 \\ -0.000137 & -0.000001 & -0.000033 & 0.000295 \end{bmatrix}$$

and the error in x is 46 MeV/c.

Finally we give the best fit solution of the observed lambda decay.

m_1 = 307 ± 49 MeV/c
m_2 = 5°.4 ± 0°.6
m_3 = 90 ± 8 MeV/c
m_4 = 57°.2 ± 1°.0
x = 852 ± 46 MeV/c

There is at CERN one subroutine (BOECK; written by W. Koch), which makes the calculations (iii) - (vi) and (viii) above, for the general case, when we have correlated variables, (see Appendix I).

5) Results from a Ξ^--fit

A typical Ξ^- candidate is shown on Fig. 4. In Fig. 5 we give the results from the geometrical and kinematical programmes.

The notation of points and tracks is explained in Fig. 4. NTR is the number of tracks leaving a point. The nature (NAT) of a point is for example, 2 if the apex of a V^0 decay and 3 if the apex of a V^- decay starts from the point. The nature of a track is 1 if the particle stops in the chamber, 2 if the track combines two interaction vertices and 10 for beam tracks. The CODE (U = unmeasured, W = measured and F = fixed) is given for the momentum (P), dip angle (DIP), azimuth angle (PHI) and mass respectively. AD in front of a quantity means the error of this quantity. A U or an F after a variable means unfitted and fitted quantities respectively, L is the measured length of a track, H the average magnetic field and BUB the expected bubble density of a charged track.

The results concerning points and tracks are obtained from THRESH and the fit results from GRIND.

We will now look at the different fits.

a) K^0 (Vertex NN)

TYP 200 indicate a V^0 and HYP 1 is a K^0. The first fit ① is a K^0-fit of the NN vertex. The mass of K^0 is fixed (=0.4978 GeV). We see that the momenta of the pions are higher than those given in THRESH. The reason for

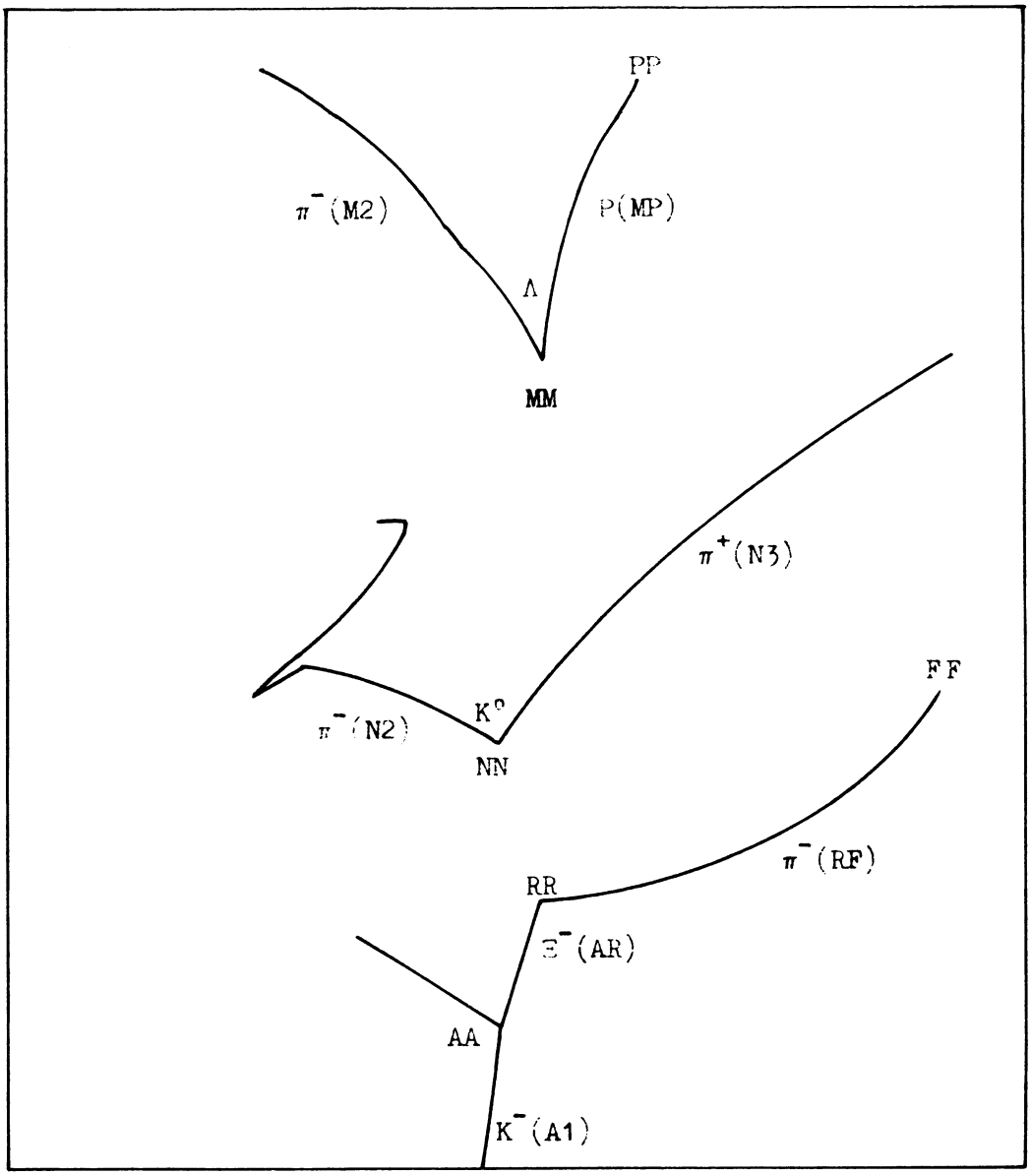


Fig. 4

A Ξ^- candidate. The production process may be

$K^- + N \rightarrow \Xi^- + K^o$.

this is of course that THRESH gives the momentum of a particle at the mean point of the measured track length, while the unfitted momentum in a fit is corrected to be valid at the interaction vertex.

The unfitted errors are greater than THRESH errors because uncertainties due to Coulomb scattering have to be included.

The K^0 is assumed to come from the point AA, (TRACK NA), and we consequently know the direction of this particle. Both pions are completely measured and we have only one unknown in the fit, the momentum of the kaon. This is a 3 C-fit (ND = 3). An unfitted value of the kaon momentum is, however, given. It has been calculated from the constraint equations, and must be available before the least squares fit can start.

At the top we find that the χ^2 of the fit is 1.01, the probability of getting a χ^2 greater than the obtained value is 0.7999 and the number of iteration steps performed to come to the solution is 3.

The K^0 hypothesis is very good for the vertex NN, and the fitted data agree well with the unfitted ones. The fitted errors are generally smaller than the unfitted. This is especially true for the relatively badly measured momenta of the pions (from 67 and 215 MeV/c to 8 and 7 MeV/c respectively).

Fit (2) differs from (1) in that the mass of the neutral particle is assumed to be unknown. We have therefore a 2 C-fit. The obtained probability (0.6048) together with the fitted mass 497.5 ± 63.8 MeV indicate that the K^0 hypothesis is still good.

GRIND has also tried to make a Λ-fit (HYP 2) and an $\bar{\Lambda}$-fit (HYP 3) with the vertex NN, but we see from the summary bank, which follows after the fits in Fig. 5, that an error 15 (ER 15) was found. This type of error indicates that a fit to the given hypothesis is impossible. We may, for example, have some obvious contradiction of a physical law, non-convergence of the iteration process, or corrections to the measured data, which are much greater than what can be expected from statistical fluctuations. The last is what has happened in our case; χ^2 is 26.8 and 41.2 for the Λ and $\bar{\Lambda}$ hypotheses after 3 and 2 steps respectively.

Fig. 5. THRESH and GRIND results for the Ξ^- candidate on Fig. 4.

EVENT 44 467683.1

POINTS

		NTR	NAT	X	Y	Z	DX	DY	DZ
1	A	2	0	6.3861	0.7826	-23.8324	0.0155	0.0149	0.0812
2	R	2	3	7.9113	0.5849	-23.6247	0.0210	0.0199	0.1086
3	M	2	2	17.2402	1.0983	-22.1280	0.0200	0.0177	0.0961
4	N	2	2	10.2983	1.3145	-25.8938	0.0161	0.0150	0.0828
5	P	0	12	27.8238	0.1450	-20.0237	0.0237	0.0191	0.1032
6	F	0	12	17.8081	-8.8863	-27.4560	0.0128	0.0114	0.0624

TRACKS		NAT	CODE	P	DIP	PHI	DP	DDIP	DPHI	L	DL	SAG	PCOSL	H	TESTS
1	AR +-	2	U W W	0.	0.0781	6.1567	0.	0.0506	0.0077	1.59	0.30	0.000	0.	0.	42
2	RF -	1	W W W	0.0650	-0.1949	5.1206	0.0018	0.1176	0.0149	15.07	0.04	2.148	0.064	17.11	0
3	M2 -	0	W W W	0.1747	0.1320	0.2950	0.0129	0.0035	0.0022	8.73	0.30	0.274	0.173	16.93	0
4	N2 -	0	W W W	0.3304	-0.5039	0.9497	0.1683	0.0269	0.0150	4.79	0.30	0.039	0.289	17.20	40
5	MP +	1	W W W	0.4422	0.1768	6.2616	0.0531	0.0037	0.0026	10.91	0.04	-0.167	0.435	16.91	0
6	N3 +	0	W W W	0.3148	-0.2907	5.7404	0.0143	0.0062	0.0029	15.16	0.30	-0.453	0.302	17.25	0
7	A1 -	10	W W W	1.3475	0.0069	3.2228	0.0168	0.0022	0.0012	-57.54	0.30	-0.090	1.348	17.09	0
8	RA +-	2	U W W	0.	-0.0781	3.0151	0.	0.0506	0.0077	-1.59	0.30	-0.000	0.	0.	42

(1)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 1 ER14 NONE CHISQ 1.01 ND 3 PROB 0.7999 STEP 3

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
NA 0	0.4978	U W W F	2.2	0.518	0.481	3.277	0.	0.023	0.005	0.505	0.497	3.277	0.012	0.017	0.005	0.
N3 +	0.1396	W W W F	1.2	0.332	-0.291	5.740	0.067	0.024	0.017	0.336	-0.280	5.743	0.008	0.022	0.017	0.
N2 -	0.1396	W W W F	1.4	0.336	-0.504	0.950	0.215	0.030	0.018	0.315	-0.488	0.948	0.007	0.025	0.018	0.

(2)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 1 ER14 NONE CHISQ 1.01 ND 2 PROB 0.6048 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
NA 0	0.4975	U W W U	2.2	0.518	0.481	3.277	0.	0.023	0.005	0.504	0.497	3.277	0.097	0.017	0.005	0.0638
N3 +	0.1396	W W W F	1.2	0.332	-0.291	5.740	0.067	0.024	0.017	0.336	-0.280	5.743	0.065	0.022	0.017	0.
N2 -	0.1396	W W W F	1.4	0.336	-0.504	0.950	0.215	0.030	0.018	0.315	-0.488	0.948	0.059	0.025	0.018	0.

(3)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 0 ER14 NONE CHISQ 0.17 ND 1 PROB 0.6763 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
MO 0	1.1154	U U U F	3.6	0.667	-0.166	3.208	0.246	0.011	0.006	0.694	-0.165	3.218	0.004	0.022	0.016	0.
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.177	6.261	0.002	0.027	0.019	0.
M2 -	0.1396	W W W F	1.4	0.188	0.132	0.296	0.058	0.037	0.027	0.216	0.132	0.300	0.002	0.037	0.025	0.

(4)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 2 ER14 NONE CHISQ 9.37 ND 3 PROB 0.0248 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
MA 0	1.1154	U W W F	3.6	0.667	-0.156	3.171	0.	0.011	0.002	0.691	-0.158	3.172	0.004	0.010	0.002	0.
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.168	6.209	0.002	0.018	0.009	0.
M2 -	0.1396	W W W F	1.4	0.188	0.132	0.296	0.058	0.037	0.027	0.214	0.128	0.267	0.003	0.033	0.022	0.

(5)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 2 ER14 NONE CHISQ 2.63 ND 2 PROB 0.2686 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
MA 0	1.0909	U W W U	4.1	0.667	-0.156	3.171	0.	0.011	0.002	0.623	-0.158	3.171	0.023	0.010	0.002	0.0068
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.166	6.240	0.002	0.015	0.014	0.
M2 -	0.1396	W W W F	2.0	0.188	0.132	0.296	0.058	0.037	0.027	0.143	0.126	0.276	0.024	0.035	0.023	0.

(6)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 2 ER14 NONE CHISQ 2.09 ND 3 PROB 0.5545 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
MR 0	1.1154	U W W F	3.6	0.667	-0.159	3.197	0.	0.015	0.003	0.693	-0.161	3.197	0.004	0.013	0.003	0.
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.172	6.237	0.002	0.019	0.009	0.
M2 -	0.1396	W W W F	1.4	0.188	0.132	0.296	0.058	0.037	0.027	0.215	0.129	0.285	0.003	0.034	0.022	0.

(7)

GOOD FIT NOPT 1 NOTR 3 TYP 200 HYP 2 ER14 NONE CHISQ 0.28 ND 2 PROB 0.8706 STEP 3

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
MR 0	1.0992	U W W U	3.9	0.667	-0.159	3.197	0.	0.015	0.003	0.650	-0.161	3.197	0.029	0.013	0.003	0.0101
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.171	6.256	0.002	0.018	0.016	0.
M2 -	0.1396	W W W F	1.7	0.188	0.132	0.296	0.058	0.037	0.027	0.171	0.128	0.290	0.030	0.035	0.023	0.

(8)

GOOD FIT NOPT 1 NOTR 3 TYP 320 HYP 4 ER14 NONE CHISQ 0.18 ND 2 PROB 0.9132 STEP 3

TRACK	MASS.	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
RA -	1.3195	U W W U	4.1	0.754	-0.078	3.015	0.	0.051	0.008	0.753	-0.092	3.015	0.017	0.032	0.007	0.0095
RF -	0.1396	W W W F	1.9	0.152	-0.195	5.129	0.001	0.258	0.166	0.152	-0.275	5.141	0.001	0.172	0.097	0.
RM 0	1.1154	W W W F	3.6	0.693	0.161	0.056	0.004	0.013	0.003	0.693	0.160	0.056	0.004	0.012	0.003	0.

(9)

GOOD FIT NOPT 1 NOTR 3 TYP 320 HYP 4 ER14 NONE CHISQ 0.22 ND 3 PROB 0.9738 STEP 3

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
RA -	1.3215	U W W F	4.1	0.754	-0.078	3.015	0.	0.051	0.008	0.749	-0.087	3.014	0.005	0.020	0.007	0.
RF -	0.1396	W W W F	1.9	0.152	-0.195	5.129	0.001	0.258	0.166	0.152	-0.305	5.121	0.001	0.089	0.028	0.
RM 0	1.1154	W W W F	3.6	0.693	0.161	0.056	0.004	0.013	0.003	0.693	0.160	0.056	0.004	0.012	0.003	0.

(10)

GOOD FIT NOPT 2 NOTR 6 TYP 320 HYP 4 ER14 NONE CHISQ 2.31 ND 6 PROB 0.8891 STEP 4

TRACK	MASS	CODE	BUB	P U	DIP U	PHI U	DP U	DDP U	DPH U	P F	DIP F	PHI F	DP F	DDP F	DPH F	DM
RA -	1.3215	U W W F	4.1	0.729	-0.078	3.015	0.	0.051	0.008	0.749	-0.087	3.014	0.005	0.020	0.007	0.
RF -	0.1396	W W W F	1.9	0.152	-0.195	5.129	0.001	0.258	0.166	0.152	-0.305	5.121	0.001	0.089	0.028	0.
RM 0	1.1154	U W W F	3.6	0.667	0.159	0.055	0.	0.015	0.003	0.693	0.160	0.056	0.004	0.012	0.003	0.
MP +	0.9382	W W W F	4.8	0.486	0.177	6.261	0.002	0.027	0.019	0.486	0.171	6.237	0.002	0.019	0.009	0.
M2 -	0.1396	W W W F	1.4	0.188	0.132	0.296	0.058	0.037	0.027	0.215	0.129	0.285	0.002	0.034	0.022	0.

SUMMARY BANK FOR EVENT 44 467683.1 5

	NOPT	PT	NOTR	TYP	HYP	GDNS	ER14	ER15	CHISQ	ND	PROB	STEPS
1	1	4	3	200	1	77	-	-	0.1006E 01	3	0.7999	3
2	1	4	3	200	2	17	-	FIT 34 NO FIT	0.2679E 02	3	0.0000	3
3	1	4	3	200	3	17	-	FIT 34 NO FIT	0.4123E 02	3	0.0000	2
4	1	3	3	200	2	57	-	-	0.9366E 01	3	0.0248	4
5	1	3	3	200	2	77	-	-	0.2087E 01	3	0.5545	4
6	1	2	3	320	4	77	-	-	0.1816E-00	2	0.9132	3
7	1	2	3	320	4	77	-	-	0.2228E-00	3	0.9738	3
8	2	2	6	320	4	0	-	-	0.2310E 01	6	0.8891	4
9	2	2	6	320	4	0	-	-	0.2310E 01	6	0.8891	4

An error 14 (ER 14), of which we have none in our example, shows that some minor contradiction has been found in the fit, for example, that the momentum of a particle derived from its range and curvature disagree. The fit will in these cases go on, but the contradiction is flagged at the top of the fit results and also in the summary bank.

b) Λ (Vertex MM)

Results from good V^0 fits of vertex MM are given in (3) to (7).

The lambda is assumed to be completely unknown in (3) (HYP 0, CODE U U U F). We have then a 1 C-fit, which gives $\chi^2 = 0.17$ and probability 0.6763. This shows that the lambda hypothesis is possible.

In (4) and (5) we assume that the lambda comes from the primary vertex AA. Fit (4), where the lambda mass is fixed, results in a very high χ^2 and gives a low probability (0.0248). Fit (5) with the mass of the neutral particle unknown gives a high probability, but the derived mass 1090.9 ± 6.8 MeV is 3.6 standard deviations from the lambda mass. We conclude that the hypothesis that the lambda comes from vertex AA is almost disproved by the fit results, or at least shown to be a very improbable solution.

The hypothesis that the lambda comes from the kink RR is a very good solution according to the two fits (6) and (7).

c) Ξ^- 1-vertex fit (Vertex RR)

When a lambda is shown to come from the kink of a negative track, we test the hypothesis: $\Xi^- \rightarrow \Lambda + \pi^-$.

We assume in the 1-vertex fit that the fitted lambda (RM in our notation) is measured and we have a 3 C-fit with the Ξ^- mass known (9), and a 2 C-fit with the mass unknown (8).

The two fits give very high probabilities, and the derived mass, 1319.5 ± 9.5 MeV, is in good agreement with the known Ξ^- mass. We conclude that the Ξ^- hypothesis is a good explanation for this event.

d) Ξ^- 2-vertices fit (Vertices RR and MM)

If a good 1-vertex Ξ^--fit is obtained, we go on by combining the two fits (Ξ^- and Λ decay) in a 2-vertices fit, (10). We then have 8 constraint equations and in our case 2 unknowns (P_{Ξ^-} and P_Λ). The high probability

(0.8891) of the 6 C-fit means that our conclusion above has a good chance of being correct.

A 2-vertices E^--fit is also tried when we do not get a good 1-vertex fit. The 2-vertices fit should in principle be superior, and we have observed a few events where the 2-vertices fit is good, while the 1-vertex fit fails. However, in most cases we obtain both fits, and the fitted data agree extremely well.

V. COMPARISON OF RESULTS FROM AN EXPERIMENT WITH THEORETICAL PREDICTIONS

1) Introduction

Most experiments are performed to test some hypothesis. The observed quantities will of course deviate from the theoretical ones. The purpose of a test is to find out whether the deviation between experimental and theoretical values could be due to random sampling variations, or whether the deviation is too great, from which we may conclude that the hypothesis is probably wrong.

In the following we describe two types of hypotheses which are often tested.

In the first type (Chapter V.2) the hypothesis gives the magnitude of some parameter associated with the population, e.g. the mean value. The test is in general performed in the following way. The sampling distribution of the parameter in question is determined and the measured quantity is compared with its theoretical distribution.

The theoretical frequency distribution is known in the second type of hypothesis. The agreement between the distribution of the observed sample and the hypothesis is in general tested by a χ^2 test of significance (Chapter V.3).

The two types of test will be illustrated by an example taken from an investigation of leptonic decay modes (Physics Letters 6, 186 (1963)). About 90 lambda hyperons decaying to electrons ($\Lambda \rightarrow P + e^- + \bar{\nu}$) were observed.

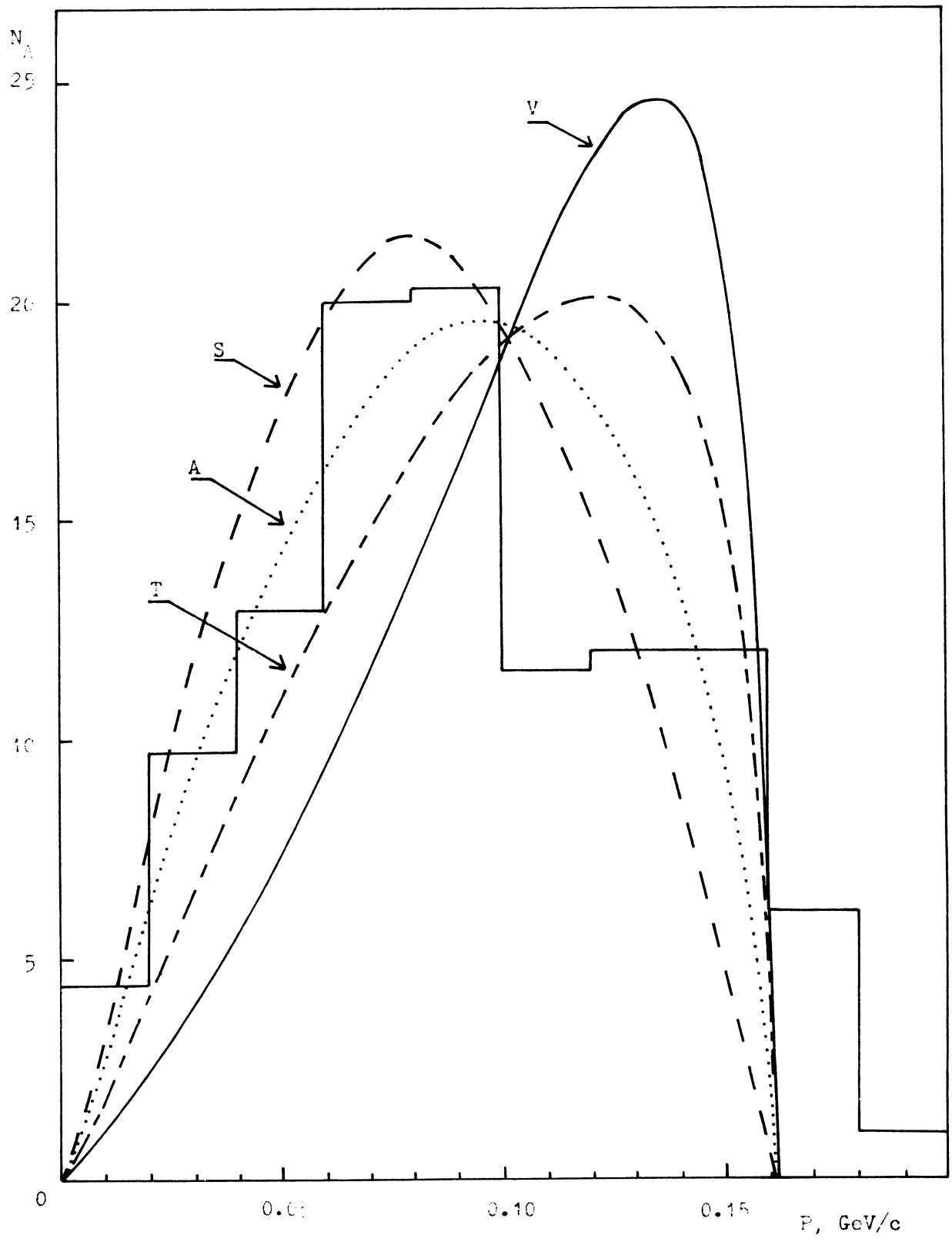


Fig. 6

The four curves show different theoretical transverse momentum spectra of the proton for Lambda hyperons decaying to electrons. The histogram gives the observed distribution. (Physics Letters 6, 185 (1963)).

There are different forms of interaction (V = vector, S = scalar, A = axial vector and T = tensor), which might be responsible for the decay. We give the transverse momentum spectrum of the proton ($P_\perp = P_p \sin \Theta_{\Lambda p}$) derived from the four theories in Fig. 6. We have also given the observed spectrum, which is corrected for detection efficiency. To make the following tests easier, we assume that the histogram contains observed events only (110 in number).

There are some events in Fig. 6 which have transverse momenta above the theoretically maximum possible value. The reason for this is of course uncertainties in the measured variables. One should therefore, in a treatment which is more strict than that below, take these uncertainties into consideration. One possibility is, for example, to modify the theoretical curves in such a way that the uncertainties in the measured variables will be included.

2) Test of a mean value

The mean value ($<P_\perp>$) of the theoretical distributions takes the following values:

V	106	MeV/c
T	98	"
A	89	"
S	81	"

The measured spectrum has the mean value $(P_\perp)_{exp} = 91$ MeV/c.

The theoretical $P_\perp$ distributions are not normal, but the distribution of the mean value of a sample will in most cases approach the normal distribution when the sample size increases. This is, for example, the case, if the population has finite variance (σ_p^2) and mean. The mean value distribution will have the same mean as the population and the variance σ_p^2/n. The standard deviations of the four theoretical distributions are about the same (34 - 38 MeV/c), which means that the mean value distribution will have a standard deviation (σ_{mv}) of about 3.5 MeV/c (n = 110).

The deviation between the theoretical and observed mean values is then:

V	4.3	σ_{mv}
T	2.0	"
A	0.6	"
S	2.9	"

The probability that $\langle P_\perp \rangle_{exp}$ will deviate by more than $\alpha.\sigma_{mv}$ from the mean value of the population is of course:

$$Pr = \frac{2}{\sqrt{2\pi}} \int_{\alpha}^{\infty} e^{-\frac{(P_\perp - \langle P_\perp \rangle)^2}{\sigma^2_{mv}}} dP_\perp \ . \qquad (57)$$

This probability can be found in most statistical tables. In our case we have:

V	<	0.01%
T		4.6%
A		55 %
S		0.4%

The level of significance for a test is arbitrarily fixed at, for example, 5%, 1% or in the more stringent tests 0.1%. Let us fix the significance level at 1%. We then conclude that the pure V and S hypotheses are apparently disproved by the experiment, while the A and T hypotheses are reasonably practical interpretations of the measured mean value.

3) χ^2 test of distributions

This test (ref. D. Hudson, CERN 63-29) is used when one wants to find out how well the whole sample distribution agrees with a known population distribution. It is therefore more general than the test described above.

The distributions are divided in class intervals of the variable ($P_\perp$ in our case). The number (N_i) of observed events in an interval i, is compared with the expected number (N_i^h) from the given hypothesis. The following quantity is calculated:

$$\chi^2 = \sum_{i=1}^{r} \frac{(N_i - N_i^h)^2}{N_i^h} \quad . \tag{58}$$

The distribution of χ^2 will approach the χ^2 distribution given in Chapter IV.3 when the size (n) of the sample increases. One may use the limiting distribution if the size of the sample is so large that each N_i^h is greater than 10.

$P_\perp$ MeV/c	N_i	N_i^h			
		V	T	A	S
0 - 40	14.1	5.7	9.1	12.8	15.7
40 - 80	32.8	20.0	26.6	32.5	39.3
80 - 120	31.9	38.5	38.6	39.3	39.3
> 120	31.2	45.8	35.7	25.4	15.7
χ^2		26.4	6.0	2.8	18.0

Table 2

In our case we divide the distributions into four classes. The expected and observed number of events in each interval is given in Table 2 together with the χ^2 values calculated with the formula above.

The number of degrees of freedom is r- 1 (3 in our case). This follows from the fact that one can only choose r- 1 of the N_i^h values independently when the total number of events in the distribution is fixed.

The probabilities ($P_3\%$) to obtain χ^2 values greater than given values (χ_0^2) are given in Table 3 for 3 degrees of freedom (see Chapter IV.3).

χ_0^2	2.4	3.7	4.6	6.3	7.8	9.8	11.3	16.2
$P_3\%$	50	30	20	10	5	2	1	0.1

Table 3

We conclude that our experimental data are not consistent with hypotheses V and S even if we select the significance level to be as low as 0.1%. The agreement is, however, good between both of the hypotheses A and T and the observed distribution.

The χ^2 test may be used even when some parameters of the population distribution are unknown. In this case one has first to estimate the unknown parameters with the help of the experimental distribution. The number of degrees of freedom will now be r- 1 - a, where a is the number of unknown parameters in the population distribution.

Acknowledgement

I wish to thank Dr. F. Müller for reading this article and making many valuable suggestions.

7863/p/cm

APPENDIX I

DESCRIPTION OF THE SUBROUTINE BOECK

BOECK is a FORTRAN subroutine, which performs needed matrix operations for one step of the best fit calculations.

Input quantities:

NF = Number of constraint equations.
NM = Number of measured variables.
NX = Number of unknown variables.
F(NF) = Constraint equations.
B(NF,NM) = Derivative matrix of measured variables.
A(NF,NX) = Derivative matrix of unknown variables.
GI(NM,NM) = Error matrix of measured variables.

Output quantities:

C(NM) = Corrections of measured quantities; $m^{\nu+1} = m^{0} + C$ (C is put equal to 0 before the first step).
DX(NX) = Corrections of unknown variables; $x^{\nu+1} = x^{\nu} + DX$.
GMFI(NM,NM) = Error matrix of fitted measured variables.
GXI(NX,NX) = Error matrix of unmeasured variables.
B(NM,NX) = Correlation matrix between measured and unmeasured variables.
CHI = χ^2 for the last step.

Some further remarks:

1. The dimensions must be at least as big as those given within the brackets.
2. H(NM,NM), HH(NM,NM), R(NF) and AL(NF) are working matrices.
3. Some of the input matrices are re-defined in later stages of the programme and thus used as working matrices.
4. One must have NM ≥ NF ≥ NX

5. A 2 dimensional array A(1,1) ... A(m,n) is in FORTRAN stored column-wise, i.e. in order A(1,1), A(2,1), ... A(m,1), A(1,2), A(2,2), ... A(m,2), ... A(m,n). It must for this programme be stored row-wise, i.e. in order A(1,1), A(1,2), ... A(1,n), A(2,1), A(2,2), ... A(2,n), ... A(m,n).

6. K is put equal to 0 as long as a further step in the iteration process is needed and equal to 1 when the iteration is finished and the error matrices have to be evaluated.

7. Equations and notations from Böck (CERN 60-30).

8. All matrix operations are performed by a series of subroutines collected under the name MXPACK and described in the GRIND manual. From this we copy the introduction and also descriptions of subroutines used in BOECK.

MXPACK is a summary name for various subroutines written in 709 FAP language for the fast execution of matrix operations. All entry names start with the letter pair MX. All routines assume that matrices are stored row-wise and without gaps (this is important in case of FORTRAN double indexing) in FORTRAN order (i.e. in absolute descending locations).

Description of subroutines:

MXEQU (A,B,I,J) "Matrix Equations"
solves A(I,I) × X(I,J) = B(I,J) for X.
The result (X) is stored into B, A is transformed.
A is assumed to be positive definite. No pivoting is done.

MXUTY (A,I) "Matrix Unity"
writes a (I,I) Unit matrix into A.

MXADD (A,B,C,I,J) "Matrix Addition"
effects A(I,J) + B(I,J) → C(I,J)

MXSUB (A,B,C,I,J) "Matrix Subtraction"
effects A(I,J) - B(I,J) → C(I,J)

MXTRA (A,B,C,I,J) "Matrix Transfer"
effects A(I,J) → C(I,J). The B-address is irrelevant.

MXMTR (A,B,C,I,J) "Matrix Multiplied Transfer"
effects B × A(I,J) → C(I,J)
B is a scalar factor.

MXMPY (A,B,C,I,J,K) "Matrix Multiplication"
effects A(I,J) × B(J,K) → C(I,K)

The following entries use the same sequence of arguments:

MXMPY1 for $A \times B^T \rightarrow C$ (B is a (K,J) matrix)
MXMPY2 for $A^T \times B \rightarrow C$ (A is a (J,I) matrix)
MXMAD for $A \times B + C \rightarrow C$ "Matrix Multiplication and Addition".

```
C     MATRIX OPERATIONS FOR ONE STEP OF LEAST SQUARES CALCULATIONS
      SUBROUTINE BOECK(K)
      DIMENSION F(3),B(12),A(3),GI(16),C(4),DX(1),GMFI(16),GXI(1),
     1H(16),HH(16),R(3),AL(3)
      COMMON NF,NM,NX,F,B,A,GI,C,DX,GMFI,GXI,CHI
      IF(K) 2,1,2
    1 CALL MXMPY(B,C,H,NF,NM,1)
      CALL MXSUB(F,H,R,NF,1)
C               R IS DEFINED IN (15')
      CALL MXMPY1(GI,B,HH,NM,NM,NF)
      CALL MXMPY(B,HH,H,NF,NM,NF)
C               H IS EQUAL TO S, DEFINED IN (16')
      CALL MXUTY(GMFI,NF)
      CALL MXEQU(H,GMFI,NF,NF)
C               GMFI IS THE INVERSION OF S
      CALL MXMPY(GMFI,A,H,NF,NF,NX)
      CALL MXMPY2(A,H,HH,NX,NF,NX)
      CALL MXUTY(GXI,NX)
      CALL MXEQU(HH,GXI,NX,NX)
      CALL MXMPY2(H,R,C,NX,NF,1)
      CALL MXMPY(GXI,C,DX,NX,NX,1)
      CALL MXMTR(DX,-1.,DX,NX,1)
C               DX IS EQUAL TO THE SECOND EXPRESSION IN (25)
      CALL MXMAD(A,DX,R,NF,NX,1)
      CALL MXMPY(GMFI,R,AL,NF,NF,1)
C               AL IS THE SOLUTION (24)
      CALL MXMPY2(AL,R,CHI,1,NF,1)
      CALL MXMPY2(B,AL,H,NM,NF,1)
      CALL MXMPY(GI,H,C,NM,NM,1)
      CALL MXMTR(C,-1.,C,NM,1)
C               C IS EQUAL TO THE SECOND EXPRESSION IN (12')
      RETURN
C               CALCULATION OF ERROR MATRICES (34-36)
    2 CALL MXMPY2(A,GMFI,H,NX,NF,NF)
      CALL MXTRA(H,0,A,NX,NF)
      CALL MXMPY(B,GI,H,NF,NM,NM)
      CALL MXTRA(H,0,B,NF,NM)
      CALL MXMPY(GMFI,B,H,NF,NF,NM)
      CALL MXMPY2(B,H,HH,NM,NF,NM)
      CALL MXSUB(GI,HH,GMFI,NM,NM)
      CALL MXMPY(A,B,H,NX,NF,NM)
      CALL MXTRA(H,0,HH,NX,NM)
      CALL MXMPY2(HH,GXI,B,NM,NX,NX)
      CALL MXMTR(B,-1.,B,NM,NX)
      CALL MXMPY(B,HH,H,NM,NX,NM)
      CALL MXSUB(GMFI,H,HH,NM,NM)
      CALL MXTRA(HH,0,GMFI,NM,NM)
      RETURN
      END
```

APPENDIX II

GRAPHICAL METHODS OF TESTING THE PROBABILITY DISTRIBUTION A SAMPLE IS THOUGHT TO HAVE COME FROM

Contributed by D. Hudson,
Data and Documents Division, CERN

Suppose we have arranged a sample of size n in increasing order of magnitude to get

$$x_1 < x_2 < \ldots < x_n \tag{1}$$

and we wish to test whether it comes from a continuous distribution with probability density function f(x), and cumulative distribution

$$F(x) = \int_{-\infty}^{x} f(t)\, dt \ . \tag{2}$$

In the first instance it is assumed that f(x) is completely known. Later on the technique is extended to the case where a location parameter μ and a scale parameter σ are unknown, and only the general form $f(x; \mu,\sigma)$ is given.

Example (i)

The χ^2_2 distribution has density function

$$\begin{aligned} f(x) &= 0 \qquad\quad , \quad -\infty < x < 0 \ , \\ f(x) &= \tfrac{1}{2}\, e^{-x/2} \quad , \quad 0 \leq x < \infty \ . \end{aligned} \tag{3}$$

The cumulative distribution is

$$\begin{aligned} F(x) &= 0 \qquad\quad , \quad -\infty < x < 0 \ , \\ F(x) &= 1 - e^{-x/2} \quad , \quad 0 \leq x < \infty \ . \end{aligned} \tag{4}$$

Example (ii)

The normal distribution has density function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-(x-\mu)^2/2\sigma^2} \quad , \quad -\infty < x < \infty \tag{5}$$

and so has to be treated by the second method when μ and σ are unknown.

Large samples

When the sample size is large it is possible to draw a histogram and compare the resulting diagram with the expected frequency curve. On page 104 there is a histogram of a sample of size 80 from a χ^2_2 distribution, together with the curve

$$N(x) = 80 \times \tfrac{1}{2}\, e^{-x/2} \qquad (6)$$

Small samples

It can be difficult to decide whether the 'bumps' and 'holes' in a histogram are significant, especially if the sample size is small. A rough guide can be obtained by using the graph of the cumulative distribution $F(x)$. We may interpret $F(x)$ as follows:

Given a number x, the proportion of random variables X in a very large (actually infinite) sample for which $X \leq x$ is $F(x)$. In a finite sample of size n, we can estimate points on the curve $F(x)$ by calculating proportions of the sample less than or equal to x.

The n points $x_1, x_2, \ldots, x_n$ give rise to $(n+1)$ intervals on the x axis, viz.

$$(-\infty, x_1)\ ,\ (x_1, x_2)\ ,\ \ldots\ ,\ (x_{n-1}, x_n)\ ,\ (x_n, \infty) \qquad (7)$$

and it is conventional to say that $1/(n+1)$ of the sample lies in each such interval. Thus $1/(n+1)$ of the sample is $\leq x_1$, so $1/(n+1)$ estimates $F(x_1)$; $2/(n+1)$ of the sample is $< x_2$; ..... ; and $n/(n+1)$ estimates $F(x_n)$. [If we add the points $x_0 = -\infty$ and $x_{n+1} = \infty$ to the sample, then $0/(n+1)$ and $(n+1)/(n+1)$ are the correct values of $F(-\infty)$ and $F(+\infty)$ respectively]. A useful convention therefore is that the graph of $F(x)$ is to be estimated by plotting the n points

$$[x,\ F(x)] = \left[x_i\ ,\ \frac{i}{n+1}\right]\ ,\ i = 1, 2, \ldots, n\ . \qquad (8)$$

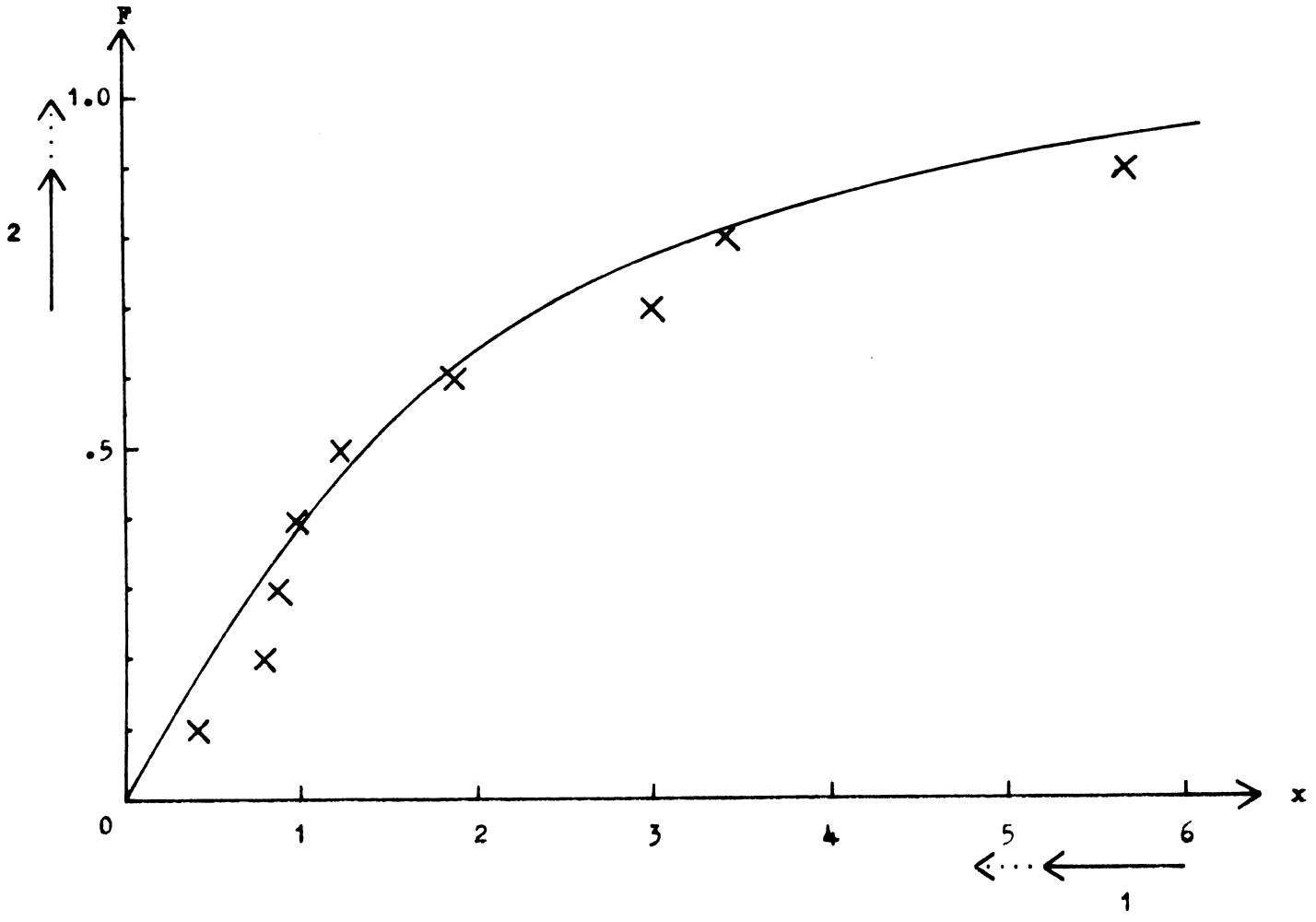
Example

The following is a sample of size nine from the χ^2_2 distribution.

.40, .78, .86, .96, 1.21, 1.86, 2.96, 3.41, 5.68

The points (.40, .1), (.78, .2), etc., are plotted next to the curve

$$F(x) = 1 - e^{-x/2} \tag{9}$$



Probability paper

We next show how to straighten out the curve of F(x) on the above graph so that the plotted points may be compared with a straight line. There are two alternative methods when f(x) is known completely.

(i) We transform the (horizontal) x axis to a new variable z = z(x) in such a way that we 'contract' the x axis most where the graph of F(x) is flat, as indicated by ①←. The transformation is

$$z = \int_{-\infty}^{x} f(t)\, dt \ . \tag{10}$$

The curve Eq. (9) becomes the straight line

$$F(z) = z \ . \tag{11}$$

(ii) We may alternatively transform the (vertical) F axis to a new variable y = y(F) in such a way that we 'stretch' the F axis most where the graph of F(x) is flat, as indicated by ②↑. The transformation is

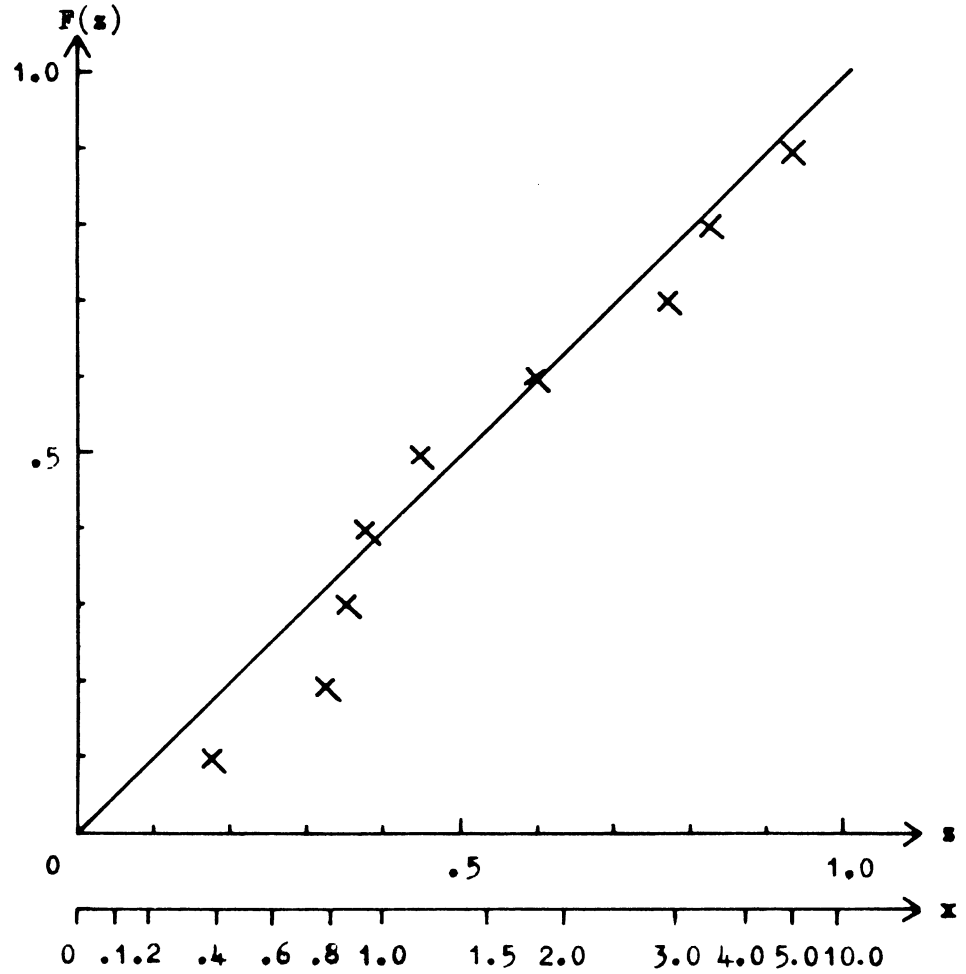
$$F = \int_{-\infty}^{y(F)} f(x)\, dx \ . \tag{12}$$

The curve Eq. (9) becomes the straight line

$$y = x \ . \tag{13}$$

The table required for graph (i) is completed by using 'Table 7: Probability integral of the χ^2_2 distribution and the cumulative sum of the Poisson distribution' in the Biometrika Tables.

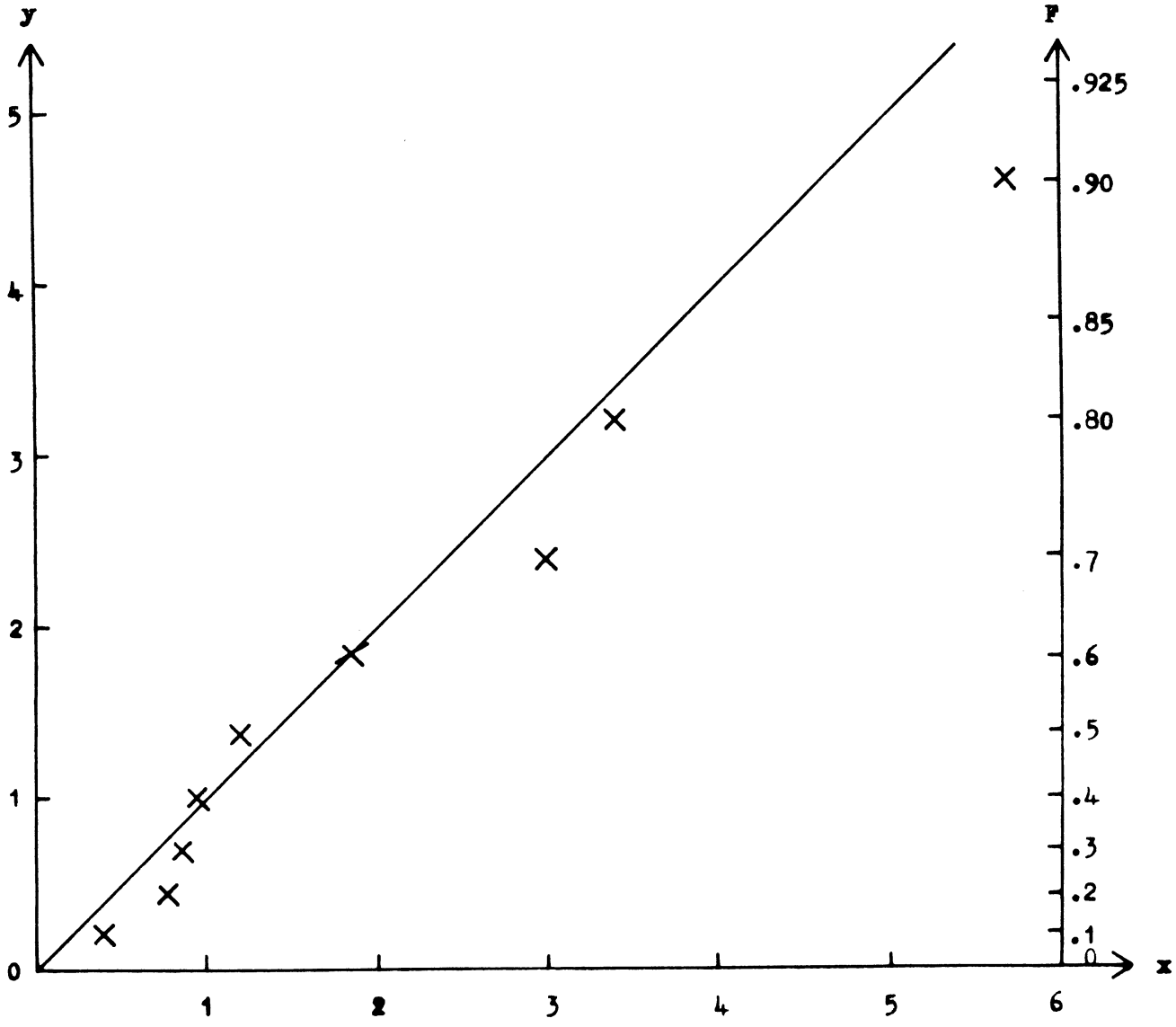
$x = \chi^2_2$	.40	.78	.86	.96	1.21	1.86	2.96	3.41	5.68
z	.18	.32	.35	.38	.45	.60	.77	.82	.94
F(z)	.1	.2	.3	.4	.5	.6	.7	.8	.9



The words 'probability paper' would refer to the above graph paper with only the x and the F scales printed. It would then not be necessary to look up the z values.

The table required for graph (ii) is completed similarly. (An augmented table of percentage points of the χ^2 distribution has been compiled at CERN, using the library tape subroutines referred to in the GRIND manual).

$x = \chi^2_2$	.40	.78	.86	.96	1.21	1.86	2.96	3.41	5.68
F	.1	.2	.3	.4	.5	.6	.7	.8	.9
y(F)	.21	.45	.71	1.02	1.39	1.83	2.41	3.22	4.61



The words 'probability paper' would refer to the above graph paper with only the x and the F scales printed. It would then not be necessary to look up the y values.

Probability paper of type (ii) is used more often in practice. The plotted points will be very bunched at parts of the graph where the original curve of F(x) is steep. Conversely, the data corresponding to 'tail areas' is well spread out. Usually we are particularly interested in these extreme values.

Further example

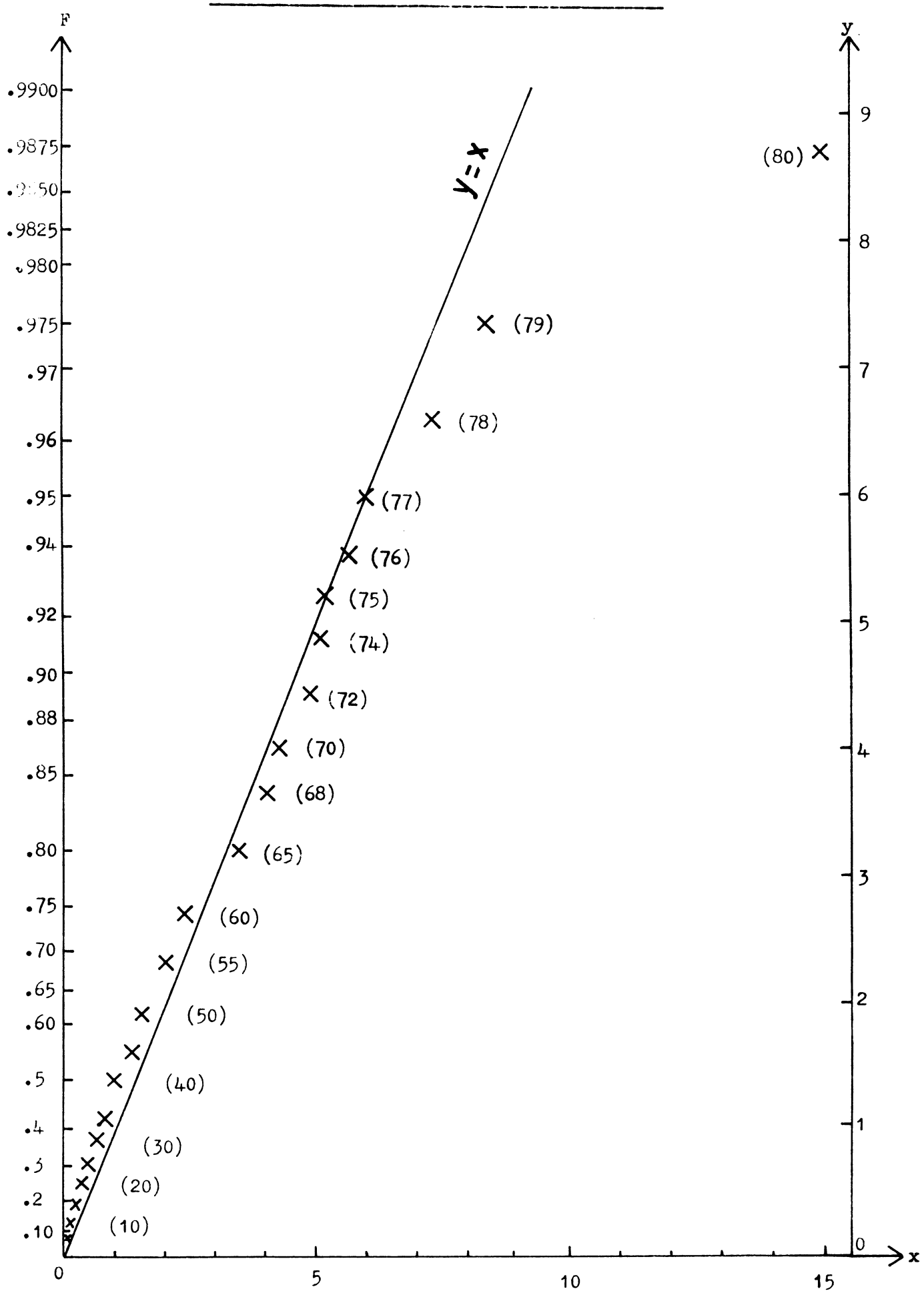
We use probability paper of type (ii) to plot the sample of size 80 on page 104. We wish to do a rough visual test to see whether the sample can reasonably be considered to have come from the X_2^2 distribution. The plotted points are given below. (In order not to crowd the graph, not every possible point is plotted.)

i	5	10	15	20	25	30	35	40	45	50
$x_i = X_2^2$	.08	.18	.27	.37	.49	.64	.82	.98	1.31	1.53
$F_i = i/81$	.06	.12	.18	.25	.31	.37	.43	.49	.56	.62

i	55	60	65	68	70	72	74	75	76
x_i	2.05	2.44	3.46	4.05	4.23	4.95	5.14	5.19	5.65
F_i	.68	.74	.802	.840	.865	.890	.914	.925	.938

i	77	78	79	80
x_i	5.99	7.37	8.32	14.98
F_i	.950	.963	.975	.987

Sample of size 80 from the X_2^2 distribution



Conclusions from the graph

The graph indicates that

(a) on the whole the data follow the χ^2_2 distribution fairly well;

(b) the smaller values (i = 1 to 60) tend to be a bit smaller than expected;

(c) the largest value x_{80} appears to be too large.

Exact test

We can find the exact level of significance of $x_{80} = x_{max}$.

We have $\Pr(x \leq k) = F(k)$

Let $\Pr(x_{max} \leq k) = H(k)$

Then $H(k) = \Pr(\text{All } x_i \leq k)$

$= [F(k)]^{80}$

So $H(14.98) = [F(14.98)]^{80}$

$= (1 - e^{-7.49})^{80}$

$= 1 - 0.044$

$\therefore \Pr(x_{max} \geq 14.98) = 4.4\%$.

The conclusion is that x_{max} is significantly larger than we expect the largest value of χ^2_2 to be in a sample of size 80. The value $x_{80} = 14.98$ may indicate that a different physical hypothesis is required for the relevant event.

Case of unknown parameters

Suppose that the probability density function of x, $f(x; \mu, \sigma)$, contains an unknown location parameter μ and an unknown scale parameter σ such that

$$w = \frac{x - \mu}{\sigma} \tag{14}$$

is a standardized variable with density function $f(w; 0, 1)$ which is completely known.

Let $$F(w) = \int_{-\infty}^{w} f(t;\ 0,\ 1)\ dt \qquad (15)$$

be the standardized cumulative distribution. We can prepare probability paper of type (ii) by making the transformation from the F scale to the y scale

$$F = \int_{-\infty}^{y(F)} f(t;\ 0,\ 1)\ dt\ . \qquad (16)$$

Comparison with Eq. (15) shows that the curve F(w) becomes the straight line

$$y = w\ . \qquad (17)$$

From Eq. (14) we see that if we measure x on the horizontal axis, Eq. (17) becomes the straight line

$$y = \frac{x-\mu}{\sigma}\ . \qquad (18)$$

Thus, when $y = 0$, $x = \mu$;
when $y = 1$, $x = \mu + \sigma$;
when $y = -1$, $x = \mu - \sigma$;

so the parameters can be read off the graph.

Example

A sample of size 7 is available and we wish to do a rough test to see whether they come from a normal distribution. The density function for x is

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\ .\ e^{-(x-\mu)^2/2\sigma^2}$$

and the standard density function for w is

$$f(w) = \frac{1}{\sqrt{2\pi}}\ e^{-w^2/2}\ .$$

The required transformation from the F to the y scale is

$$F = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{y(F)} e^{-w^2/2}\, dw$$

which is tabulated in the Biometrika Tables.

The data are given below in increasing order of magnitude.

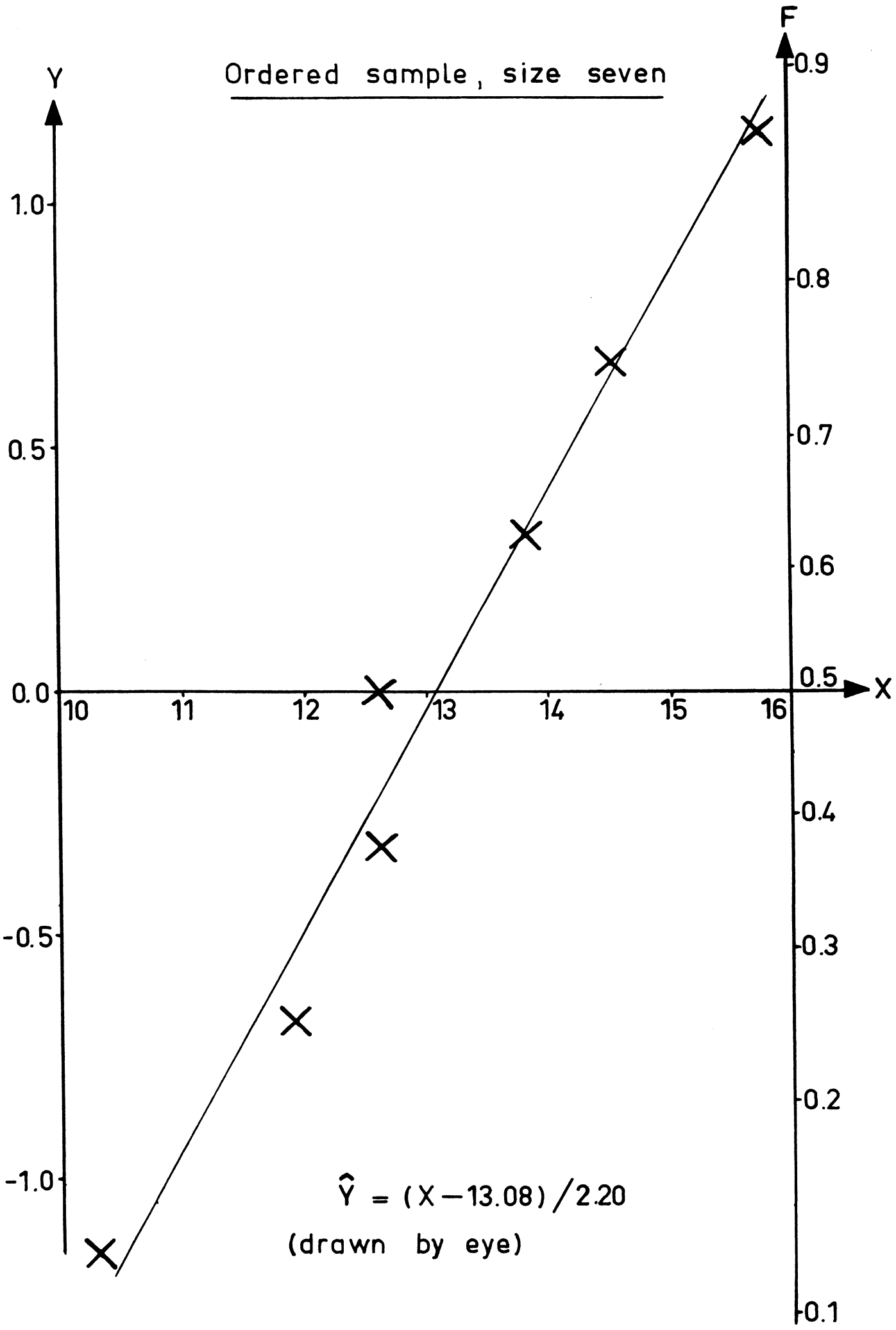
i	1	2	3	4	5	6	7
x_i	10.3	11.9	12.6	12.6	13.8	14.5	15.7
F_i	.125	.250	.375	.500	.625	.750	.875
y_i	-1.150	-.674	-.319	0	.319	.674	1.150

The 'normal probability plot' of the 'order statistics' is shown on page 144. The linearity shown by the plot is a rough assurance that the data are normally distributed. A line drawn by eye through the points gives the estimates

$$\mu = 13.08 \quad , \quad \sigma = 2.2 \ .$$

(The maximum likelihood estimates are

$$\hat{\mu} = 13.06 \quad , \quad \hat{\sigma} = 1.8 \ ).$$


Ordered sample, size seven
Y
X
F
1.0
0.5
0.0
-0.5
-1.0
10
11
12
13
14
15
16
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
$\hat{Y} = (X - 13.08)/2.20$
(drawn by eye)

REFERENCES

1) W. Dixon and F. Massey, Chapter 5.5 'Normal probability paper' and Chapter 13.7 'Binomial probability paper' in "Introduction to statistical analysis" - McGraw-Hill, 1957.

2) H. Chernoff and G. Lieberman, 'Use of normal probability paper' - J.Amer.Statist.Assn. 49, p. 778 (1954).

3) E. Crow, F. Davis and M. Maxfield, Chapter 4 'Tests of distributions as a whole' in "Statistics manual" - Dover, 1960.

4) E. Pearson and H. Hartley, "Biometrika tables for statisticians" - Cambridge U.P., 1958.

5) M. Kendall and A. Stuart, Chapter 14 'Order statistics' in "The advanced theory of statistics, Vol. I" - Charles Griffin, 1958.

NOTES ON THE MONTE CARLO METHOD

A. Werbrouck,
Istituto Nazionale di Fisica Nucleare
Sezione di Torino

I. INTRODUCTION

Many processes, real physical processes or imaginary ones, can be idealized as a sequence of choices. If it is possible to approximate each choice by some probability function, then one can establish a model which simulates the process. The most common such model is Monte Carlo. Many real processes of nature can be approximated in this way.

Some examples are:

1) The decay in time of an unstable particle.
2) The laboratory emission of some particle from a bombarded target.
3) The multiple scattering of a fast charged particle.
4) An entire experiment as visible in a finite volume.

To study any of the above processes in nature, one observes and counts many examples or events of the given type. As is well known the results are subject to statistical errors.

The Monte Carlo method functions in the same way. One generates many "events" (pseudo-events or fictitious events) according to the simulating model. Each event is the result of a particular sequence of choices. These events are then counted, classified and distributed according to criteria as if they were real events. One can then make comparisons with existing real data, or predictions of what should be the outcome of a given real experiment, provided that the established model simulates nature sufficiently well. For comparison with any real data one must always consider the statistical error in both the real events and the pseudo Monte Carlo events. For that reason one usually wants more pseudo events than the number of available real events. Since most Monte Carlo models can be

written into a computer programme where the number of pseudo-events is limited only by the computer time available, one usually chooses this method of calculation. In general one makes various approximations in the model for sake of simplicity and because we often do not have complete knowledge of a natural process. Thus the reduction of similarity to nature is compensated by a greater number of generated events (since each generation requires less time) and smaller statistical error. These two compensating factors moderated by the computer size and availability (or the perseverance of the human calculator) will affect strongly actual Monte Carlo calculations.

While the basic ideas of the Monte Carlo description are valid for either hand or machine calculations, much of the following discussion will be presented from the machine point of view.

Many times it is useful to envisage the Monte Carlo method as the evaluation of an integral I:

$$I = \int_{u_1}^{u_2} P(u)\,du \int_{v_1(u)}^{v_2(u)} P(u,v)\,dv \;\ldots\ldots \int_{z_1(u,v..)}^{z_2(u,v..)} P(u,v,\ldots z)\, f(u,v,\ldots z)\,dz \;.$$

I could in example four be the average efficiency to detect a $K \to e$ decay of a stopped K^+ in a heavy liquid bubble chamber, where the electron is detected when it suffers a large fractional energy loss due to bremsstrahlung ($\Delta E/E \leq 1$). This average efficiency is the result of integrating the efficiency $f(u,v,\ldots z)$ for detecting the electron over the variables on which it depends, where each variable in turn has a probability distribution, $P(v)$. In this application the variables may be:

1) The x,y,z coordinates of the K decay point given by a distribution function $\rho(x,y,z)$ determined by observing and measuring a type of event with probability of detection = 1 (τ decay).

2) The electron initial laboratory momentum q, given by the c.m. electron spectrum $w(q)$, because in this simple case the K^+ decays at rest.

3) The electron initial direction in azimuth Φ and polar Θ taken from appropriate distribution functions, $P(\Phi)$ and $P(\Theta)$, (isotropic for decay at rest), with respect to a convenient coordinate system.

4) The x,y,z limits of the fiducial volume of the chamber, beyond which the electron may pass without revealing its identity. These limits enter as boundary conditions.

5) The magnetic field H(x,y,z).

The probability of escape without detection might be approximated as $\propto e^{-L/\lambda}$ where L is the potential path length within the fiducial volume calculated for a selected decay point, emission direction and momentum q in the magnetic field H, and λ is the mean free path for detecting an electron of momentum q. If λ varies too rapidly as the electron loses momentum, it might be necessary to evaluate λ and the probability of detection for successive segments of the potential path.

Such an integration could be very difficult analytically. By the Monte Carlo method it is quite easy. One simply generates events (called trials) at the decay points (selected either from those measured or from a smoothed function derived from the measured points) where the electron momentum and direction are determined as we shall illustrate below. Each electron is followed to see if it is detected or escapes. If it is detected (called success) it may be useful to classify it in the same way as the observed real events for later comparison. The efficiency then becomes the number of detected events divided by the number of generated ones (or the number of successes divided by the number of trials). If desired the efficiency can be calculated in different zones of the chamber or as a function of the initial electron momentum, by classifying appropriately the trials and successes.

In general one can consider the method as a purely statistical generator of fictitious events or as a multifold integration. In the above example many events are generated and treated as if real events in a purely statistical way. However, one can consider equally well the events as contributions to the final integral, properly weighted by the probability distributions of the relevant variables and the imposed boundary conditions.

In the analytic evaluation of I, one passes from right to left. In the Monte Carlo evaluation one passes from left to right. The first choice is the value of u, which is necessary to know the distribution function P(u,v) from which one selects v, and so on. Obviously one must pass this sequence of choices many times to approximate the analytic value of the integral. In the above example the variables were listed in a suitable order for choosing.

II. CHOICES

The type of choice of a variable in Monte Carlo is a random choice according to the chosen probability function for that variable. Although the probability function may be modified or parameterized by previous choices, the value of the variable must not be predictable a priori. To satisfy this characteristic the probability interval is compared with a uniform random number distribution.

$$P(v)\, dv = K(n)\, dn \qquad (1)$$

That is, the probability that the variable has a value between v and v+ dv is set proportional to the probability that the random number RN has a value between n and n+ dn.

Eq. (1) is the fundamental formula of the Monte Carlo method. Since we choose a uniform RN distribution, K(n) is simply a constant of normalization. A mathematical proof of Eq. (1) is given in Appendix I.

It is convenient to consider the following three types of probability distributions as determined from their relations with the random number distribution.

A) The probability distribution is continuous and conveniently integrated analytically.

B) The probability distribution is continuous and not conveniently integrated analytically.

C) The probability distribution is discrete.

We now present many examples according to the above classification, all of which are based on Eq. (1). We assume that the random number generator gives us a distribution uniform between 0 and 1. Most of these examples are useful in various Monte Carlo models for nuclear physics.

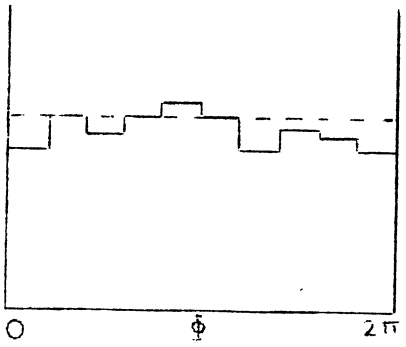
Type A

1. Isotropic azimuthal angle

$$P(\Phi)\, d\Phi \propto d\Phi = K\, dn\,, \quad \int_0^{\Phi} d\Phi = K \int_0^{n} dn\,, \quad \Phi = Kn$$

at $\Phi = 0,\ n = 0$; at $\Phi = 2\pi,\ n = 1$ $\therefore$ $\Phi = 2\pi(RN)$.

This means that if a series of RN from a distribution are transformed in this way, the differential distribution is reproduced, or the histogram in Φ is consistent with a flat distribution.

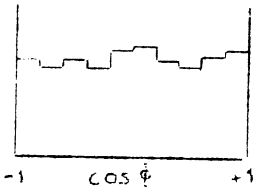


2. Isotropic polar angle Θ

$$P(\Theta)\, d\Theta \propto d(\cos\Theta) = K\, dn\,, \quad \int_{-1}^{\cos\Theta} d(\cos\Theta) = K \int_0^{n} dn\,, \quad \cos\Theta + 1 = Kn$$

at $\cos\Theta = -1,\ n = 0$; at $\cos\Theta = +1,\ n = 1$ $\therefore$ $\cos\Theta = 2(RN) - 1$.

If one transforms a series of RN in this way, one finds a histogram in $\cos\Theta$ consistent with uniform.

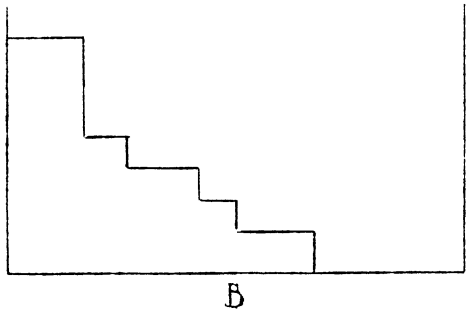


3. Exponential decay or absorption (distance B and λ mean free path chosen for example).

$$P(B)\,dB = e^{-B/\lambda}\,\frac{dB}{\lambda} = Kn\,, \quad \int_0^B e^{-B/\lambda}\,\frac{dB}{\lambda} = K\int_0^n dn\,, \quad -e^{B/\lambda} + 1 = Kn$$

at $B = 0\,,\ n = 0\ ;\quad B = \infty,\ n = 1 \quad \therefore\ e^{-B/\lambda} = 1 - n\,.$

Of course, if n is a RN, so is 1-n and we write $B = -\lambda \ln(RN)$. If one transforms a series of RN in this way, one finds a histogram in B that is consistent with an exponential decay.

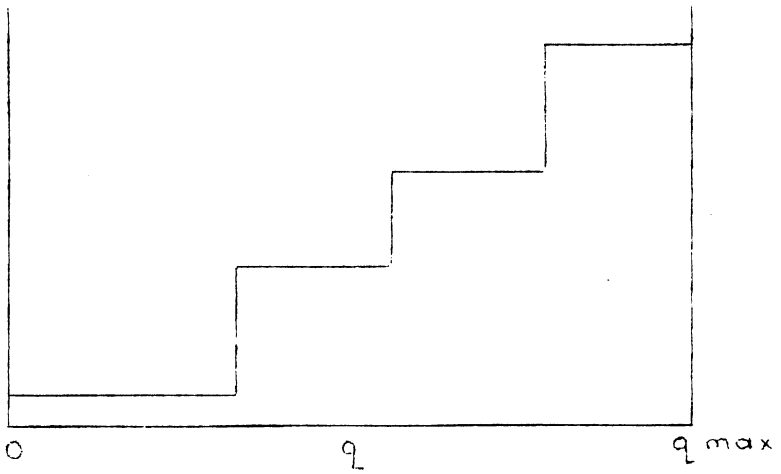


4. Fermi gas model of nucleon momentum q in the nucleus (cf. Rossi, High-Energy Particles, p. 357).

$$P(q)\,dq \propto q^2 dq = K\,dn\,, \quad \int_0^q q^2 dq = K\int_0^n dn\,, \quad \frac{q^3}{3} = Kn$$

at $q = 0,\ n = 0\ ;\quad q = q_{max},\ n = 1 \quad \therefore\ q = q_{max}\,(RN)^{1/3}\,.$

Here the histogram would have the form



5. Impact parameter b for uniform flux incident normally on scattering centre.

$$P(b)\,db \propto d(\text{Area}) \propto bdb = Kdn, \quad \int_0^b bdb = K\int_0^n dn, \quad \frac{b^2}{2} = Kn$$

at $b = 0,\ n = 0$; at $b = b_{max},\ n = 1$ $\therefore$ $b = b_{max}\,(RN)^{1/2}$.

If one transforms a series of RN, one to give b_n, the next to give Φ_n, and so on, one would soon have a uniformly populated scatter diagram in polar coordinates, bounded by a circle of radius b_{max}.

One sees that all these relations between a random number and the variable that must be chosen in the Monte Carlo model, follow very simply from Eq. (1). For the electron detection, example above, one uses the relations 1, 2 and 3 of Type A to know the electron's emission direction (Θ and Φ) and the distance R at which the electron is detected. If $R \geq L$, the electron is not detected. If $R \leq L$, the electron is detected within the fiducial volume.

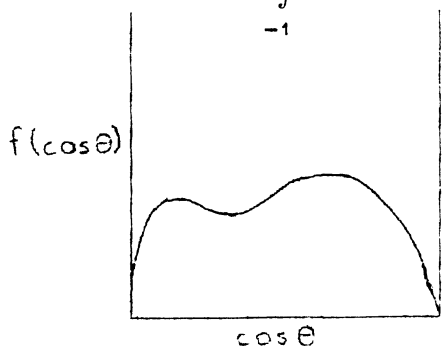
Type B

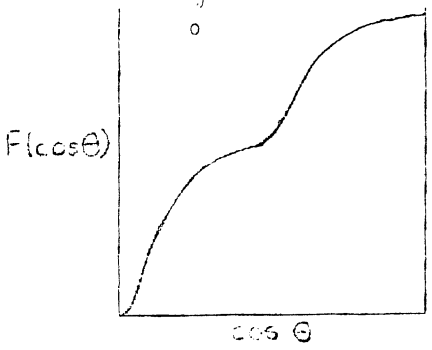
Among Type B relations, one finds a large fraction of the continuous variables in a physical process; cross-sections, angular distributions, centre-of-mass spectra for production of, or decay into, three or more bodies. Again Eq. (1) provides the basic relation. Let us take, for example, an emperical angular distribution

$$\frac{1}{\sigma_{total}}\frac{d\sigma}{d\Omega} = f(\cos\Theta) \quad \text{(azimuthal symmetry)},$$

which is not conveniently integrated analytically.

$$\int_{-1}^{\cos\Theta} f(\cos\Theta)\,d(\cos\Theta) = K\int_0^n dn = F(\cos\Theta)$$





index	$\cos\Theta_n$ value
0	-1
1	.
.	.
.	.
.	.
N	+1

One simply integrates the left integral numerically and normalizes $F(\cos\Theta)$ so that $F(1) = 1$. Then one constructs a Table of $\cos\Theta_n$ with index n ($n = 0,1,2,\ldots N$) where $F(\cos\Theta_n) = n/N$. The Table will have N+1 entries. One must choose N sufficiently large that straight segments between the $F(\cos\Theta_n)$ follow well the curve $F(\cos\Theta)$. To find the corresponding value of $\cos\Theta$, one multiplies the random number by N and separates the resulting integral part α from the fractional part β at the decimal point.

α = integral part of (N times RN)
β = fractional part of (N times RN)

The number α is integer and can serve as an index to the Table, while β is a fraction less than 1. Thus,

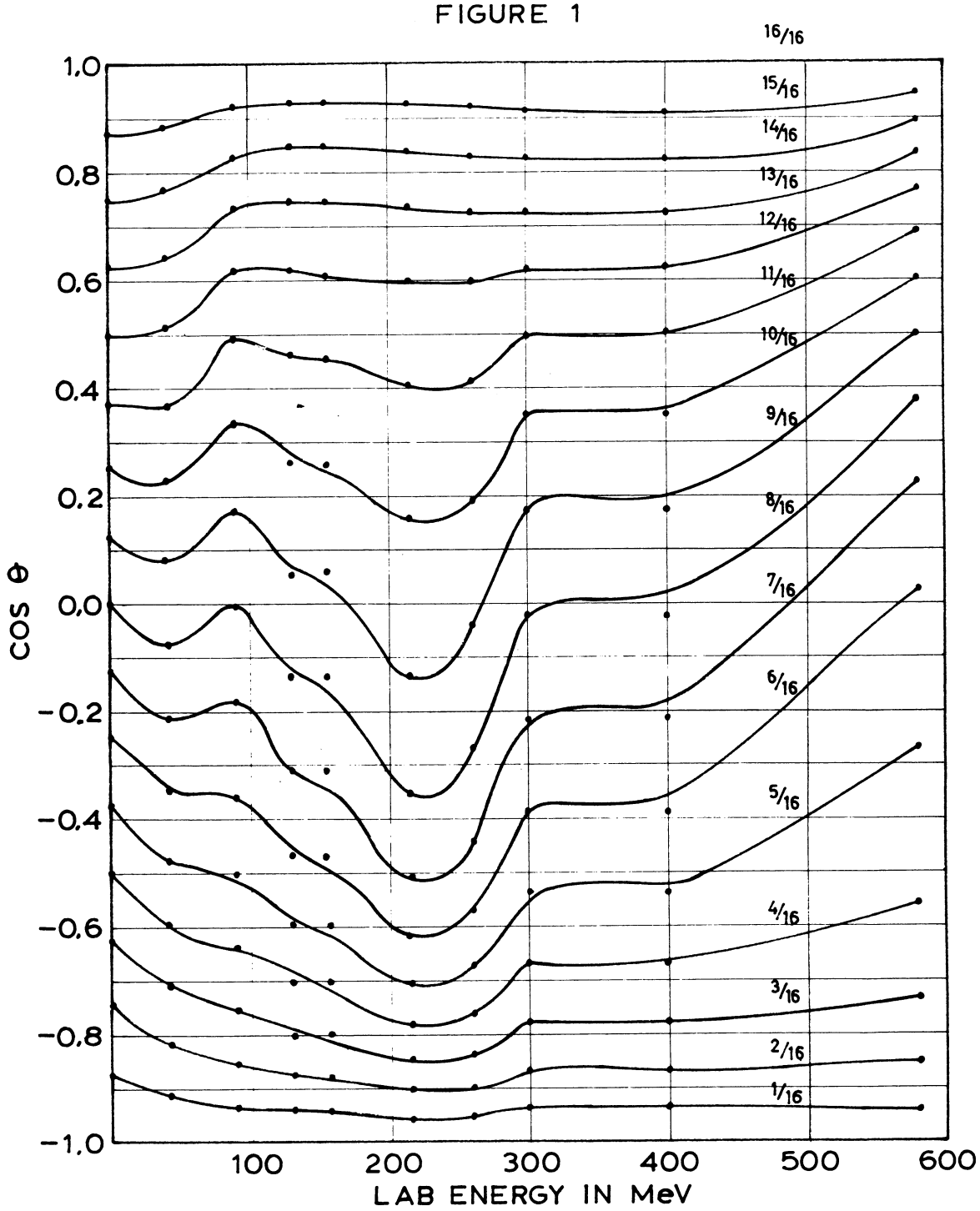
$$\cos\Theta\,(RN) = \cos\Theta_\alpha + \beta\,[\cos\Theta_{\alpha+1} - \cos\Theta_\alpha]\ . \qquad (2)$$

Obviously this is simply an application of linear interpolation almost written in the programming language FORTRAN. If the angular distribution is a function of energy E, one could enter the cosine Table, once each for E_1 and E_2 where $E_1 \leq E \leq E_2$. For the same random numbers, one would then by Eq. (2) have two values for $\cos\Theta$. The final $\cos\Theta$ would be given by

$$\cos\Theta = \cos\Theta_1 + \frac{(E - E_1)}{(E_2 - E_1)}\,(\cos\Theta_2 - \cos\Theta_1)\ ,$$

a simple extension of linear interpolation. Here we see a situation where a probability distribution (that for $\cos\Theta$) is affected by a previous choice or calculation (that of the energy). In Fig. 1, is shown a convenient representation of an angular distribution as a function of energy, from which it is easy to construct the $\cos\Theta$ Tables for several energies. The points result from integrating experimental $f(\cos\Theta)$. The curves are the variation with energy and angle of $F(\cos\Theta) = n/N$, with n remaining constant, i.e., constant probability lines. Here N = 16 since the figure was prepared to represent n-p scattering in a large binary computer. From such a representation one can easily see at which E values the Tables should be prepared in order that linear interpolation be sufficiently accurate.

FIGURE 1



CURVES OF CONSTANT INTEGRAL PROBABILITY IN THE CM N-P ELASTIC SCATTERING ANGLE AS A FUNCTION OF NEUTRON OR PROTON LAB ENERGY

The cos Θ entries for a given energy are simply read at the intersection of the successive $F(\cos\Theta) = n/N$ lines and the vertical constant energy line. For example, suppose that we are constructing in a Monte Carlo model a proton-neutron collision that corresponds to a proton laboratory energy of 500 MeV on a stationary neutron. From Fig. 1, Tables of cos Θ_n are in the computer for 400 and 580 MeV. The RN selected is 0.57, slightly greater than $9/16$. Application of the above formulae for $E_1 = 400$ MeV and $E_2 = 580$ MeV, would result in a cos $\Theta \sim +0.35$.

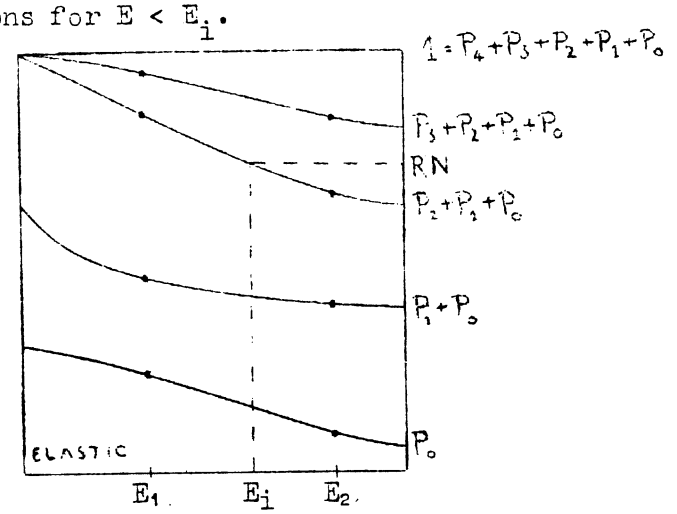
Type C

Whenever the variable to be chosen in the Monte Carlo model is discrete, the application of Eq. (1) is somewhat analogous to that in Type B. Examples are the number of particles produced in a collision, or the decay mode when more than one is possible. The random number is still continuously distributed, so the N discrete choices, each with relative probability $P_m(m=1,\ldots N)$ are to be compared with partial integrals on the RN distribution. Since the random number must fall between 0 and 1,

$$P_1 + P_2 + \ldots P_N = \int_0^{P_1} dn + \int_{P_1}^{P_1+P_2} dn + \ldots \int_{1-P_N}^{1} dn = 1 = (P_1 - 0) + (P_1 + P_2 - P_1) + \ldots$$

In other words, if a RN is found between 0 and P_1, the variable has its first value, between P_1 and $P_1 + P_2$, the second value, and so on. Of course, the list of values may depend upon previous choices or calculations, such as the multiplicity of pion production as a function of c.m. energy. In this case a new Table of P_m must be established by interpolating in the continuous energy variable E between E_1 and E_2 ($E_1 \leq E \leq E_2$) before comparing with the random number since one cannot interpolate a discrete variable. To illustrate this procedure, consider this representation of the relative probability of various pion multiplicities in a nucleon-nucleon collision as a function of c.m. energy. The points represent values of probability put into a Table for $E = E_1$ and $E = E_2$. By interpolation between these points one establishes a new Table of relative probabilities for the energy E, $E_1 \leq E \leq E_2$. Comparison with RN then gives the pion multiplicity.

In the illustration the shown RN would lead to production of three pions for $E > E_i$ and two pions for $E < E_i$.



The normal distribution is often useful in Monte Carlo models. By the direct application of Eq. (1), we see that it is conveniently classified in Type B.

$$\int_{-\infty}^{x} e^{-x^2/2}\, dx = K \int_{0}^{n} dn$$

at $x = -\infty$, $n = 0$; at $x = +\infty$, $n = 1$ $\therefore$ $K = \sqrt{2\pi}$.

Since the function is symmetric, one can double the precision of a given length (N+ 1) Table, by inserting only positive values, letting α and β be the integral and fractional part of $2N|\frac{1}{2} - RN|$, and then setting v negative for $RN < \frac{1}{2}$ and positive for $RN \geq \frac{1}{2}$. Here $||$ means absolute value and

$$v = v_\alpha + \beta[v_{\alpha+1} - v_\alpha] .$$

One can also treat the normal distribution as Type A One method uses the properties of the RN distribution itself which has mean $\frac{1}{2}$ and variance

$$\int_{0}^{1} (n - \tfrac{1}{2})^2\, dn = \tfrac{1}{12} .$$

By the central limit theorem the deviation of the mean of N random numbers is

$$\sigma_m^2 = \frac{1}{12N} \quad \text{or} \quad \sigma_m = \frac{1}{\sqrt{12N}} .$$

Thus the variable

$$v = \sigma^{-1} \left(\sum_{i=1}^{N} \frac{n_i}{N} - \frac{1}{2} \right) = \left(\sum_{i=1}^{N} \frac{n_i}{N} - \frac{1}{2} \right) \sqrt{12N}$$

has an average zero and standard deviation one, i.e., the normal distribution. A reasonable N is 12 for which

$$v = 6 - \sum_{i=1}^{12} RN .$$

Another method is based on applying Eq. (1) twice in a Type A relation.

$$\int_{-\infty}^{x} e^{-x^2/2}\, dx \int_{-\infty}^{y} e^{-y^2/2}\, dy = \int_{0}^{r} e^{-r^2/2}\, r dr \int_{0}^{\Phi} d\Phi = K_1 \int_{0}^{n_1} dn\; K_2 \int_{0}^{n_2} dn_2$$

where

$$x^2 + y^2 = r^2 \text{ and } \Phi = \tan\, y/x \; ; \quad -e^{-r^2/2} + 1 = n_2 \text{ or } e^{-r^2/2} = n_1$$

by the same observation on n and 1 - n as made in Type A3. By A1,

$$\Phi = 2\pi n_2 \quad \text{so that} \quad v = (-2\ell n RN_1)^{1/2} \cos 2\pi RN_2 .$$

Since we assigned the two RN quite arbitrarily, there is another value of v available by interchanging

$$v = (-2\ell n RN_2)^{1/2} \sin 2\pi RN_1 .$$

While the last method is preferred for a large computer, all are given, as each illustrates a different application of Eq. (1).

It is stated above that the value of the variable, within its established limits, must not be predictable a priori. In practice it is very difficult to obtain a true random number generator that is free of bias. A binary counter of pulses due to electron emission fluctuations from a hot cathode has been suggested. This counter would have to receive many impulses between interrogations. Usually one investigates Monte Carlo models on a digital computer. Thus it would be necessary to connect the counter to the computer to make available the RN. Even if connected without bias, this arrangement would have a disadvantage because the sequence of RN would not be reproducible for possible programme checking. On the other hand, a reproducible generator does not satisfy perfectly the non-predictability criterion. However, if the choice B which follows a given choice A, reproduces the B probability distribution within statistical fluctuations in the course of the entire calculation, the process has been simulated. Thus one can use a reproducible RN generator if the sequence is not correlated, i.e., if the distribution of numbers which follow, for example, a 6 is uniform, or the distribution of the third number after a 2 is uniform. In general, the distribution of the nth number after any given number N should be uniform within statistical fluctuations at any point in the calculation. Another important requirement is that the sequence of RN does not repeat itself during the calculation. If such a repetition should occur, the same number might be used to begin a new sequence, and the whole calculation would be simply repeated without improving the Monte Carlo statistics. In Appendix II, we give an example of a simple RN generator routine, along with reference to more advanced versions, based on the power residues development of number theory.

In all the above discussion we have applied a random selection from each probability distribution. This characterizes the Monte Carlo method. In some instances it is more practical to use a uniform sampling of the probability distribution, i.e., values of the variables corresponding to equal probability intervals.

The practical basis of such a choice is often that of increasing markedly the number of generated events with the same calculational effort. For example, suppose that after a sequence of choices, one has generated a

π^0 with definite direction and momentum in a finite bubble chamber. To generate rapidly the various decay configurations one could let this π^0 decay at i equal cosine c.m. intervals and j azimuthal angle intervals where the former intervals are 2/i wide and the latter $2\pi/j$ wide.

In these cases where these variables are cycled many times it is advisable to determine the starting value of the variable at random to avoid correlations between cycles.

III. ERROR

In general some classifying of pseudo-events is effected to arrive at the final Monte Carlo results. In the first example, every generated $K \rightarrow e$ decay was finally classified as detected or not detected in order to arrive at the efficiency. Consider a sample of N events of which r are in, and s out of, a certain class. Let t be the probability of an event being in the class. Then the likelihood function for the result is

$$L = t^r(1-t)^s \quad \text{or} \quad w = \ln L = r \ln t + s \ln(1-t)$$

setting $dw/dr = 0$, we find, quite expectedly, $t = r/N$.

The error in t is

$$\sigma_t = \left[- \frac{\partial^2 w}{\partial t^2} \right]^{-1} = \sqrt{\frac{t(1-t)}{N}} .$$

Whenever $t << 1$, the error becomes

$$\sqrt{\frac{t}{N}} \quad \text{or} \quad \sigma_t = \frac{\sigma_r}{N}$$

where $\sigma_r = \sqrt{r}$.

IV. NUCLEAR CASCADE

In this section we outline the nuclear cascade problem as solved by Monte Carlo techniques, and give a skeletal FORTRAN programme which illustrates this solution. The object is to simulate the processes

following the collision of a single fast particle with a complex nucleus. The name cascade is used because many more interactions in the same nucleus are expected to follow the initial collision. In this case, an integral I as written in the introduction, is not simply defined because a single particle may interact a variable number of times.

Such an approach to the collision with a complex nucleus ($Z >> 1$) of a simple particle (pion, proton, kaon) becomes reasonable when the de Broglie wave length of the incident particle is of the order of, or less than, the nuclear force range (1 fermi corresponds to 197 MeV/c) and its kinetic energy is considerably greater than the relevant real potentials. With these conditions, the incident particle can be considered a projectile which comes upon a collection of nucleons, and interacts with only one at a time, although it may interact several times before leaving the nucleus or being absorbed.

The nuclear model assumed here is the Fermi gas model. Here the nucleons are confined in a sphere of radius $R_0 = r_0 A^{1/3}$ and have the isotropic momentum distribution described as example A4 with

$$q_{max} = \left(\frac{A}{4}\right)^{1/3} \left(\frac{3}{4\pi}\right)^{2/3} \frac{h}{R_0} \frac{300}{r_0} \text{ fermi MeV/c}$$

(h is Planck's constant). The nuclear density is constant within the radius R and zero beyond. The mean free path in such nuclear matter becomes from $\lambda\bar{\sigma}p = 1$

$$\lambda = \frac{4\pi A r_0^3}{3[Z\sigma_p + (A - Z)\sigma_n]}$$

where $\sigma_p(\sigma_n)$ is the total interaction cross-section with a proton (neutron). To obtain a statistically significant result, one must "follow" many incident particles, and also the collision products until they leave the nucleus, are captured by the nuclear potential or have an energy so low to be no longer of interest. Every escaping particle must be counted and classified according to criteria, in such a way that meaningful predictions or comparisons are possible.

Here we present a sequence of choices in an order that can be used to simulate the nuclear cascade process.

1. Select an energy or momentum of the incident particle. The variable could be a constant, selected from a non-simple spectrum by the Type B relation, or selected from a Gaussian beam spread centred at E_o with half-width ΔE. For the second method, one RN is necessary. For the third, two must be available if one uses the third method of reproducing the normal distribution. In the latter case

$$E = E_o + \frac{\Delta E}{\sqrt{2 \ell n Z}} v$$

where v is the normal variable and

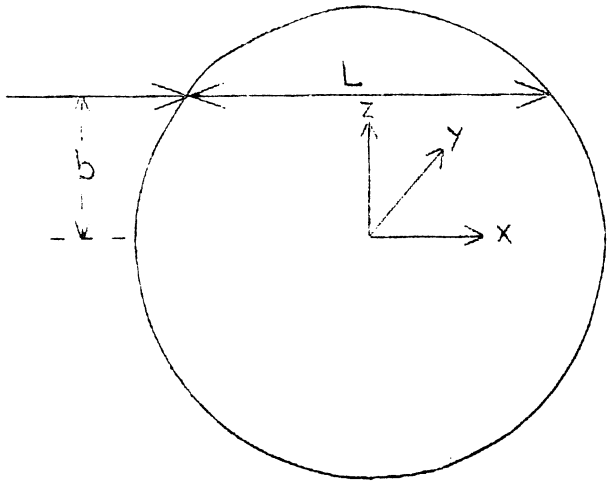
$$\frac{1}{\sqrt{2 \ell n Z}}$$

is the ratio of standard deviation to half width.

2. With the next RN, select the impact parameter b by the method A5 where b_{max} equals the nuclear radius. At this point we are beginning geometry, so a coordinate system is necessary. Let the incident direction be x in a cartesian system centred at the initial centre of the nucleus and fixed in the laboratory (Fig. 2). Since there is azimuthal symmetry about the incident direction the point of incidence is considered to be in the x-z plane. Thus the point of incidence is

$$z = b, x = \sqrt{b_{max}^2 - z^2}, y = 0 .$$

3. With the next RN, find the interaction distance B by method A3 using the above defined mean free path. If B is greater than the potential path L in nuclear matter for the chosen incident point, the incident particle did not interact and one returns to 1 to select the next incident particle. If this distance is less than the potential path, an interaction occurred and must be followed.



4. Choose the nature of the struck particle, proton or neutron, by a Type C choice. If the next RN is less than $Z\,\sigma_p/(Z\sigma_p + (A-Z)\sigma_n)$, the interaction is on a proton; if greater on a neutron.

5. Choose the struck nucleon momentum with the next RN by method A4 $q = q_{max}\,(RN)^{1/3}$

6. Choose the direction of the struck nucleon with respect to the incident particle. To remain consistent with Fig. 2, the polar angle between the incident particle (called 1) and the struck nucleon (called 2) is $\cos^{-1}\mu$. Since the distribution of nucleon momenta is isotropic, $\mu = 1 - 2$ (RN) by A2. With the next RN, the azimuthal angle Φ is chosen by A1, $\Phi = 2\pi$ (RN). The complete kinematic treatment of an arbitrary collision between 1 and 2, leading to the emission of the collision products is given in Appendix II. Here we select the variables necessary to reconstruct the collision.

7. Choose the nature of the collision (elastic or inelastic) by Type C with the next RN. If elastic, choose the scattering angle Θ in the c.m. (in general by Type B). If inelastic, choose the particles, their c.m. momenta, and their directions with respect to a plane containing the c.m. initial momentum direction of 1 and 2 as x axis and the c.m. laboratory momentum direction (separated by the angle δ in Fig. 2). If no more than three particles are emitted, all must lie in this plane.

8. Choose the azimuthal angle of rotation of the above plane about the c.m. initial momentum direction of 1 and 2. This angle is α in Fig. 2 and by A1, $\alpha = 2\pi$ (RN).

9. At this point one is ready to transform the collisions products back to the laboratory system by the transformations described in Appendix III. In practice one first transforms the energies of the nucleons to see if the collision is allowed by the Pauli exclusion principle, i.e. if the nucleon final state is not already occupied. In this simple model, the

laboratory kinetic energy of the emitted nucleon would have to be more than $p_{max}^2/2M$ in order that the collision be allowed. If the collision is not possible, the incident particle with the same momentum and direction is followed onward from the point with a new choice 3, etc. If the collision is allowed, one of the particles is followed in its new direction with resultant momentum and a new choice 3, etc. The other particle may be stored to be followed later if its energy is still interesting. When all the interesting particles have been followed, one starts with another incident at step 1.

Many modifications and refinements are of course possible. Here we list a few which are desirable for certain problems.

If the energies of interest are not always large compared to the real potentials, potential corrections should be applied at entry and exit. If directions are very important, diffraction effects at the change of potential should perhaps be included. The nuclear density here was constant. For the lighter nuclei, the outer volume, in which the nuclear density is much lower than at the nuclear centre, is a large fraction of the total volume. In order to improve such nuclei, one can use a suitable density as a function of radius. In this case the mean free path is no longer a constant but must be calculated for each trajectory. A simple way to include considerations of this type is the differential sampling approach. One compares a random number with the probability to interact with the nuclear matter in the next unit of distance (~ internucleon spacing). In this way the nuclear density, and the variation of the cross-sections due to charge and relative velocity and energy of the immediately ahead nuclear matter, can all enter into the probability of interaction which becomes

$$\frac{\Delta}{\lambda} \rightarrow \frac{\sigma(\beta_r)\ \beta_r \bar{\rho} \Delta}{\beta_i} \qquad \text{where}$$

$\sigma(\beta_r)$ is the cross-section for interacting with the immediately ahead nucleon (target) chosen at random in direction and momentum from the nuclear model

β_r is the relative velocity of the projectile and target

β_i is the velocity of the projectile in the laboratory where the nuclear centre was initially at rest

Δ is the finite differential element ($\sim$ 1 fermi)

$\bar{\rho}$ is the average nuclear density in the next differential element.

In this way the nuclear matter traversed by the projectile is sampled as near the random way as possible.

REFERENCES

1) "Symposium on Monte-Carlo Methods", edited by H. Meyer - Wiley, 1954.

2) E. Cashwell and C. Everett, "A practical manual on the Monte Carlo Method for random walk problems" - Pergamon Press, 1959.

3) "The Monte-Carlo Method", W.F. Baner, Industrial and Applied Mathematics, Vol. 6, No. 4, December 1958.

```
NUCLEAR CASCADE PROBLEM IN SKELETAL FORTRAN FORM WRITTEN FOR
        NUCLEUS OF MASS A,CHARGE Z,RADIUS=RZERO*CUBRT(A)
        INCIDENT PION GAUSSIAN SPECTRUM OF ENERGY EZERO AND STD DEVIATION ENORM

STATEMENT NUMBERS REFER TO PARAGRAPH NUMBERS IN SECTION IV OF TEXT
OTHER NECESSARY STATEMENT NUMBERS HAVE BEEN REPLACED BY MNEMONIC LABELS

RANDOM NUMBER GENERATOR RDM IS REFERENCED IN APPENDIX II
EACH TIME RN=RDM(X) APPEARS,A NEW RANDOM NUMBER IS GENERATED

        INITIATE
READ ADJUSTABLE CONSTANTS
        A,Z,RZERO,EZERO,ENORM,MASS AND NUMBER OF INCIDENT PARTICLES,
        TOTAL INTERACTION CROSS SECTIONS,
        ANGULAR DISTRIBUTIONS FOR POSSIBLE INTERACTIONS

PREPARE SECONDARY CONSTANTS
        RADIUS=R=RZERO*CUBRT (A)
        MAX FERMI MOMENTUM=QMAX=300/RZERO

START   IF ENOUGH INCIDENT PARTICLES FOLLOWED,GO TO FINISH
        IF NOT,SELECT INCIDENT ENERGY

    1   RN1=RDM(X)
        RN2=RDM(X)
        V=SQRTF(-2.*LOGF(RN1))*COSF(6.28*RN2)
        EN=EZERO+ENORM*V

SELECT IMPACT PARAMETER BY METHOD A5
        RN=RDM(X)
    2   Z=R*SQRTF(RN)
        X=-SQRTF(R*R-Z*Z)
        Y=0
SET INITIAL DIRECTION COSINES
        DIRX=1.0
        DIRY=0
        DIRZ=0
        IPART=IPART+1

FOLLOW INTERESTING PARTICLES,IF ANY
        IF NOT,GO TO 1

CALCULATE AVERAGE CROSS SECTION
        SIGAV=(Z*SIGP(EN)+(A-Z)*SIGN(EN))/A

CALCULATE MEAN FREE PATH
        LAMBDA=(1.33*3.14*R**3)/SIGAV

CALCULATE DISTANCE B TO NEXT INTERACTION BY METHOD A3
        RN=RDM(X)
    3   B=-LAMBDA*LOGF(RN)

CALCULATE INTERACTION POINT
        XINT=X+DIRX*B
        YINT=Y+DIRY*B
        ZINT=Z+DIRZ*B

CHECK IF INTERACTION POINT IS IN THE NUCLEUS
        TEMP=XINT**2+YINT**2+ZINT**2
        GO TO RECORD IF TEMP IS GREATER THAN OR EQUAL TO R**2
        OTHERWISE,FIND THE RESULTS OF THIS INTERACTION

CHOOSE THE NATURE OF THE TARGET
    4   RN=RDM(X)
        PROFR=FRACTION OF INTERACTIONS ON A PROTON
        PROFR=Z*SIGP(EN)/(A*SIGAV)

 IF RN IS LESS THAN PROFR,TARGET IS PROTON
 OTHERWISE,TARGET IS NEUTRON

CHOOSE TARGET MOMENTUM
    5   RN=RDM(X)
        Q=QMAX*CUBRT(RN)

CHOOSE DIRECTION OF TARGET WITH RESPECT TO INCIDENT PARTICLE
    6   RN=RDM(X)
        MU=1.-2.*RN
        RN=RDM(X)
        PHI=6.28*RN

CALCULATE TOTAL CM ENERGY=ETOT

FIND FRACTION OF INTERACTIONS ELASTIC AT THIS ENERGY=ELFR(ETOT)
        RN=RDM(X)
    7   IF RN IS LESS THAN ELFR(ETOT),GO TO ELASTIC
        OTHERWISE,INELASTIC

ELASTIC CHOOSE CM SCATTERING ANGLE
        GO TO 8

INELASTIC CHOOSE FINAL STATE PARTICLES,CM EMISSION ANGLES AND MOMENTA
        GO TO 8

CHOOSE AZIMUTHAL ANGLE OF ROTATION OF CM PRODUCTION PLANE
    8   RN=RDM(X)
        ALPHA=6.28*RN

TRANSFORM TO LAB THE COLLISION PRODUCTS WITH THE SUBROUTINE LORENT,WHICH APPLIES
THE LORENTZ TRANSFORMATIONS DESCRIBED IN APPENDIX III
    9   CALL LORENT

STORE INTERESTING PRODUCTS FOR FURTHER FOLLOWING
ADD LOW ENERGY NON ESCAPING PRODUCTS TO EXCITATION ENERGY
        GO TO FOLLOW

RECORD AND CLASSIFY ESCAPING PARTICLE
        GO TO FOLLOW

FINISH  WRITE RESULTS OF THIS MONTE CARLO CALCULATION
        END
```

APPENDIX I

THE BASIC EQUATIONS FOR THE MONTE CARLO METHOD

Contributed by D. Hudson,
Data and Documents Division, CERN

It is assumed that we have available a source variable R which generates random numbers $\{r\}$ which are uniformly distributed over the unit interval,

$$\text{i.e.} \qquad \Pr[R \leq r] = r \quad , \qquad 0 \leq r \leq 1 \, . \tag{1}$$

Appendix II deals with a method for generating random numbers on a computer.

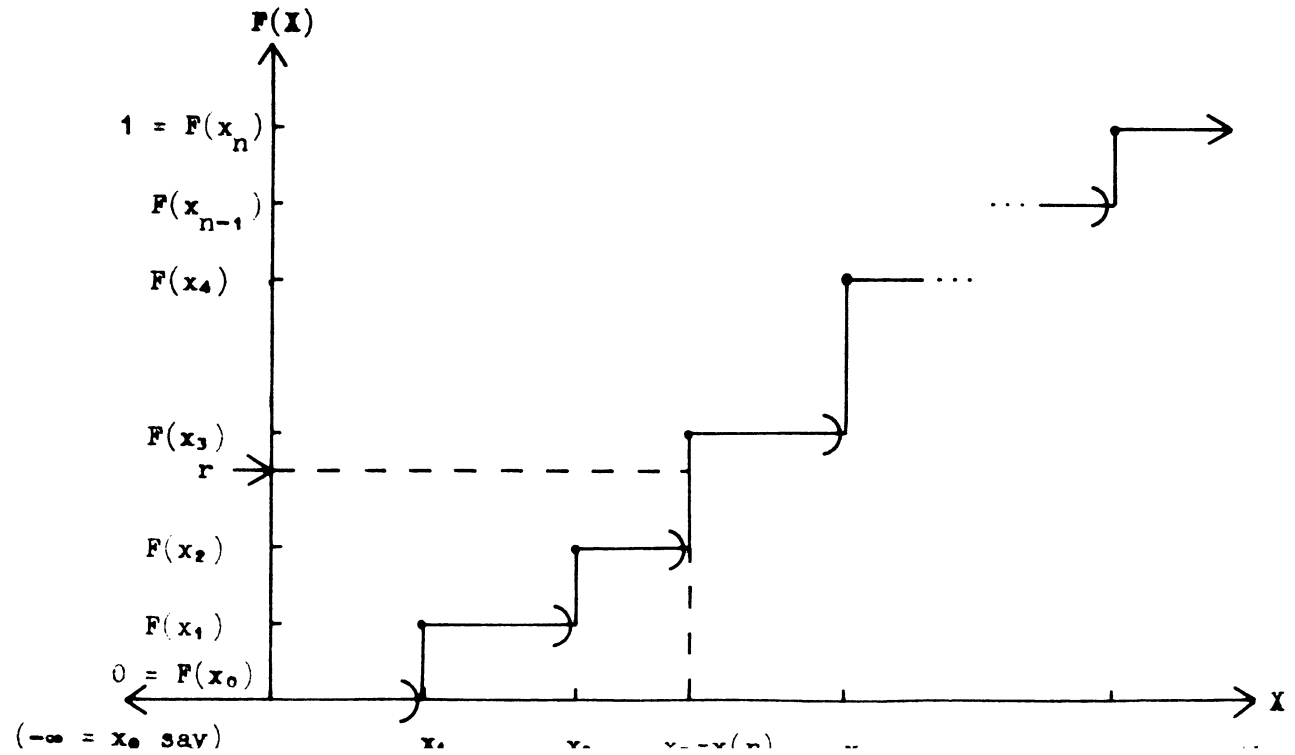
We require to generate values $\{x\}$ of a random variable X with given cumulative distribution $F(x)$,

$$\text{i.e.} \qquad \Pr[X \leq x] = F(x) \quad , \qquad 0 \leq F \leq 1 \, . \tag{2}$$

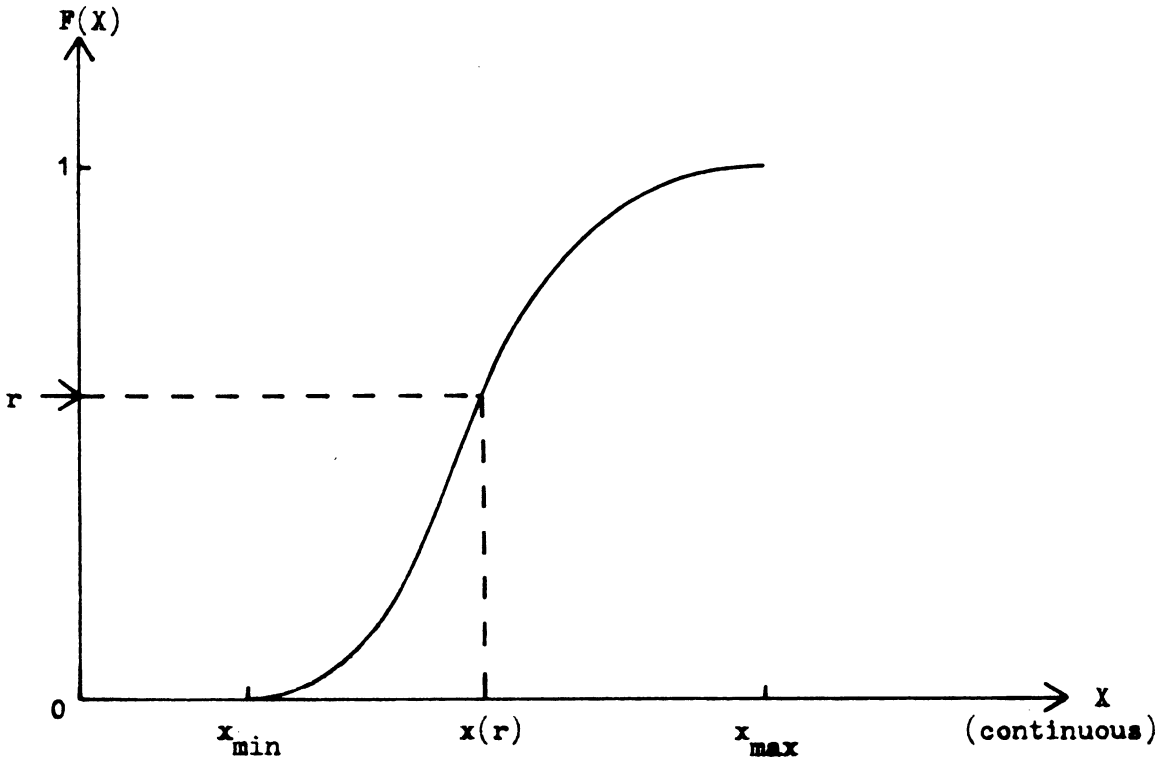
In the case of a discrete variable X taking only the values

$$x_1, x_2, \ldots, x_n \, ,$$

the function $F(X)$ looks like



In the case of a continuous variable X taking all values in a given interval (which may be infinite), the function F(X) looks like*



*) For simplicity, we ignore values of X for which F(X) remains constant, since these values of X are 'impossible'. With this convention, F(X) is only defined at points where F(X) is strictly increasing.

We require a transformation from R to X such that X has the distribution (2).

Theorem Suppose we have a specific value r from the distribution (1).

(i) When X has a discrete distribution, find x_i such that

$$F(x_{i-1}) < r \leq F(x_i) \tag{3}$$

and put $X = x(r) = x_i$ (see first sketch).

(ii) When X has a continuous distribution, find x(r) such that

$$F[x(r)] = r \tag{4}$$

and put $X = x(r)$. (See second sketch). In both cases, X follows the required distribution.

Proof

(i) For a discrete distribution, we see from Eq. (3) that $X \leq x_i$ implies $R \leq F(x_i)$.

Hence
$$\begin{aligned} \Pr[X \leq x_i] &= \Pr[R \leq F(x_i)] \\ &= F(x_i), \quad \text{from Eq. (1)} . \end{aligned}$$

Comparison with Eq. (2) shows that X follows the required distribution.

(ii) When X has a continuous distribution, the equation (4) implies a transformation $X = X(R)$ in the implicit form

$$F(X) = R . \tag{5}$$

We also see from Eq. (2) that the given function F(X) is a strictly increasing function of X.

Hence
$$\begin{aligned} \Pr[X \leq x] &= \Pr[F(X) \leq F(x)] \\ &= \Pr[R \leq r], \text{ from Eqs. (5) and (4)} \\ &= r \qquad , \text{ from Eq. (1)} \\ &= F(x) \qquad , \text{ from Eq. (4)}. \end{aligned}$$

Again we see that X follows the required distribution.

In the continuous case, we can write

$$F(x) = \int_{-\infty}^{x} f(t)\, dt \qquad (6)$$

where f(x) is the probability density function. The basic equation (4) can then be written

$$r = \int_{-\infty}^{x(r)} f(t)\, dt \qquad (7)$$

or

$$dr = f(x)\, dx \qquad (8)$$

A computer programme may require an iterative procedure to solve the equation (7).

REFERENCE

1) J. Butler, 'Machine sampling from given probability distributions' in "Symposium on Monte Carlo methods", edited by H. Meyer - Wiley, 1954.

APPENDIX II

GENERATING RANDOM NUMBERS ON A COMPUTER

Contributed by D. Hudson,
Data and Documents Division, CERN.

Strictly speaking, a random number exists only as the result of a random process. On a computer, however, we often use some arithmetical sequence

$$Z_{n+1} = g(Z_n) \quad , \quad 0 \leq Z_n \leq 1 \qquad (1)$$

with some starting value Z_0 , $0 \leq Z_0 \leq 1$.

The numbers produced by such a rule are of course not random, since they can be predicted in advance. The best we can hope for is that the numbers will appear to be random - that is, the sequence of 'random' numbers must satisfy certain statistical tests concerning the distribution of the numbers over the unit interval; the correlation between Z_n and Z_{n+1} should be low, and so on.

Congruences of whole numbers

We read

$$r \equiv x \text{ Mod } m \qquad (2)$$

as "r is congruent to x, modulo m." In the present context, this can best be interpreted to mean that r, x and m are non-negative integers and that r is the remainder when x is divided by m. Thus

$$0 \leq r \leq m-1 \ . \qquad (3)$$

Congruences are particularly useful as a means of generating a sequence of type (1). We start with a sequence of integers

$$x_{n+1} \equiv \lambda x_n + \mu \text{ Mod } m \ . \qquad (4)$$

Such a sequence often has good random properties if λ and μ are carefully chosen for a given m. We then convert the integers to fractions by putting

$$Z_n = x_n/m \ . \qquad (5)$$

This sequence will produce up to a maximum of m different $\{Z_n\}$ before repeating itself, so m should be a large number.

Example A five bit computer, with m = 32, can generate at most 32 RN before repeating because there exist only 32 stable states of the computer. We choose

$$x_0 = 1, \quad \lambda = 5, \quad \mu = 7 \ . \qquad (6)$$

The sequence x_1, x_2, ... is generated by

$$x_{n+} \equiv 5x_n + 7 \quad \text{Mod } 32 \qquad (7)$$

and is

12,3,22,21,16,23,26,9,20,11,30,29,24,31,
2,17,28,19,6,5,0,7,10,25,4,27,14,13,8,15
18,1, ...

and it then repeats from 12 again. We obtain the required sequence $\{Z_i\}$ on the unit interval by putting

$$Z_i = x_i/32 \ .$$

A computer programme to evaluate Eq. (7) would normally be written in basic code. Remaindering is performed by keeping only the last five bits after a multiplication. Division of these five bits by 32 is performed by placing a decimal point on the left. A FORTRAN version is given below, for comparison. (It is assumed that the numbers 32 and 32.0 will not cause an overflow).

```
      RANDOM NUMBER GENERATOR
      DIMENSION Z(32)
C
C     SET PARAMETERS
      LAMBDA = 5
      MU = 7
      MODLUS = 32
      IX = 1
C
      DO 1 N=1,32
      IX = XMODF(LAMBDA*IX + MU , MODLUS)
    1 Z(N) = FLOATF(IX)/32.0
C
C     START NEW PAGE OF MONITOR OUTPUT
      WRITE OUTPUT TAPE 2,100
  100 FORMAT(1H1)
C
C     OUTPUT RESULTS
      WRITE OUTPUT TAPE 2,101,(Z(N), N=1,32)
  101 FORMAT(4F10.5/)
      CALL EXIT
      END
```

The 32 'random numbers' are

0.37500	0.09375	0.68750	0.65625
0.50000	0.71875	0.81250	0.28125
0.62500	0.34375	0.93750	0.90625
0.75000	0.96875	0.06250	0.53125
0.87500	0.59375	0.18750	0.15625
0.	0.21875	0.31250	0.78125
0.12500	0.84375	0.43750	0.40625
0.25000	0.46875	0.56250	0.03125

It is clear that the less significant digits do not satisfy elementary notions of randomness. The random numbers must therefore only be used as a whole, or alternatively, the left-hand digits may be used to produce random digits.

REFERENCES

1) G. Hardy and E. Wright, "An introduction to the theory of numbers", Oxford, Clarendon Press, 1954.

2) O. Taussky and J. Todd, 'Generation and testing of pseudo-random numbers' in "Symposium on Monte-Carlo methods" edited by H. Mayer - Wiley, 1956.

3) A. Rotenburg, 'A new pseudo-random number generator', J.Assn. for Computing Mach., Vol. 7, p. 75 (1960).

4) R. Coveyou, 'Serial correlation in the generation of pseudo-random numbers', J.Assn. for Computing Mach., Vol. 7, p. 72 (1960).

5) A. Kaercher, 'RDM - Random number - Rectangular distribution'. - SHARE library programme for the IBM 7090 computer, written in FAP. Code number is G5XGC 0008.

6) Random Number Generation and Testing, IBM Reference Manual. (This Manual does not contain a description of the method which produces the longest obtainable sequence.)

APPENDIX III

LORENTZ TRANSFORMATIONS FOR GENERAL COLLISION

Here we describe the transformations necessary to treat the most general collision of two arbitrary particles in a completely relativistic manner. Fig. 2 shows all these transformations from the laboratory system up to the point where one begins transforming the products back to the laboratory by the inverse transformations. In practice one must apply only the inverse transformations. However, it seems easier conceptually to see the transformations and, since they are orthogonal, the inverses are simply the transposes. While several translations appear in Fig. 2, these are included only for clarity as the collision occurs at the point (R_x, R_y, R_z) in the nucleus. Primes on x,y,z are used in the figure to indicate effects of rotations while x,y,z in the descriptions is generic and not written with subscripts or primes. Starred quantities are c.m. quantities. For convenience some transformations are combined.

We start with a fixed laboratory cartesian system having origin at the initial nuclear centre and with the incident beam along the x axis. The momentum vectors of incident and target particles are $\vec{p}_1$ and $\vec{p}_2$.

The transformations are described in the order of their appearance, first verbally and then explicitly.

1) S, a combined rotation of the laboratory coordinate system through angles M and N until the x axis is coincident with the momentum vector $\bar{p}_1$ of the projectile particle.

2) Φ, a rotation about x through a random azimuthal angle Φ until the z axis lies in the plane formed by $\bar{p}_1$ and $\bar{p}_2$, and points in the sense of $\bar{p}_2$.

3) w, a counter-clockwise rotation about the y axis by the angle w until the x axis is coincident with the direction of the c.m. This angle is a function of p_1, p_2 and μ (the cosine of the angle between $\bar{p}_1$ and $\bar{p}_2$).

4) L, the Lorentz transformation to the centre of mass.

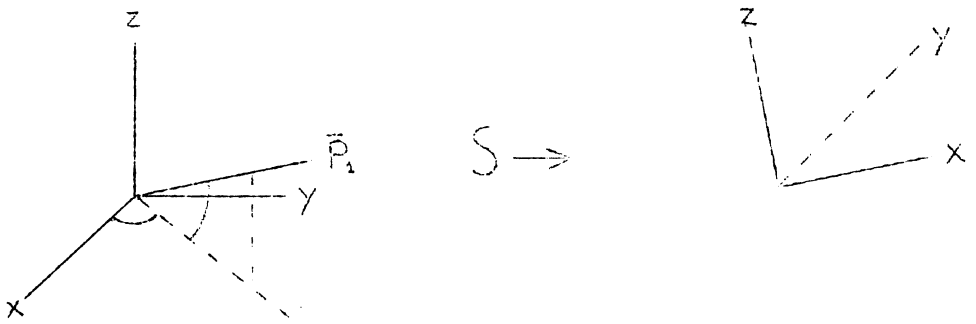
5) δ, the rotation about the y axis by the angle δ until the x axis is parallel to the line $\bar{p}_1^*\bar{p}_2^*$ in the c.m. With our conventions, sin δ is always negative.

We are now in the physically significant system, with x axis along the direction of approach of 1 and 2 in their c.m. In this system the directions and momenta of the selected reaction products must be selected with respect to the plane containing the x axis and the c.m. motion. If no more than three particles result, all these lie in this plane. The following rotation of momenta and transformations of coordinate system are applied, whereas none of the previous coordinate transformations were applied.

6) α, a rotation of each outgoing p* through the same random azimuth angle α about the x axis which is at this point the $\bar{p}_1^*\bar{p}_2^*$ line in the c.m. This is the only rotation of a vector necessary, all the other transformations are those of coordinate systems.

The formal operations that are applied to the outgoing vectors in the physically significant system, that with x parallel to $\bar{p}_1^*\bar{p}_2^*$, are then in operator order, S^{-1} Φ^{-1} W^{-1} L^{-1} δ^{-1} α, first α, then δ^{-1}, and so on.

We will now present the transformations in more detail with simple diagrams indicating the effect of each. All coordinate systems are right-handed. The unit vector $\bar{p}_1/|p_1|$ has laboratory components α,β,γ.



$$S = \begin{pmatrix} \cos M & 0 & \sin M \\ 0 & 1 & 0 \\ -\sin M & 0 & \cos M \end{pmatrix} \begin{pmatrix} \cos N & \sin N & 0 \\ -\sin N & \cos N & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos M \cos N & \cos M \sin N & \sin M \\ -\sin N & \cos N & 0 \\ -\sin M \cos N & -\sin M \sin N & \cos M \end{pmatrix}$$

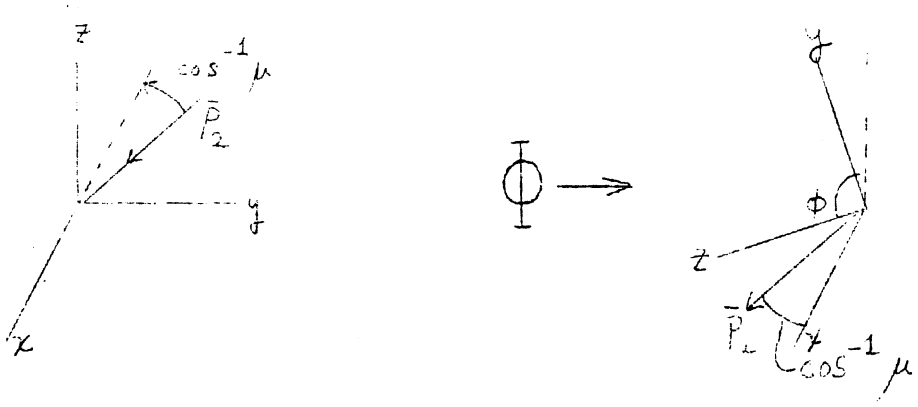
where $\cos M = \sqrt{\alpha^2 + \beta^2}$, $\sin M = \gamma$, $\cos N = \alpha/\sqrt{\alpha^2 + \beta^2}$, $\sin N = \beta/\sqrt{\alpha^2 + \beta^2}$, and $Q = \sqrt{\alpha^2 + \beta^2} = \sqrt{1 - \gamma^2}$.

$$\text{Then } S^{-1}\begin{pmatrix} D \\ E \\ F \end{pmatrix} = \begin{pmatrix} \alpha & -\beta/Q & -\alpha\gamma/Q \\ \beta & \alpha/Q & -\beta\gamma/Q \\ \gamma & 0 & Q \end{pmatrix}\begin{pmatrix} D \\ E \\ F \end{pmatrix} = \begin{pmatrix} \alpha D - \dfrac{(\beta E + \alpha\gamma F)}{Q} \\ \beta D \quad \dfrac{(\alpha E - \beta\gamma F)}{Q} \\ \gamma D \qquad QF \end{pmatrix} = \begin{pmatrix} G \\ H \\ J \end{pmatrix}$$

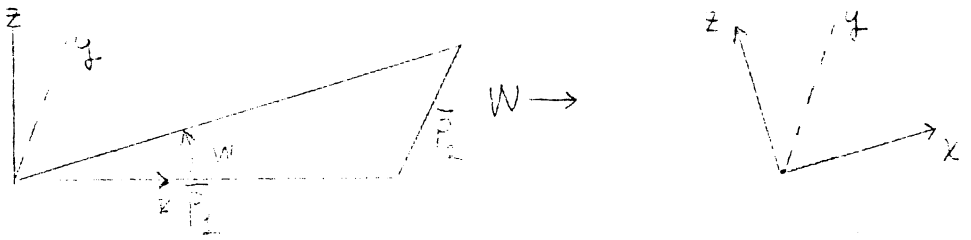
where in this one transformation, we have included operands.

If $\gamma = \pm 1$, $\frac{1}{\gamma}$ diverges, and we must use

$$S^{-1} = \begin{pmatrix} 0 & 0 & \mp 1 \\ 0 & 1 & 0 \\ \pm 1 & 0 & 0 \end{pmatrix}$$

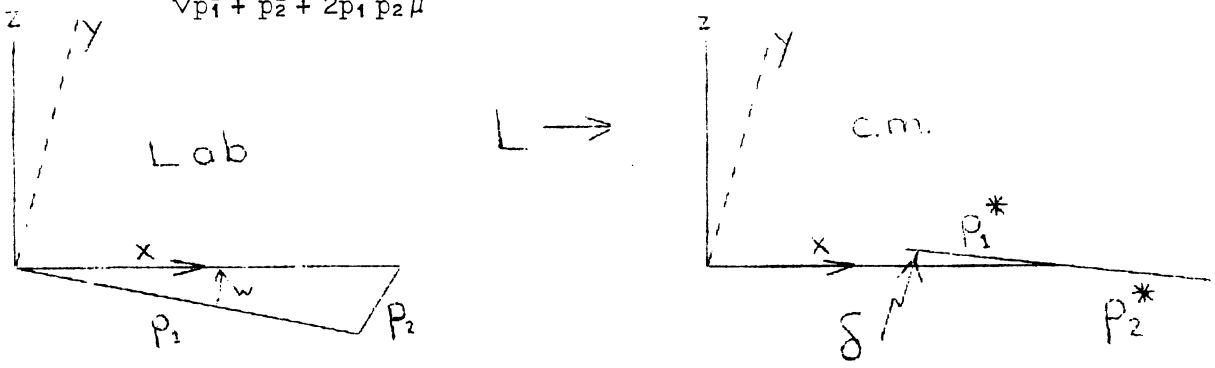


$$\Phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & \sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{pmatrix} \text{ and } \Phi^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & -\sin\Phi \\ 0 & \sin\Phi & \cos\Phi \end{pmatrix}$$



$$w = \begin{pmatrix} \cos w & 0 & \sin w \\ 0 & 1 & 0 \\ -\sin w & 0 & \cos w \end{pmatrix} \text{ and } w^{-1} = \begin{pmatrix} \cos w & 0 & -\sin w \\ 0 & 1 & 0 \\ \sin w & 0 & \cos w \end{pmatrix}$$

where $\cos w = \dfrac{p_1 + p_2 \mu}{\sqrt{p_1^2 + p_2^2 + 2p_1 p_2 \mu}}$



$$L = \begin{pmatrix} E/M & 0 & 0 & -p/M \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -p/M & 0 & 0 & E/M \end{pmatrix} \text{ and } L^{-1} = \begin{pmatrix} E/M & 0 & 0 & p/M \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ p/M & 0 & 0 & E/M \end{pmatrix}$$

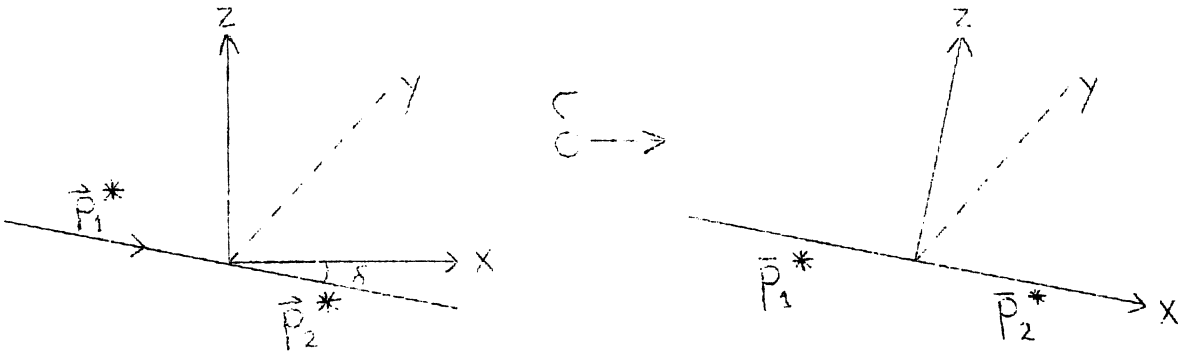
where E, p, and M are the total energy, momentum, and mass of the c.m. as determined in the laboratory.

$$E = E_1 + E_2$$
$$M = [m_1^2 + m_2^2 + 2E_1 E_2 - 2P_1 P_2 \mu]^{1/2} = [m_1^2 + m_2^2 + 2m_1 m_2 g]^{1/2}$$
$$p = \sqrt{E^2 - M^2}$$
$$g = \gamma_1 \gamma_2 - n_1 n_2 \mu \, .$$

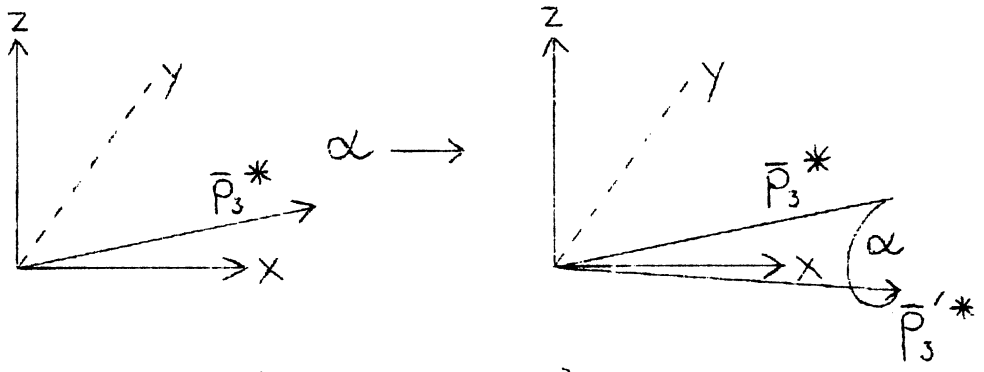
The first quantities to be transformed back are the total laboratory energies. If either particle is a nucleon, a violation of the Pauli exclusion principle negates the collision and prevents pointless transforming of the momentum components. Otherwise we continue

$$\cos \delta = \frac{\gamma_1 (m_1 g + m_2) - \gamma_2 (m_1 + m_2 g)}{p \sqrt{g^2 - 1}}$$

$$\sin \delta = -\sqrt{1 - \cos^2 \delta}$$



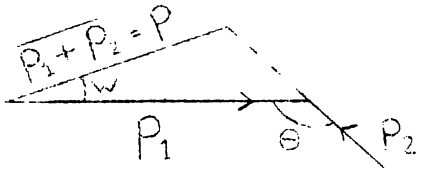
$$\delta = \begin{pmatrix} \cos\delta & 0 & \sin\delta \\ 0 & 1 & 0 \\ -\sin\delta & 0 & \cos\delta \end{pmatrix} \quad \text{and} \quad \delta^{-1} = \begin{pmatrix} \cos\delta & 0 & -\sin\delta \\ 0 & 1 & 0 \\ \sin\delta & 0 & \cos\delta \end{pmatrix}$$



$$\alpha = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}$$

We add here a derivation of the angle δ, the angle between the direction of motion of the c.m. and the direction $\bar{p}_1^*\bar{p}_2^*$ along which the projectile and target approach each other in the c.m.

First re-write the direction of motion of the c.m. when $\bar{p}_2$ makes an angle ϑ with $\bar{p}_1$.



In Fig. 2 $\cos \vartheta = \mu$. The direction of motion of the c.m. was given by the angle w, where

$$\cos w = \frac{p_1 + p_2 \mu}{p}$$

and p was written as

$$p = \sqrt{p_1^2 + p_2^2 + 2p_1 p_2 \mu} .$$

Now
$$\cos \delta = \frac{\gamma(p_i \cos w - \beta E_1)}{p}$$

where $\gamma = E_1 + E_2/M$, $\beta = p/M$. An expression for p^* is

$$p^* = \frac{M}{2}\left[1 - 2\left(\frac{m_1^2 + m_2^2}{M^2}\right) + \left(\frac{m_1^2 - m_2^2}{M^2}\right)^2\right]^{1/2} .$$

After substituting γ, β, p^* and cos w, we find

$$\cos \delta = \frac{\gamma_1(m_1 g + m_2) - \gamma_2(m_2 g + m_1)}{p\sqrt{g^2 - 1}}$$

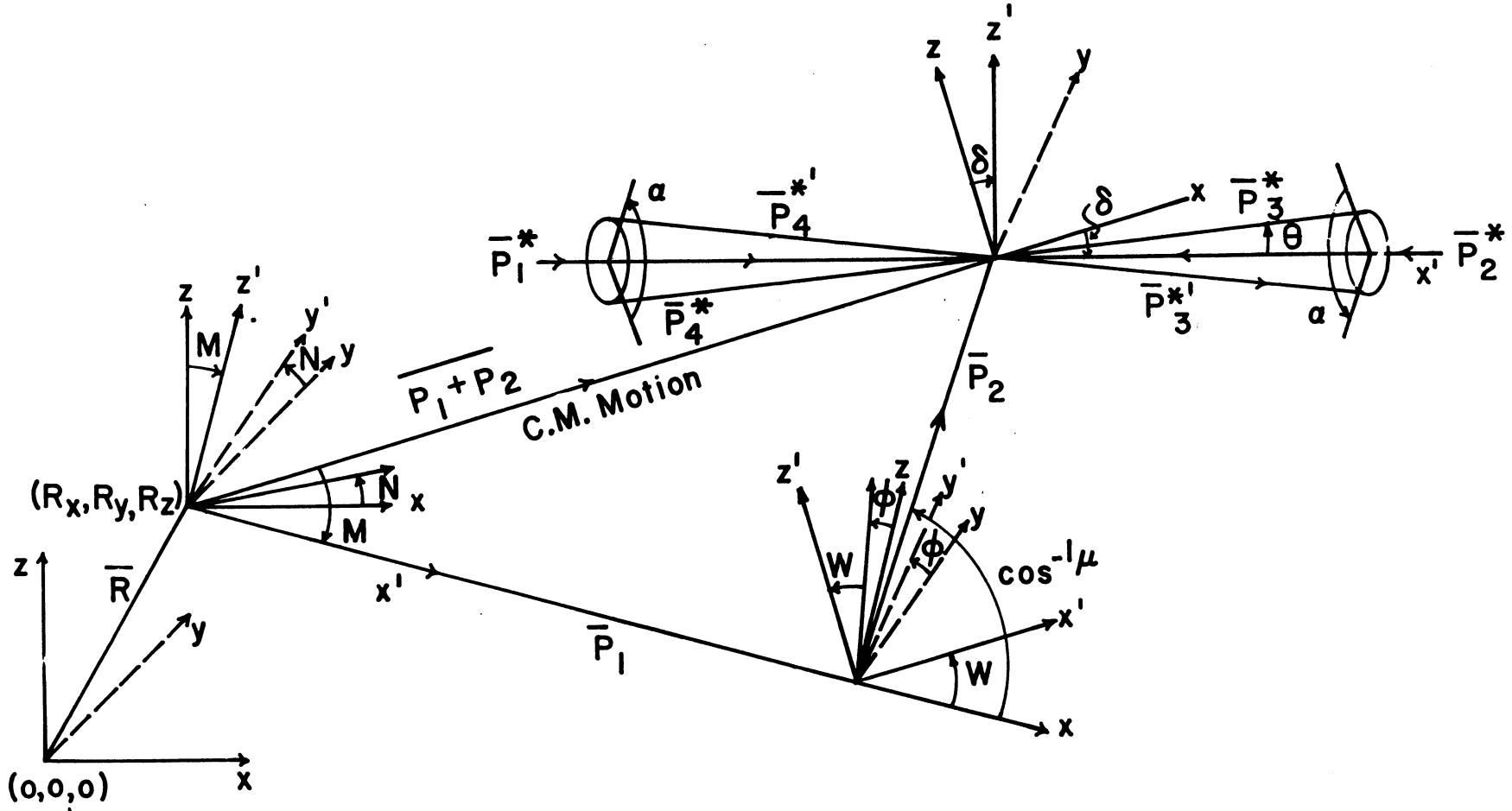


Figure 2

ERRATA

Page	Au lieu de :	Il faut :
4	$E(\xi^2) = E(\eta^2) + E(\zeta^2) + E(\eta\ \zeta)$	$E(\xi^2) = E(\eta^2) + E(\zeta^2) + 2\ E(\eta\ \zeta)$
9	$E(X^2)$ et $D(X)$	$E(X^2)$ et $D(X)$
10	$f(x)dx = \frac{1}{\sqrt{2\pi}}\ e^{-\frac{(x-\Theta)^2}{2\ \sigma^2}}\ \frac{dx}{\sigma}$	$f(x)dx = \frac{1}{\sqrt{2\pi}}\ e^{-\frac{(x-\Theta)^2}{2\ \sigma^2}}\ \frac{dx}{\sigma}$
11	$\varphi_X(t) = \sum_i pi\ e^{it\ x_i}$	$\varphi_X(t) = \sum_i p_i\ e^{it\ x_i}$
12	$E(X^2)$	$E(X^2)$
12	$\ldots = \frac{e^{-\frac{+^2}{2}}}{\sqrt{2\pi}}\ \ldots$	$\ldots = \frac{e^{-\frac{t^2}{2}}}{\sqrt{2\pi}}\ \ldots$
21	$Y - \rho X/1 - \rho^2$	$(Y - \rho X)/(1 - \rho^2)^{1/2}$
21	$f(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}}\ \ldots$	$f(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}}\ \ldots$
22	$\ldots \sqrt{4\pi \times 137\ m_e\ u^2} = 21$ MeV	$\ldots \sqrt{4\pi \times 137\ m_e\ c^2} = 21$ MeV
24	$\omega_i = \frac{D_i}{t} = \frac{y_i + 1 - y_i}{t}$	$\omega_i = \frac{D_i}{t} = \frac{y_{i+1} - y_i}{t}$

7863/p/mh

Page	Au lieu de :	Il faut :
28	$\varphi = E[1 + \vec{it},\vec{X} \ldots$	$\varphi = E[1 + \vec{it}\cdot\vec{X}$
28	$+ 2\, t_1 t_2\, X_1 X_2 + \ldots)$	$+ 2\, t_1 t_2\, X_1 X_2 + \ldots) + \ldots$
28	$+ 2\, t_1 t_2\, \sigma_1\sigma_2\rho_{12} + \ldots)$	$+ 2\, t_1 t_2\, \sigma_1\sigma_2\rho_{12} + \ldots) + \ldots$
28	$\varphi = 1 - \frac{1}{2} \sum_{ij} t_i t_j\, E(X_i X_j))$	$\varphi = 1 - \frac{1}{2} \sum_{ij} t_i t_j\, E(X_i X_j) + \ldots)$
31	$u_k = f_n(x_1, x_2 \ldots x_n)$	$u_k = f_k(x_1, x_2 \ldots x_n)$
34	$\rho = \frac{E[n_1 - np_1)(n_2 - np_2)]}{\sqrt{np_1 q_1}\quad\sqrt{np_2 q_2}} \ldots$	$\rho = \frac{E[(n_1 - np_1)(n_2 - np_2)]}{\sqrt{np_1 q_1}\quad\sqrt{np_2 q_2}} \ldots$
51	$\chi^2 = \sum_{i=1} \frac{(n_i - np_i)^2}{np_i}$	$\chi^2 = \sum_{i=1}^{N} \frac{(n_i - np_i)^2}{np_i}$
58	- Estimation de la variance σ^2 d'une série de n observations gaussiennes indépendantes :	- Estimation de la variance σ^2 d'une série de n observations gaussiennes indépendantes, dans le cas où m est connu.
59	$np_i^1(\Theta)$ et $p_i^1(\Theta)$	$np_i'(\Theta)$ et $p_i'(\Theta)$
59	croquis :	La valeur de Θ au point où la ligne oblique croise l'axe de Θ est $\Theta = t$.
70	$y = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}$	$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$

Page	Au lieu de :	Il faut :
71	$\begin{vmatrix} S_1 & S_2 \\ S_3 & S_4 \end{vmatrix}$ et $\begin{vmatrix} \Sigma & S_1 \\ S_2 & S_3 \end{vmatrix}$	$-\begin{vmatrix} S_1 & S_2 \\ S_3 & S_4 \end{vmatrix}$ et $-\begin{vmatrix} \Sigma & S_1 \\ S_3 & S_4 \end{vmatrix}$
73	$\frac{\partial}{\partial x_0}\left\{\sum_1^n \left(\sum_j^m - x_0 - x_1 x_j - x_2 u_j^2\right)\right\}$ (3 fois)	$\frac{\partial}{\partial x_0}\left\{\sum_1^n \left(\sum_j^m - x_0 - x_1 u_j - x_2 u_j^2\right)^2\right\}$ (3 fois)
73	G_α^{-1}	G_Y^{-1}

	Appears as :	Should be :
105	$f_2 \equiv m_1 - \sin m_2 - m_3 \sin m_4 = 0$	$f_2 \equiv m_1 \sin m_2 - m_3 \sin m_4 = 0$
174	$x_{n+} \equiv 5x_n + 7 \text{ Mod } 32$	$x_{n+1} \equiv 5x_n + 7 \text{ Mod } 32$

7863/p/mh