Practical Statistics for Particle Physicists

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CERN Academic Lectures

October 2006

Topics

1) Introduction

   Learning to love the Error Matrix

2) Do's and Dont's with $\mathcal{L}$ikelihoods

3) χ^2 and Goodness of Fit

4) Bayes, Frequentism and Limits

5) Discovery and p-values

Books

Statistics for Nuclear and Particle Physicists

Cambridge University Press, 1986

Available from CUP

Errata in these lectures

Other Books

J. OREAR "NOTES ON STATISTICS FOR PHYSICISTS
UCRL-8417 (1958)

D J HUDSON 'Lectures on elementary statistics + prob.'
+ "Max like + least squares theory"
CERN reports 63-29 + 64-1

S. BRANDT STATISTICAL + COMPUTATIONAL METHODS IN
DATA ANALYSIS (North Holland 1973)

W T EADIE et al STATISTICAL METHODS IN
EXPTL PHYSICS (North Holland 1971)

S L MEYER DATA ANALYSIS FOR SCIENTISTS +
ENGINEERS (Wiley 1975)

A FRODESON et al PROBABILITY + STATISTICS IN
PARTICLE PHYSICS (Bergen 1979)

R. BARLOW "STATISTICS (Wiley, 1993)

G COWAN, STATISTICAL DATA ANALYSIS (Oxford 1998)

B. ROE PROBABILITY + STATISTICS IN EXPTL PHYSICS
(Springer-Verlag 1992)

Particle Data Book

Statistical Methods in Experimental Physics

2nd Edition

The first edition of this classic book has become the authoritative reference for physicists desiring to master the finer points of statistical data analysis. This second edition contains all the important material of the first, much of it unavailable from any other sources. In addition, many chapters have been updated with considerable new material, especially in areas concerning the theory and practice of confidence intervals, including the important Feldman–Cousins method. Both frequentist and Bayesian methodologies are presented, with a strong emphasis on techniques useful to physicists and other scientists in the interpretation of experimental data and comparison with scientific theories. This is a valuable textbook for advanced graduate students in the physical sciences as well as a reference for active researchers.

25 World Scientific YEARS OF PUBLISHING

6096 hc

ISBN 981-256-795-X

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2nd Edition

Statistical Methods in Experimental Physics

James

Frederick James

Statistical Methods in Experimental Physics

2nd Edition

CONDITIONAL PROBABILITY

$$\text{Prob}[A+B] = \frac{N(A+B)}{N_{tot}} = \frac{N(A+B)}{N(B)} \cdot \frac{N(B)}{N_{tot}}$$

$$= P(A|B) \times P(B)$$

If A + B are independent, $P(A|B) = P(A)$

$$\Rightarrow P(A+B) = P(A) \times P(B) \quad , \quad A + B \text{ indep}$$

e.g. $P[\text{Rainy} + \text{Sunday}] = P(\text{rainy}) \times \frac{1}{7}$ INDEP

$P[\text{Rainy} + \text{December}] \neq P(\text{rainy}) \times \frac{1}{12}$ ~~INDEP~~

$P[E_e \text{ large} + E_\nu \text{ large}] \neq P(E_e \text{ large}) \times P(E_\nu \text{ large})$ ~~INDEP~~

$P[\text{Beam part 1 interacts} + \text{Beam part 2 interacts}]$

$= [P(\text{beam particle interacts})]^2$ INDEP

$$\text{Prob}[A+B] = \text{Prob}[A|B] \times \text{Prob}[B]$$

$$= \text{Prob}[B|A] \times \text{Prob}[A]$$

ESTIMATE OF VARIANCE

$$s^2 = \frac{1}{N-1} \sum (x_i - \bar{x})^2$$

UNBIASSED ESTIMATE OF σ^2

$$= \frac{N}{N-1} \left(\overline{x^2} - \bar{x}^2 \right)$$

USEFUL "ON LINE"

BUT can have numerical problems

For Gaussian x_i

error on s $= \dfrac{\sigma}{\sqrt{2(N-1)}}$

e.g. $N = 3 \Rightarrow 50\%$ error

$N = 51$ for 10% error

COMBINING EXPERIMENTS

$x_i \pm \sigma_i$ (uncorrelated)

$$\hat{x} = \frac{\sum x_i/\sigma_i^2}{\sum 1/\sigma_i^2}$$

$$1/\sigma^2 = \sum 1/\sigma_i^2$$

From $S = \sum (x_i - \hat{x})^2/\sigma_i^2$

Minimise S

σ from $S_{min} + 1$

OR Propagate errors from $\hat{x} = \ldots\ldots$

Define $w_i = 1/\sigma_i^2$ = weight ~ information content

$$\hat{x} = \sum w_i x_i / \sum w_i$$

$$W = \sum w_i$$

Example : Equal σ_i $\Rightarrow$ $\hat{x} = \bar{x}$

$\sigma = \sigma_i/\sqrt{n}$

BEWARE

$$\left.\begin{matrix} 100 \pm 10 \\ 1 \pm 1 \end{matrix}\right\} \longrightarrow 2 \pm 1 \ ?$$

or 50.5 ± 5 ?

DIFFERENCE BETWEEN ADDING + AVERAGING

NO OF MARRIED MEN $= 10.0 \pm 0.5$ Million

NO OF MARRIED WOMEN $= 8 \pm 3$ Million

Total $=$ 18 ± 3 million

Average $=$ 9.9 ± 0.5

$\Rightarrow$ total $= 20 \pm 1$ million

General point: Including theoretical input can improve accuracy of answer

RELATION BETWEEN POISSON AND BINOMIAL

N people at lecture, m males + f females

Assume that these are representative of basic rates :—

ν people $\qquad$ νp males $\qquad$ $\nu(1-p)$ females

Probability of observing N people

$$P_{\text{Poisson}} = \frac{e^{-\nu}\,\nu^{N}}{N!}$$

Probability of given male/female division

$$P_{\text{Binomial}} = \frac{N!}{m!\,f!}\,p^{m}(1-p)^{f}$$

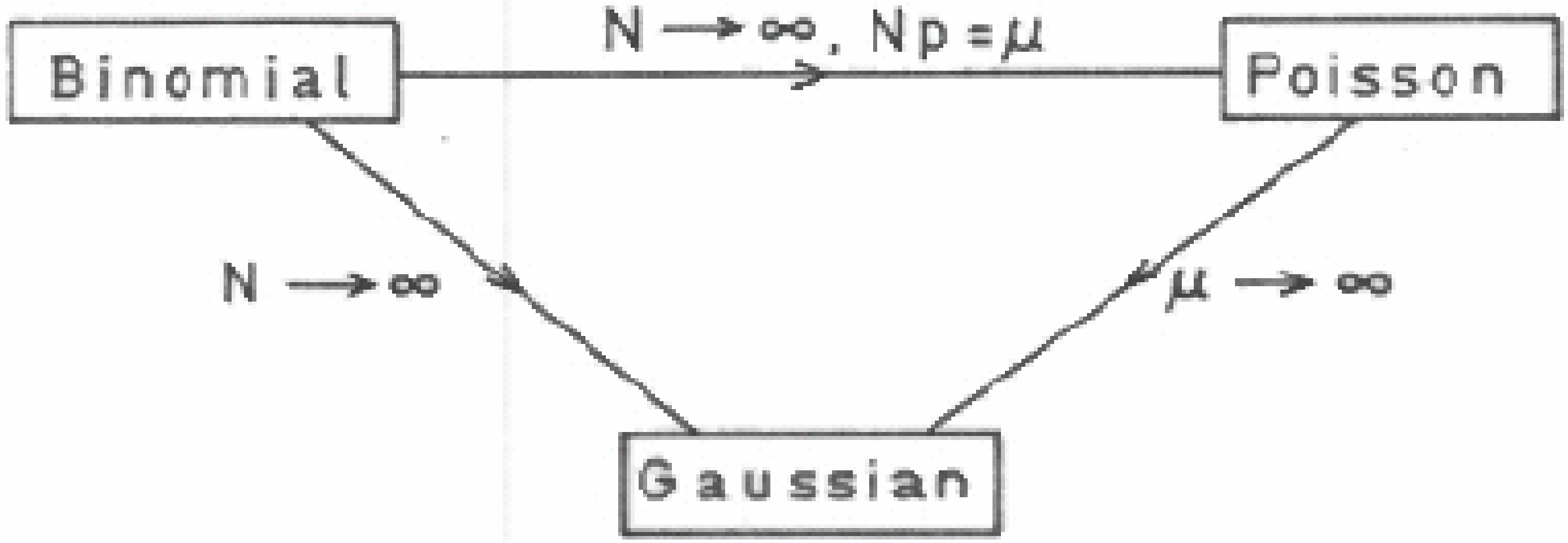
Probability of N people, m males + f females

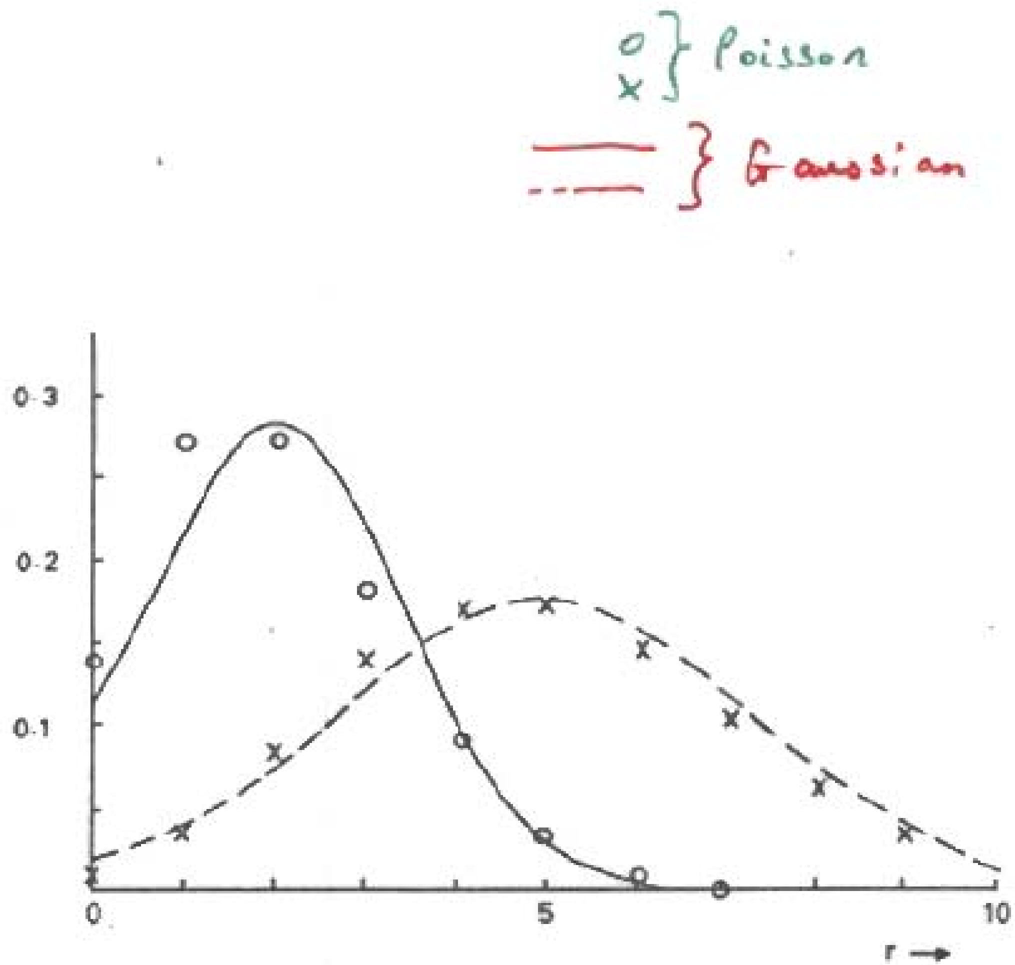
$$P = P_{\text{Poisson}}\,P_{\text{Binomial}}$$

$$= \left\{\frac{e^{-\nu p}\,\nu^{m}p^{m}}{m!}\right\} \times \left\{\frac{e^{-\nu(1-p)}\,\nu^{f}(1-p)^{f}}{f!}\right\}$$

= Poisson distribution for males × Poisson distribution for Females

People	Male	Female
Patients	Cured	Remain ill
Decaying mult.	Forwards	Backwards
Cosmic Rays	Protons	Other particles


Binomial
$N \to \infty$, $Np = \mu$
Poisson
$N \to \infty$
$\mu \to \infty$
Gaussian



Relevant for Goodness of Fit

$$y = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

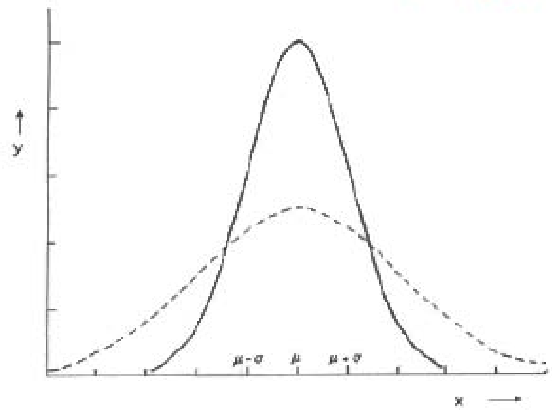


Fig. 1.5. The solid curve is the Gaussian distribution of eqn (1.14). The distribution peaks at the mean μ, and its width is characterised by the parameter σ. The dashed curve is another Gaussian distribution with the same values of μ, but with σ twice as large as the solid curve. Because the normalisation condition (1.15) ensures that the area under the curves is the same, the height of the dashed curve is only half that of the solid curve at their maxima. The scale on the x-axis refers to the solid curve.

Significance of σ

i) RMS of Gaussian $= \sigma$

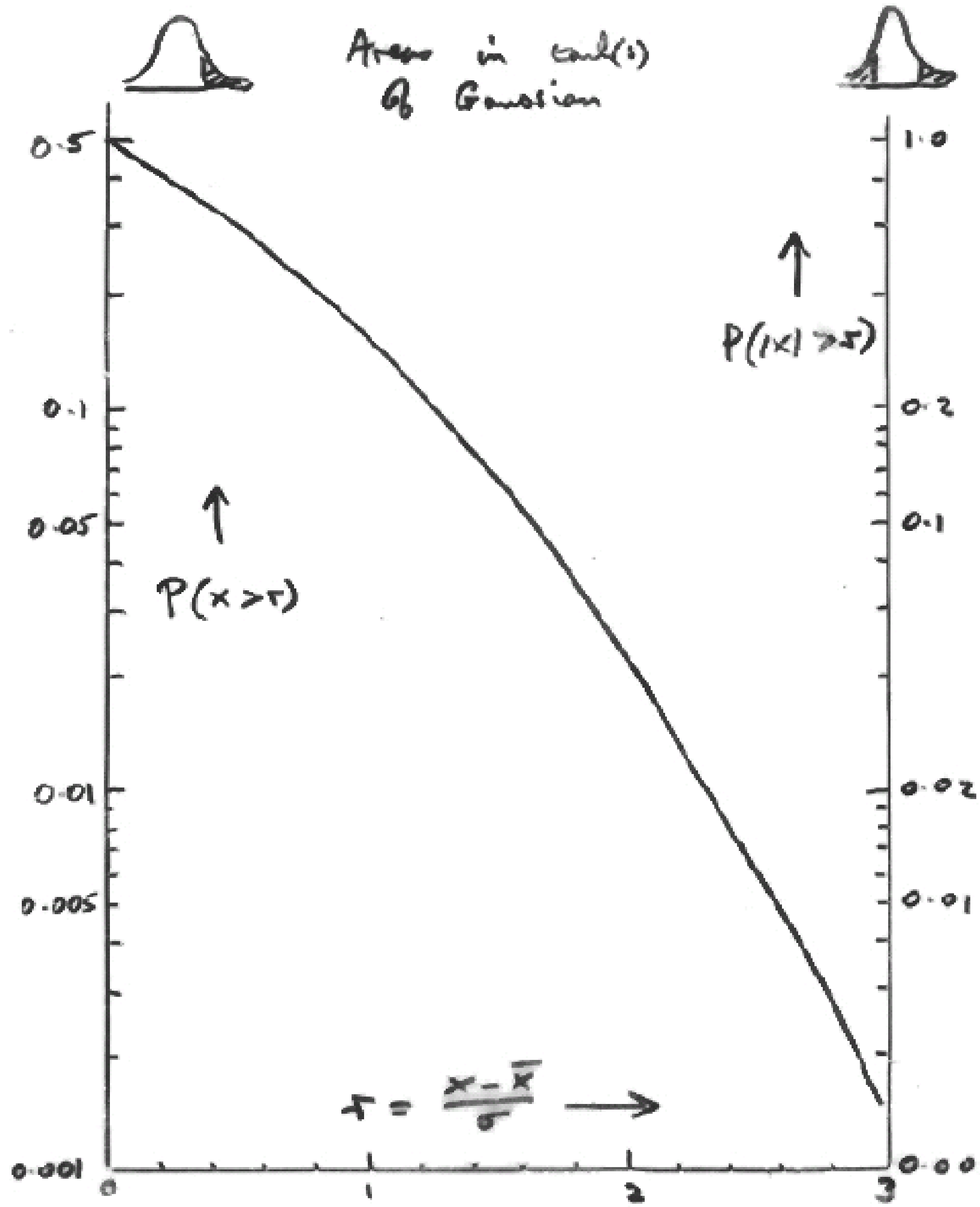
(Hence factor of 2 in defn of Gaussian)

ii) At $x = \mu \pm \sigma$, $y = y_{max}/\sqrt{e}$

(i.e. $\sigma \sim$ half-width at "half" height)

iii) Fractional area within $\mu \pm \sigma$ is 68%

iv) Height at max $= 1/\sqrt{2\pi}\,\sigma$



Areas in tail(s)
of Gaussian
0.5
0.1
0.05
0.01
0.005
0.001
1.0
0.2
0.1
0.02
0.01
0.00
P(x > τ)
P(|x| > τ)
τ = (x − x̄)/σ
0
1
2
3

STUDENT'S t

$x = \frac{\text{meas - expected}}{\sigma}$

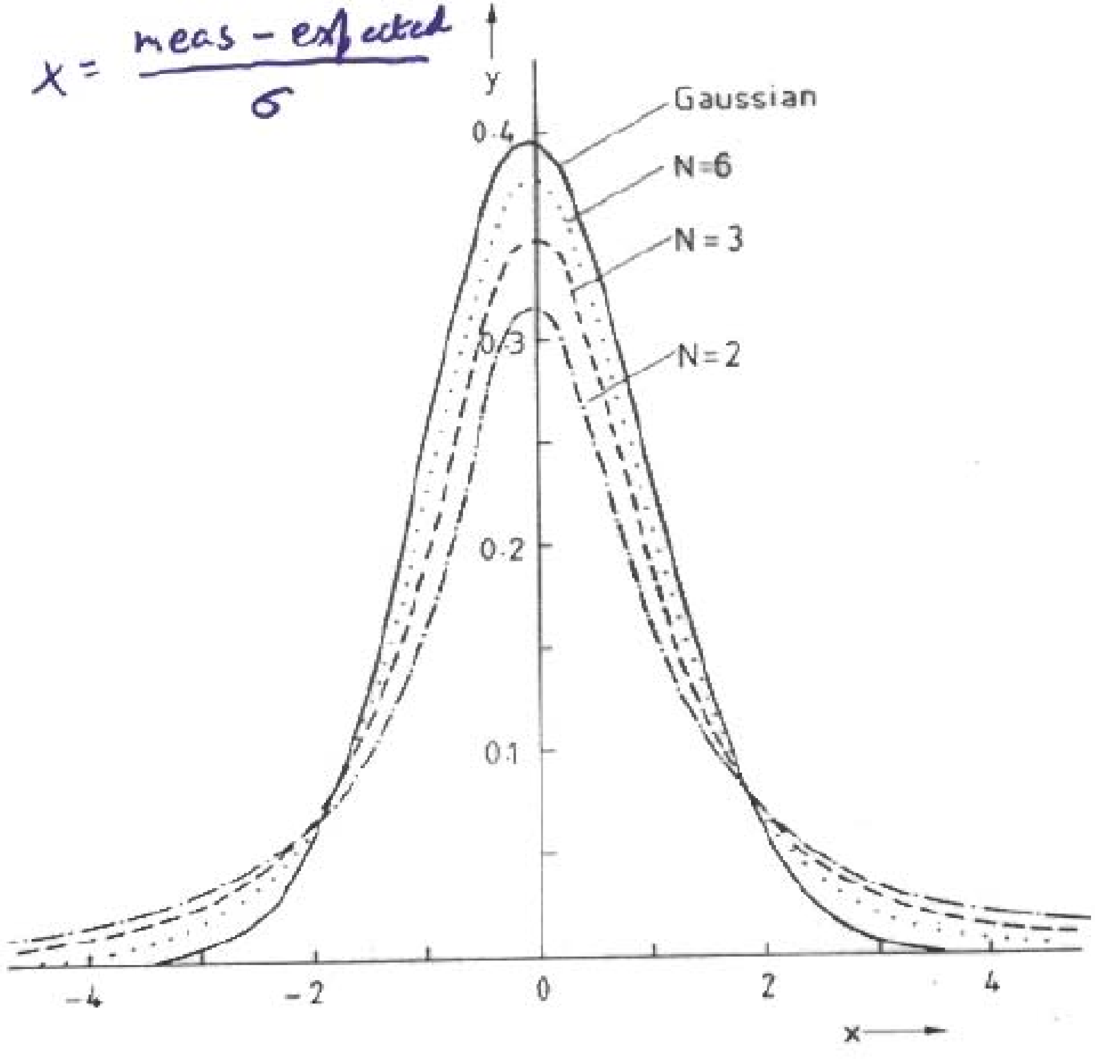
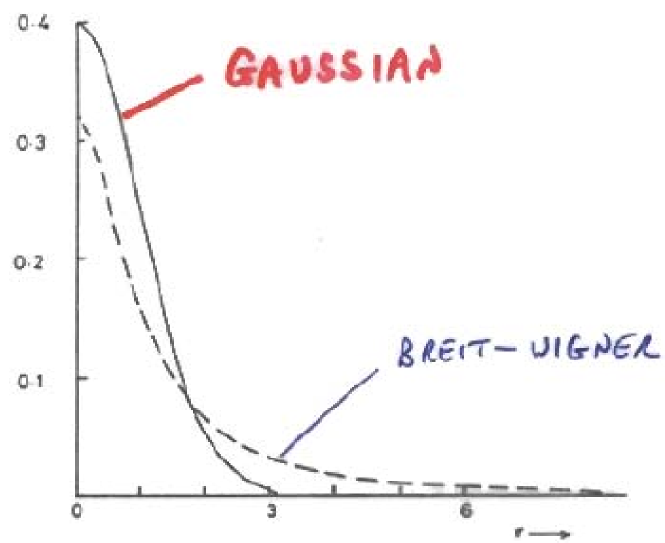


Fig. A5.1 Comparison of Student's t distributions for various values of the number of observations N, with the Gaussian distribution, which is the limit of the Student's distributions as N tends to infinity.



Gaussian = N(r, 0, 1)

Breit Wigner = $1/\{\pi * (r^2 + 1)\}$

Learning to love the Error Matrix

- Introduction via 2-D Gaussian
- Understanding covariance
- Using the error matrix

  Combining correlated measurements
- Estimating the error matrix

Gaussian in 2-variables

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

$$P(y) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_y} e^{-\frac{1}{2} y^2/\sigma_y^2}$$

x + y uncorrelated $\Rightarrow$

$$P(x,y) = \frac{1}{2\pi} \frac{1}{\sigma_x \sigma_y} e^{-\frac{1}{2}\left(\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2}\right)}$$

Down on $P(0,0)$ by $e^{-\frac{1}{2}}$ when

$$\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} = 1$$

Rewrite as

$$\begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} \frac{1}{\sigma_x^2} & 0 \\ 0 & \frac{1}{\sigma_y^2} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 1$$

Invert

$\Rightarrow$ ERROR MATRIX

$$\begin{pmatrix} \sigma_x^2 & 0 \\ 0 & \sigma_y^2 \end{pmatrix}$$

Element E_{ij} - $\overline{<}(x_i - \bar{x}_i)(x_j - \bar{x}_j)>$

Diagonal E_{ij} = variances

Off-diagonal E_{ij} = covariances

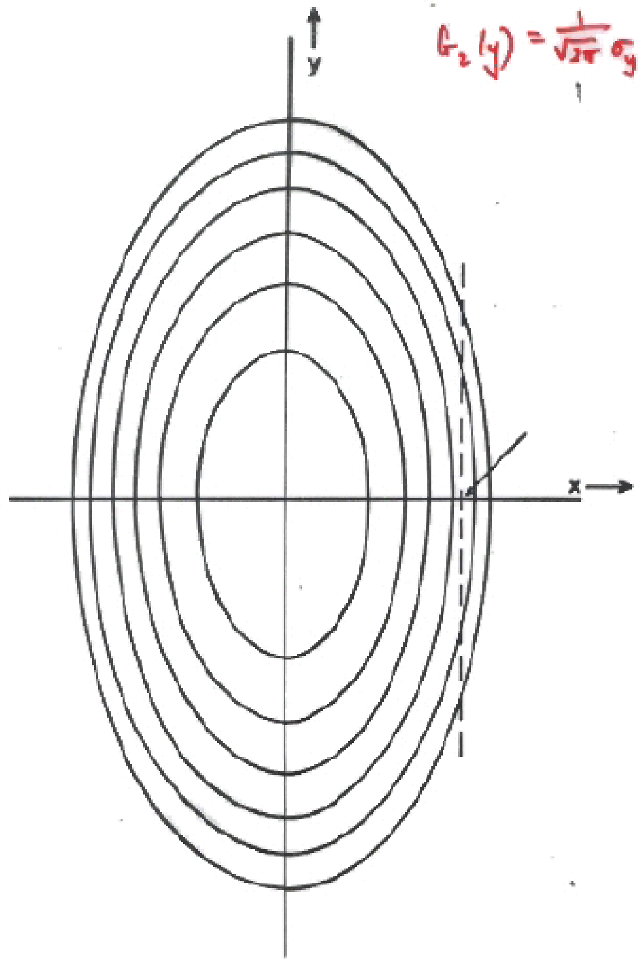
TOWARDS THE ERROR MATRIX

$x + y$ indep Gaussians

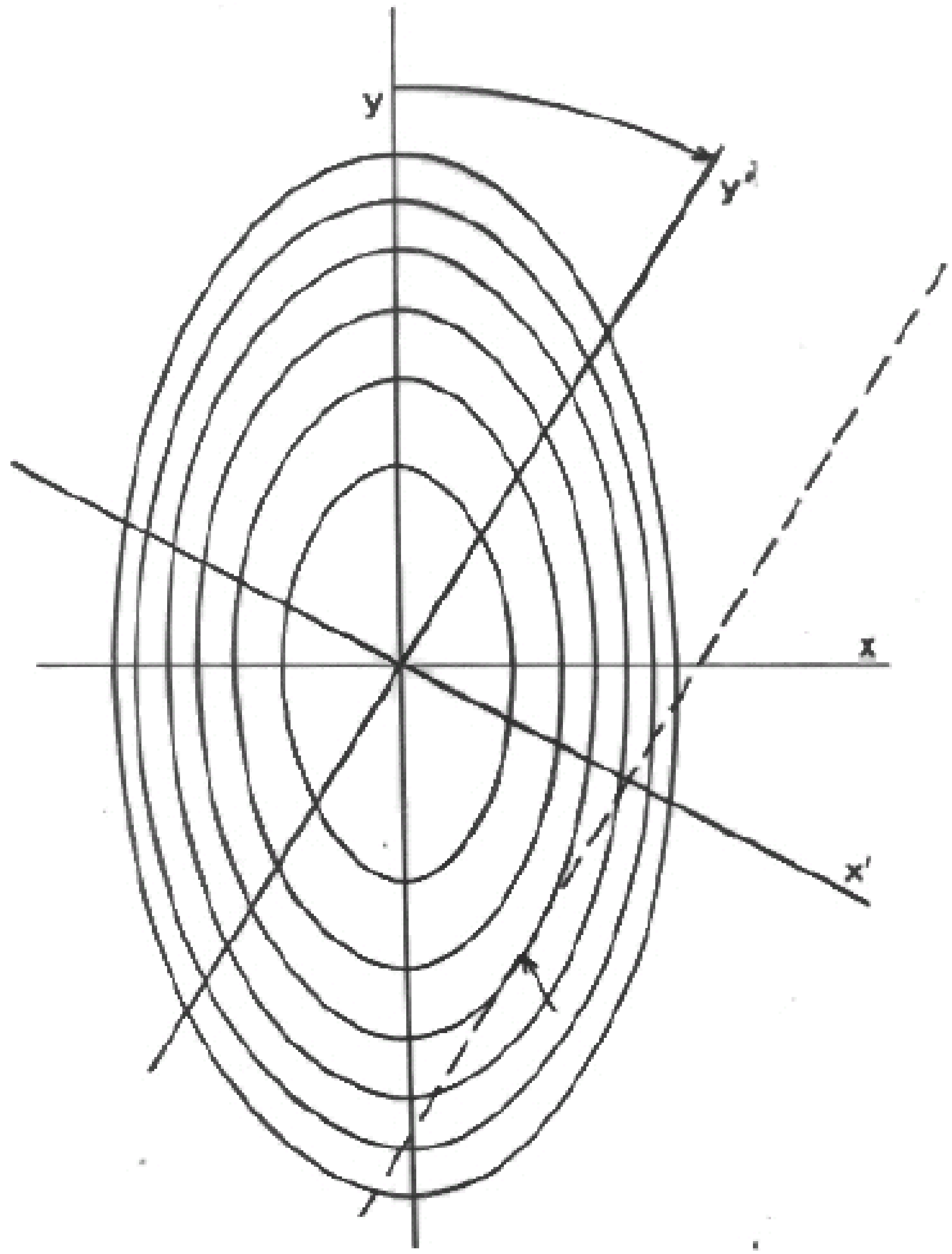
$$P(x,y) = G_1(x)\, G_2(y)$$

$$G_1(x) = \frac{1}{\sqrt{2\pi}\,\sigma_x} \exp\left[-\frac{1}{2}\frac{x^2}{\sigma_x^2}\right]$$

$$G_2(y) = \frac{1}{\sqrt{2\pi}\,\sigma_y} \exp\left[-\frac{1}{2}\frac{y^2}{\sigma_y^2}\right]$$



$$P(x,y) = \frac{1}{2\pi}\frac{1}{\sigma_x \sigma_y} \exp\left[-\frac{1}{2}\left(\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2}\right)\right]$$


y
y'
x
x'

Specific example

$\sigma_x = \frac{\sqrt{2}}{4} = \cdot 354$ $\qquad$ $\sigma_y = \frac{\sqrt{2}}{2} = \cdot 707$

Then factor of $e^{-\frac{1}{2}}$ when

$$8x^2 + 2y^2 = 1$$

Now introduce CORRELATIONS by $30°$ rotn

$$\frac{1}{2}\left[13x'^2 + 6\sqrt{3}\,x'y' + 7y'^2\right] = 1$$

$$\begin{pmatrix} \frac{13}{2} & \frac{3\sqrt{3}}{2} \\ \frac{3\sqrt{3}}{2} & \frac{7}{2} \end{pmatrix} = \text{Inverse Error Matrix}$$

$$\frac{1}{32} \times \begin{pmatrix} 7 & -3\sqrt{3} \\ -3\sqrt{3} & 13 \end{pmatrix} = \text{Error Matrix}$$

$$8x^2 + 2y^2 = 1$$

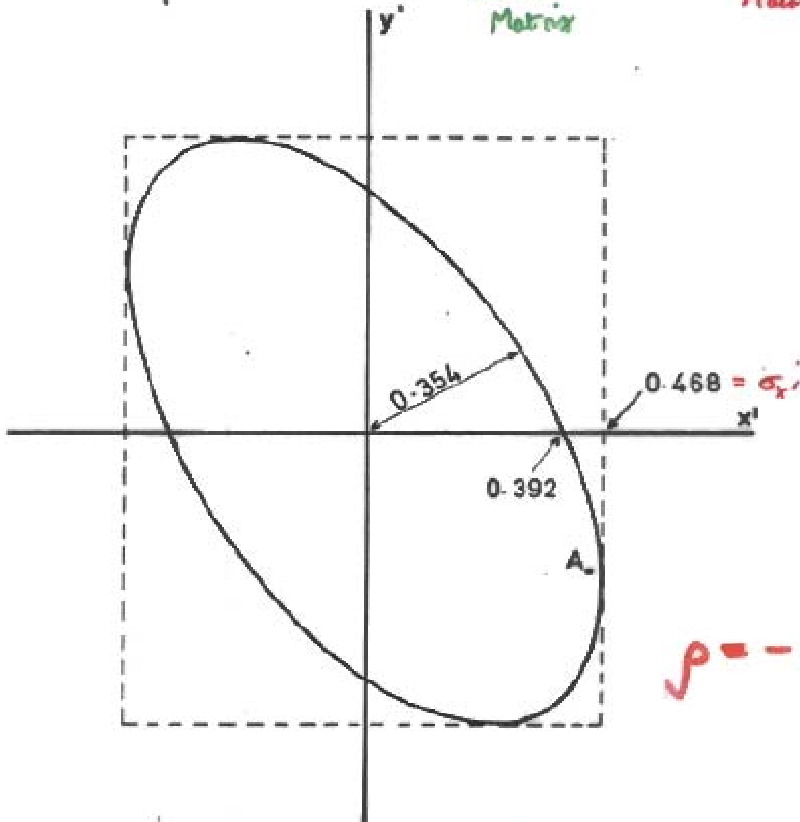
$$\tfrac{1}{2}\left[13x'^2 + 6\sqrt{3}\,x'y' + 7y'^2\right] = 1$$

$$\begin{pmatrix} \frac{13}{2} & \frac{3\sqrt{3}}{2} \\ \frac{3\sqrt{3}}{2} & \frac{7}{2} \end{pmatrix}$$

Inverse Error Matrix

$$\frac{1}{32} \times \begin{pmatrix} 7 & -3\sqrt{3} \\ -3\sqrt{3} & 13 \end{pmatrix}$$

Error Matrix



$$\rho = -0.54$$

$$(0.468)^2 = \frac{7}{32} = \sigma_{x'}^2$$

$$(0.392)^2 = 1/6.5$$

$\frac{1}{8} = (0.354)^2 =$ Eigenvalue of error matrix $= \sigma_x^2$

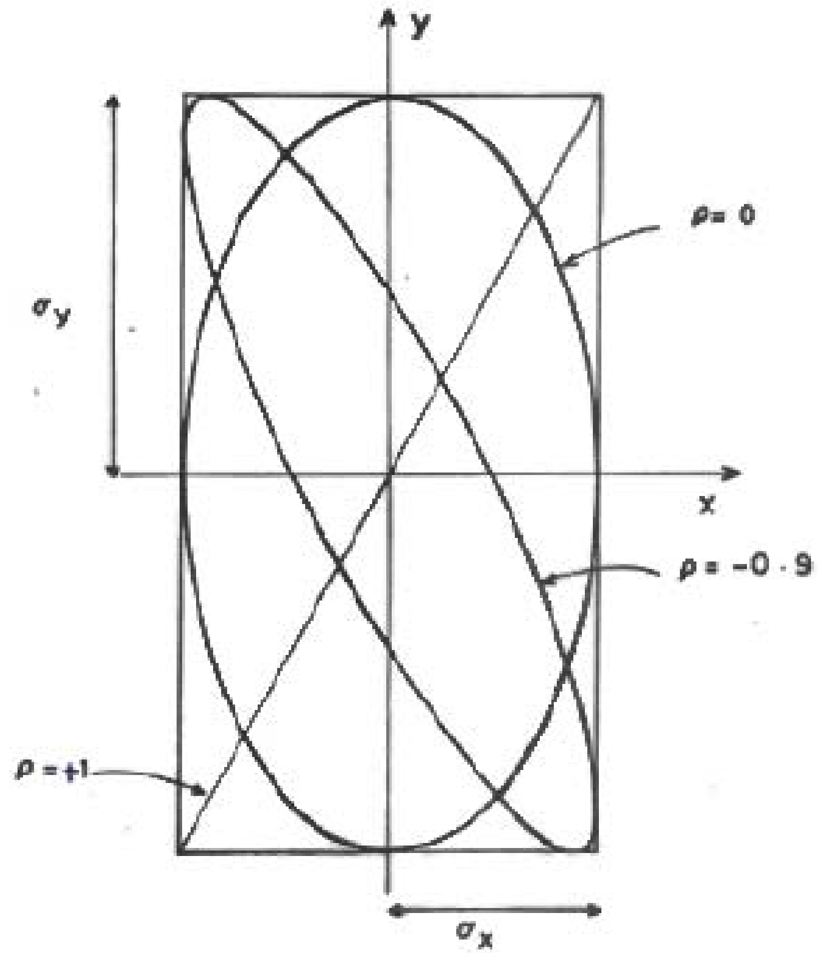
$\left.\begin{array}{l}\sigma_x \\ \sigma_y\end{array}\right\}$ constant

ρ varying

Covariance

$$\begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix}$$

Error Matrix



USING THE ERROR MATRIX

(i) Function of variables

$$y = y(x_a, x_b)$$

Given x_a, x_b error matrix, what is σ_y?

Differentiate, square, average

$$\overline{\delta y^2} = \left(\frac{\partial y}{\partial x_a}\right)^2 \overline{\delta x_a^2} + \left(\frac{\partial y}{\partial x_b}\right)^2 \overline{\delta x_b^2} + 2\frac{\partial y}{\partial x_a}\frac{\partial y}{\partial x_b}\overline{\delta x_a \delta x_b}$$

Zero if x_a, x_b uncorrelated

OR

$$\overline{\delta y^2} = \begin{pmatrix} \frac{\partial y}{\partial x_a} & \frac{\partial y}{\partial x_b} \end{pmatrix} \begin{pmatrix} \overline{\delta x_a^2} & \overline{\delta x_a \delta x_b} \\ \overline{\delta x_a \delta x_b} & \overline{\delta x_b^2} \end{pmatrix} \begin{pmatrix} \frac{\partial y}{\partial x_a} \\ \frac{\partial y}{\partial x_b} \end{pmatrix}$$

$\tilde{D}$

Error matrix

Derivative vector D

$$\sigma_y^2 = \tilde{D} E D$$

(ii) Change of variables $\quad x_a = x_a(p_i, p_j)$
$\quad x_b = x_b(p_i, p_j)$

e.g. Cartesian $\Rightarrow$ polars

or Points in x, y $\Rightarrow$ m, c of straight line fit

Given (p_i, p_j) error matrix $\Rightarrow$ (x_i, x_j) error matrix

Differentiate, $\delta x_a \delta x_b$, average

$$\delta x_a = \frac{\partial x_a}{\partial p_i}\delta p_i + \frac{\partial x_a}{\partial p_j}\delta p_j \qquad (+\text{ sim for } x_b)$$

Then
$$\overline{\delta x_a^2} = \left(\frac{\partial x_a}{\partial p_i}\right)^2 \overline{\delta p_i^2} + \left(\frac{\partial x_a}{\partial p_j}\right)^2 \overline{\delta p_j^2} + 2\frac{\partial x_a}{\partial p_i}\frac{\partial x_a}{\partial p_j}\overline{\delta p_i \delta p_j}$$

$$\overline{\delta x_a \delta x_b} = \frac{\partial x_a}{\partial p_i}\frac{\partial x_b}{\partial p_i}\overline{\delta p_i^2} + \frac{\partial x_a}{\partial p_j}\frac{\partial x_b}{\partial p_j}\overline{\delta p_j^2} + \left(\frac{\partial x_a}{\partial p_i}\frac{\partial x_b}{\partial p_j} + \frac{\partial x_a}{\partial p_j}\frac{\partial x_b}{\partial p_i}\right) \times \overline{\delta p_i \delta p_j}$$

$+ \overline{\delta x_b^2}$ like $\overline{\delta x_a^2}$

N.B. Change of variables does not have to be $N \to N$

e.g. straight line fit involves $N \to 2$

Then i) & ii) are both examples of $N \to M$ $(M \le N)$
where $M = 1$ in i) $\quad M = N$ in ii)

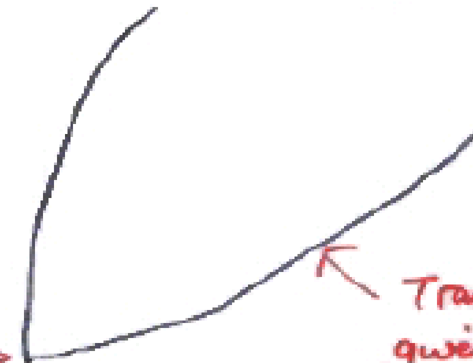
i.e.

$$\underbrace{\begin{pmatrix} \overline{\delta x_a^2} & \overline{\delta x_a \delta x_b} \\ \overline{\delta x_a \delta x_b} & \overline{\delta x_b^2} \end{pmatrix}}_{\text{New error matrix}} = \underbrace{\begin{pmatrix} \frac{\partial x_a}{\partial p_i} & \frac{\partial x_a}{\partial p_j} \\ \frac{\partial x_b}{\partial p_i} & \frac{\partial x_b}{\partial p_j} \end{pmatrix}}_{\tilde{T}} \underbrace{\begin{pmatrix} \overline{\delta p_i^2} & \overline{\delta p_i \delta p_j} \\ \overline{\delta p_i \delta p_j} & \overline{\delta p_j^2} \end{pmatrix}}_{\text{Old error matrix}} \underbrace{\begin{pmatrix} \frac{\partial x_a}{\partial p_i} & \frac{\partial x_b}{\partial p_i} \\ \frac{\partial x_a}{\partial p_j} & \frac{\partial x_b}{\partial p_j} \end{pmatrix}}_{\text{Transform matrix } T}$$

$$E_x = \tilde{T} E_p T$$

BEWARE!

e.g



Calculate effective mass here

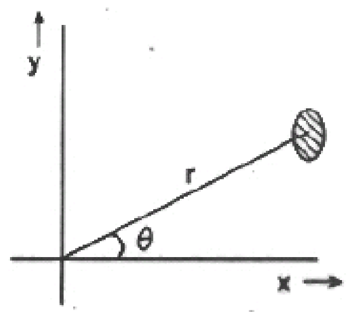
Track params given at centre of track

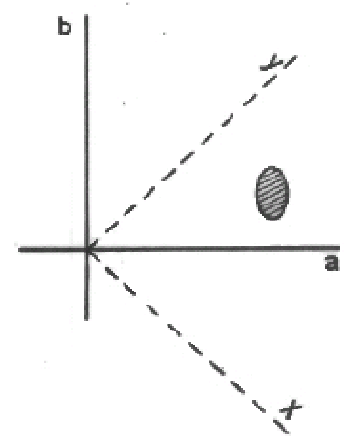
Tracks' error matrix (centre of tracks)

$$\sigma_M^2 = \tilde{D}\,\tilde{T}\,E\,T\,D$$

Deriv vector for mass in terms of track params at vertex

Transformation matrix from centre of tracks to vertex


y
r
θ
x


b
y
a
x

USING THE ERROR MATRIX

COMBINING RESULTS

If $a_i \pm \sigma_i$ are independent:

Minimise $S = \sum \left(\frac{a_i - \hat{a}}{\sigma_i} \right)^2$

$\Rightarrow \quad \hat{a} = \frac{\sum a_i w_i}{\sum w_i} \qquad w_i = 1/\sigma_i^2$

Now $a_i \pm \sigma_i$ are correlated with error matrix $\underline{\underline{E}}$

$$\underline{\underline{E}} = \begin{pmatrix} \sigma_1^2 & cov(1,2) & cov(1,3) & \cdots \\ cov(1,2) & \sigma_2^2 & cov(2,3) & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$

$$S = \sum_{i,j} (a_i - \hat{a}) \underline{\underline{E}}^{-1}_{ij} (a_j - \hat{a})$$

INVERSE ERROR MATRIX

N.B. $\hat{a}$ CAN LIE OUTSIDE a_i

$\sigma_{\hat{a}} \to 0$ AS $\rho \to \pm 1$

$$\underline{\underline{E}}^{-1} = \begin{pmatrix} 1/\sigma_1^2 & 0 & 0 & \cdots \\ 0 & 1/\sigma_2^2 & 0 & \\ \vdots & \vdots & \vdots & \end{pmatrix}$$ FOR UNCORRELATED

MORE COMBINING :

SEVERAL PAIRS OF CORRELATED MEAS.

(x_i, y_i) with $\underline{\underline{E}}_i = \begin{pmatrix} \sigma_x^2 & \text{cov} \\ \text{cov} & \sigma_y^2 \end{pmatrix}_i$

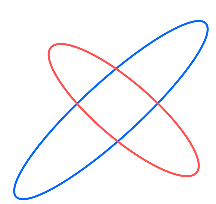
$$\chi^2 = \sum_i \left\{ (x_i - \hat{x})^2 E^{-1}_{11,i} + (y_i - \hat{y})^2 E^{-1}_{22,i} + 2(x_i - \hat{x})(y_i - \hat{y}) E^{-1}_{12,i} \right\}$$

i.e. result:—

Inverse error matrix on result $\hat{x}, \hat{y}$

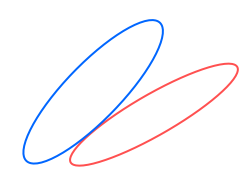
$$= \sum_i \underline{\underline{E}}_i^{-1}$$

cf $\frac{1}{\sigma^2} = \sum \frac{1}{\sigma_i^2}$ for single uncorrelated meas.



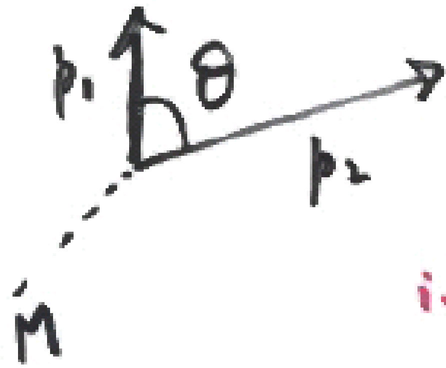
Small error

Example: Lecture 3



x_{best} outside $x_1 \rightarrow x_2$
y_{best} outside $y_1 \rightarrow y_2$

CORRELATIONS + MASS RESOLUTION



$$M^2 = (E_1+E_2)^2 - (\underline{p}_1+\underline{p}_2)^2$$

$$\sim p_1 p_2 \theta \qquad [\, p_i \gg m_i \,;\ \theta \ll 1 \,]$$

i.e. $M \uparrow$ as $p_i \uparrow$ + $\theta_i \uparrow$

As $p_i \downarrow$, $\theta \uparrow$

$\therefore$ Smaller σ_M

As $p_i \downarrow$, $\theta \downarrow$

$\therefore$ Larger σ_M

ESTIMATING THE ERROR MATRIX

1) ESTIMATE ERRORS

ESTIMATE CORRELATIONS

(Usually easiest if $\rho = 0$ or ± 1)

2) FOR INDEP SOURCES OF ERRORS, ADD ERROR MATRICES

e.g. M_W FROM $WW \to 4$ JETS
$WW \to JJl\nu$

$\underline{\underline{E}} = (M_W)_1, (M_W)_2$ ERROR MATRIX

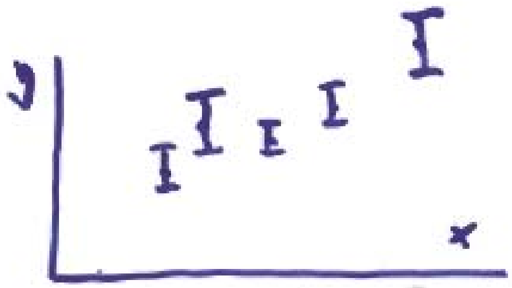
$$\underline{\underline{E}} = \underline{\underline{E}}_{stat} + \underline{\underline{E}}_{B.E.} + \underline{\underline{E}}_{E\ scale} + \underline{\underline{E}}_{FSR} + \underline{\underline{E}}_{colour\ reconn}$$

$$\begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix} \qquad \begin{pmatrix} \sigma_1^2 & \sigma_1\sigma_2 \\ \sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \qquad \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & 0 \end{pmatrix}$$

3) TRANSFORMATIONS

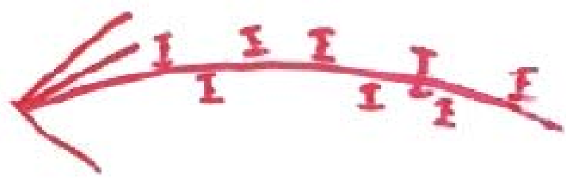
e.g. $(x \pm \sigma_x ,\ y \pm \sigma_y)$ with <u>un</u>correl. errors

$\Rightarrow$ r, θ <u>with</u> correlations



Indep data points

$\Rightarrow$ correlated a and b



Track fit

4) REPEATED OBSERVATIONS

$(x_i, y_i) \Rightarrow \sigma_x^2 \quad \sigma_y^2$ and

cov(x, y) from $\overline{(x-\bar{x})(y-\bar{y})}$

Conclusion

Error matrix formalism makes life easy when correlations are relevant

Next time: $\mathcal{L}$ikelihoods

- What it is
- How it works: Resonance
- Error estimates
- Detailed example: Lifetime
- Several Parameters
- Extended maximum $\mathcal{L}$
- Do's and Dont's with $\mathcal{L}$