χ^2 and Goodness of Fit

Louis Lyons

Imperial College & Oxford

CERN School

Sept 2024

Least Squares Best Fit

- Resume of straight line
- Correlated uncertainties
- Uncertainties in x and in y

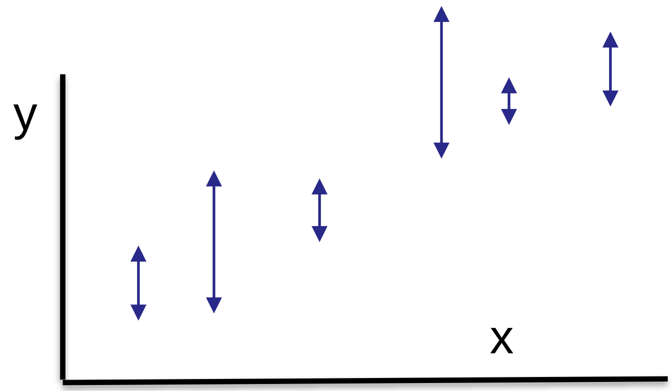
Goodness of Fit with χ^2

- Errors of first and second kind
- Kinematic fitting
  - Toy example

THE paradox

Least Squares Straight Line Fitting

Data = $\{x_i, y_i \pm \delta y_i\}$



1) Does it fit straight line?

(Goodness of Fit)

2) What are gradient and intercept?

(Parameter Determination)

Do 2) first

N.B.1 Can be used for non "a+bx"

e.g. $a + b/x + c/x^2$ or $Ae^{-\mu t}$

N.B.2 Least squares is not the only method

$$S=\Sigma\{(y_i^{th} - y_i^{obs})/\sigma_i\}^2$$

(S rather than χ^2)

N.B Mathematical χ^2 = sum of squares of standard Gaussians G(x|0,1)

σ_i is supposed to be 'uncertainty on data if it agreed with theory' * Pearson χ^2

Usually taken as 'uncertainty on expt' Neyman χ^2

i) Makes algebra simpler

ii) If theory ~ expt, not too different

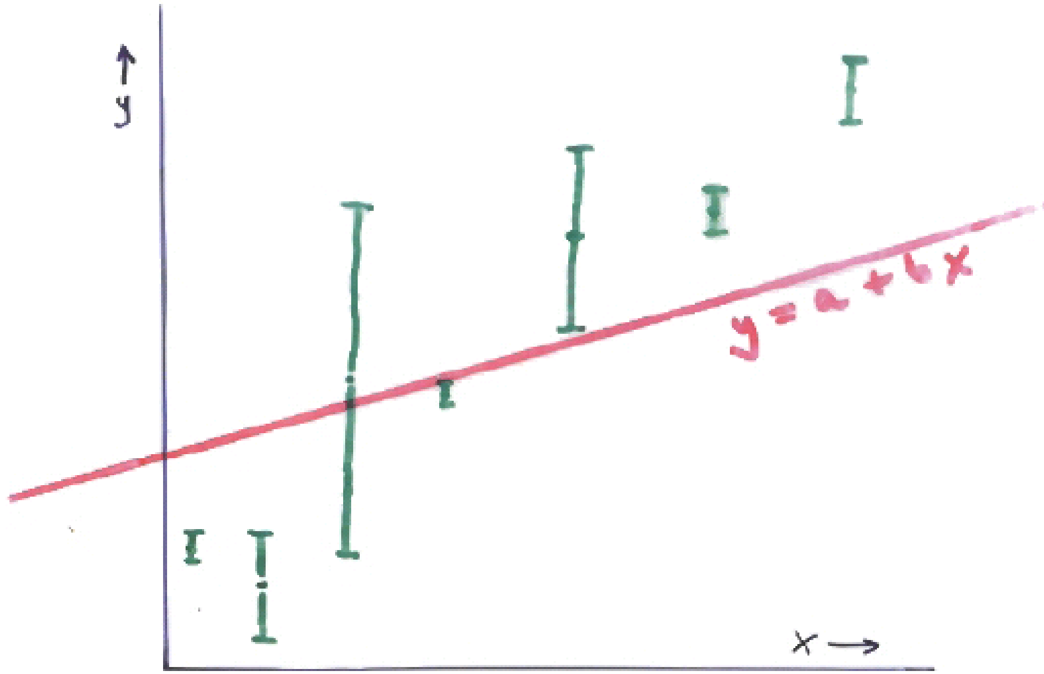
If theory and data OK:

$y^{th} \sim y^{obs}$ → S small

Minimise S → best line

Value of S_{min} → how good fit is

*	Th	Obs	σ^{th}	σ^{obs}	Cont to S
	0.01	1	0.1		98
				1	1



Criterion:

$a + bx_i$; Vert devn

$$S = \sum_i \left(\frac{y_i^{th}(a,b) - y_i^{obs}}{\sigma_i} \right)^2$$

An error for each pt.

Straight Line Fit

$$S = \sum_i \left(\frac{(a + b x_i) - y_i}{\sigma_i} \right)^2$$

i) "Draw" lots of lines $\Rightarrow$ S for each

ii) Minimise S (w.r.t. $\underline{\underline{a}}$ & $\underline{\underline{b}}$)

$$\frac{1}{2}\frac{\partial S}{\partial a} = \sum_i \frac{(a + b x_i - y_i)}{\sigma_i^2} = 0$$

$$\frac{1}{2}\frac{\partial S}{\partial b} = \sum_i \frac{(a + b x_i - y_i) x_i}{\sigma_i^2} = 0$$

2 SIM. EQNS FOR 2 UNKNOWNS ($\underline{a}$ & $\underline{b}$)

$$b = \frac{[1][xy] - [x][y]}{[1][x^2] - [x][x]} = \frac{\langle xy\rangle - \langle x\rangle\langle y\rangle}{\langle x^2\rangle - \langle x\rangle^2}$$

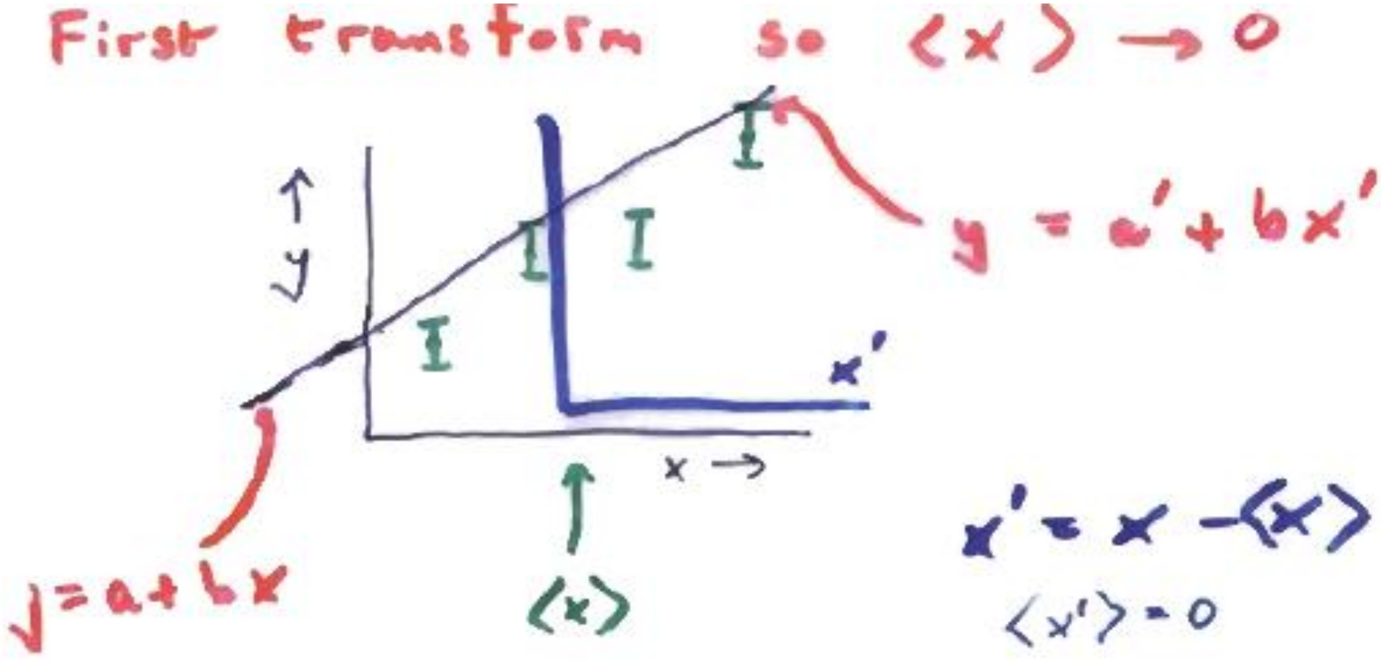
where $[f] = \sum \frac{f_i}{\sigma_i^2}$

& $\langle f\rangle = [f]/[1]$

$$\langle y\rangle = a + b\langle x\rangle$$

N.B. L.S.B.F. passes through (<x>, <y>)

Uncertainties on intercept and gradient



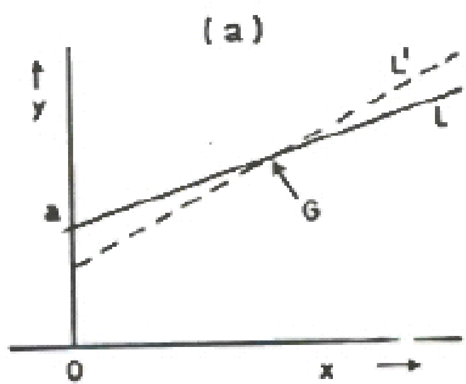
Better to use x' because

uncertainties on a' and b are UNCORRELATED

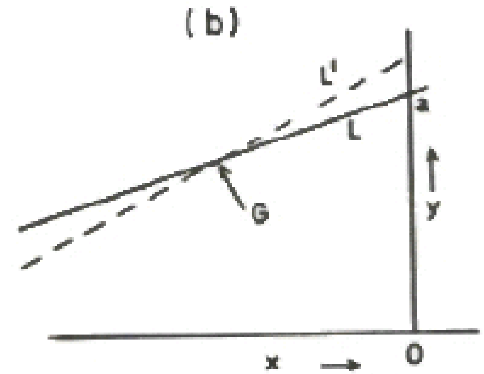
Contrast uncertainties on a and b are CORRELATED

That is why track parameters specified at track 'centre'

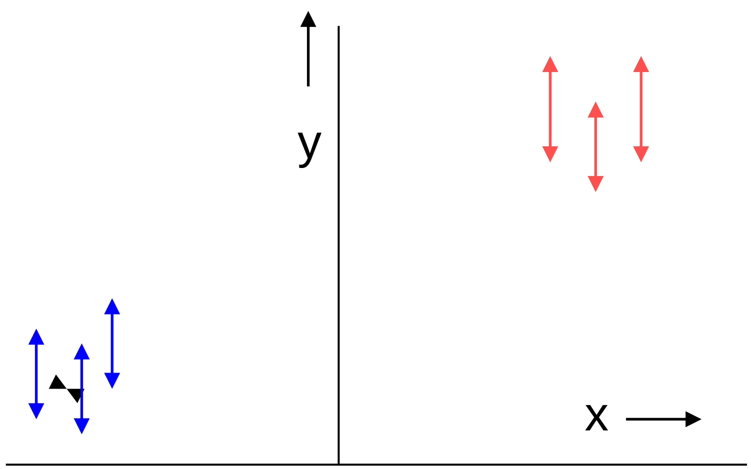
Covariance(a,b) ~ -<x>

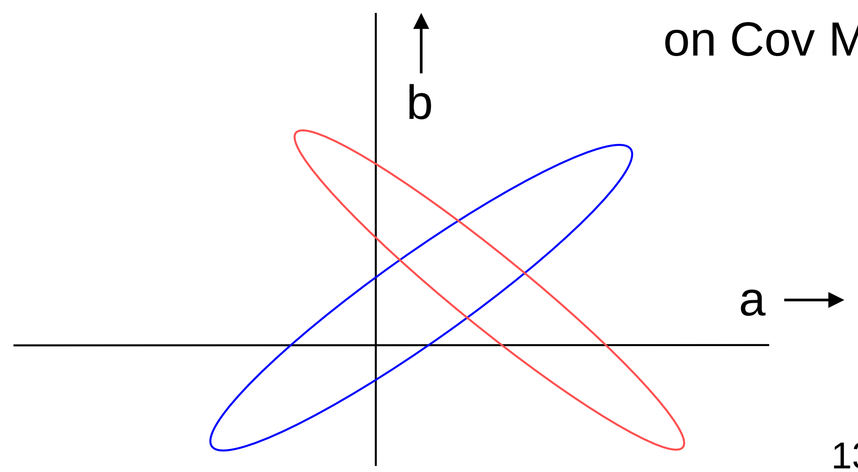


<x> positive



<x> negative





See lecture
on Cov Matrix

Comments on Least Squares method

1) Need to bin

Beware of too few events/bin   (Want Poisson ~ Gaussian)

2) Extends to n dimensions →

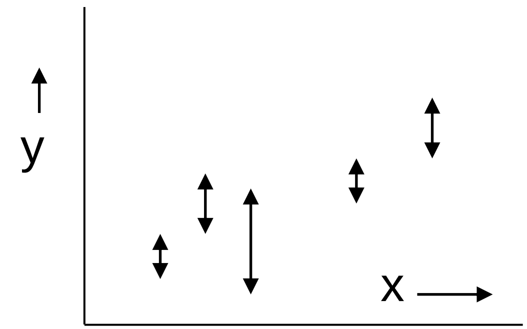
but needs lots of events for n larger than 2 or 3

3) No problem with correlated uncertainties

4) Can calculate S_{min} "on line"   i.e. single pass through data

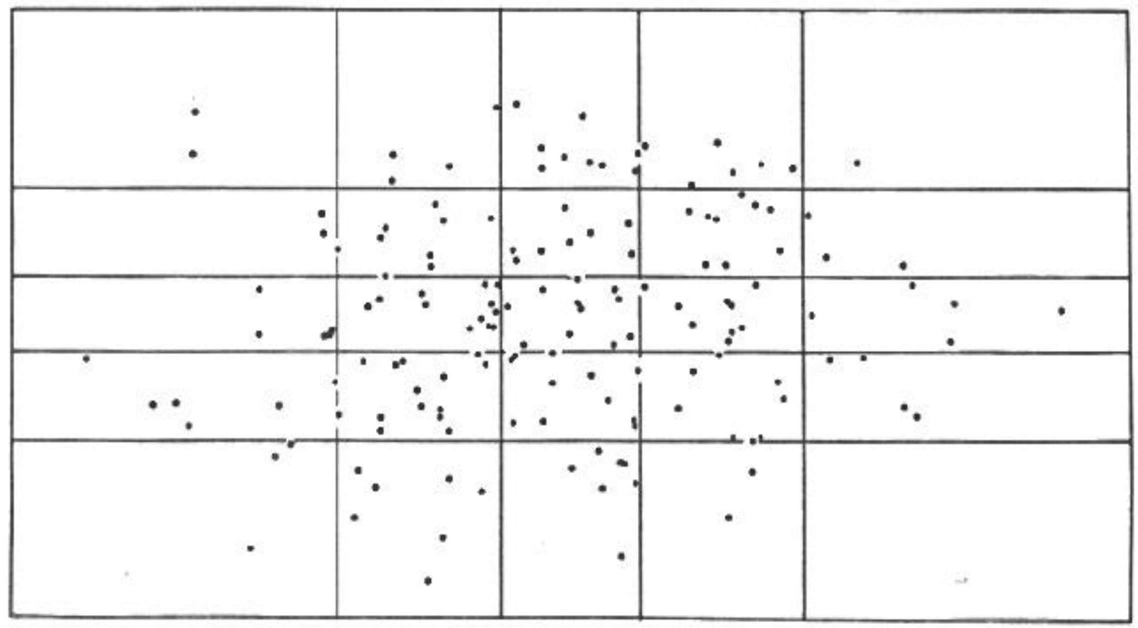
$$\Sigma (y_i - a - bx_i)^2 / \sigma^2 = [y_i^2] - b\,[x_i y_i] - a\,[y_i]$$

5) For theory linear in params, analytic solution



6) Goodness of Fit ★ ★ ★

	Individual events (e.g. in cos θ)	$y_i \pm \sigma_i$ v x_i (e.g. stars)
1) Need to bin?	Yes	No need
4) χ^2 on line	First histogram	Yes



	Moments	Max Like	Least squares
Easy?	Yes, if…	Normalisation, maximisation messy	Minimisation
Efficient?	Not very	Usually best	Sometimes = Max Like
Input	Separate events	Separate events	Histogram
Goodness of fit	Messy	No (unbinned)	Easy
Constraints	No	Yes	Yes
N dimensions	Easy if ….	Norm, max messier	Easy
Weighted events	Easy	Errors difficult	Easy
Bgd subtraction	Easy	Troublesome	Easy
Uncertainty estimates	Observed spread, or analytic	$\left\{ - \frac{\partial^2 \ell}{\partial p_i \partial p_j} \right\}^{-1/2}$	$\left\{ \frac{\partial^2 S}{2 \partial p_i \partial p_j} \right\}^{-1/2}$
Main feature	Easy	Best	Goodness of Fit

Goodness of Fit: χ^2 test

1) Construct S and minimise wrt free parameters
2) Determine ν = no. of degrees of freedom

$$\nu = n - p$$

n = no. of data points

p = no. of FREE parameters

3) Look up probability that, for ν degrees of freedom, $\chi^2 \geq S_{min}$

Works ASYMPTOTICALLY, otherwise use MC

[Assumes y_i are GAUSSIAN distributed with mean y_i^{th} and variance σ_i^2]

Properties of mathematical χ^2 distribution:

$$\overline{\chi^2} = \nu$$

$$\sigma^2(\chi^2) = 2\nu$$

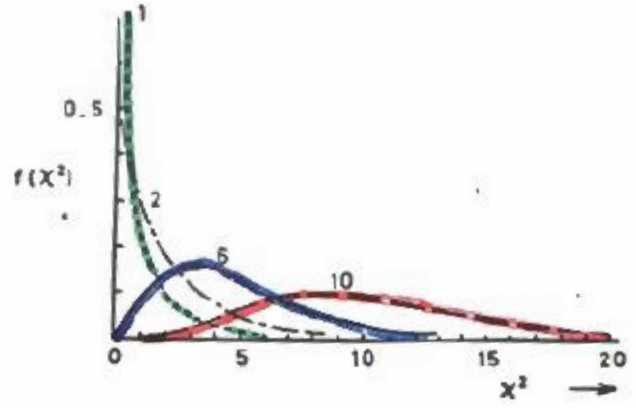
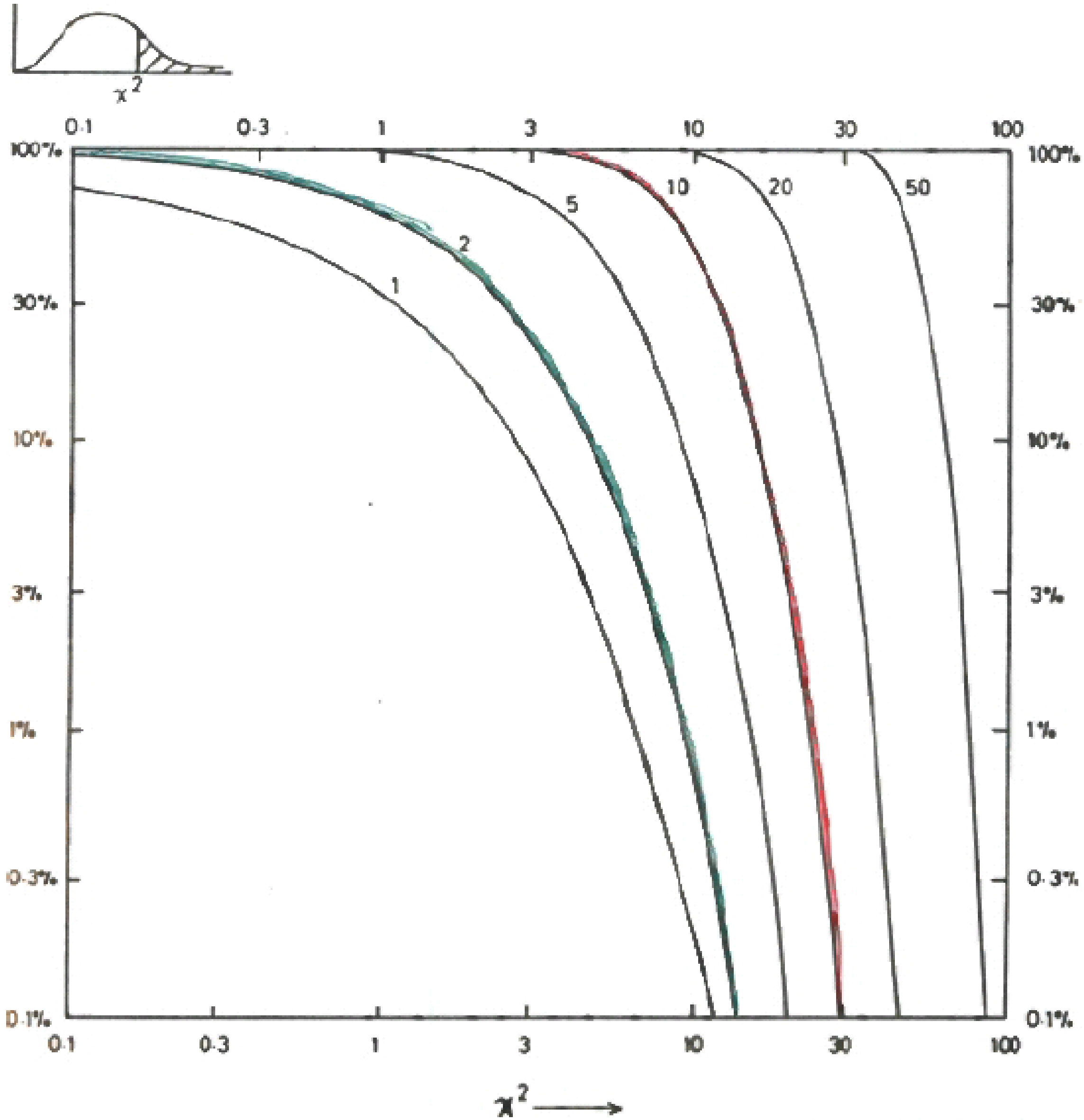


Fig. 2.6

So $S_{min} > \nu + 3\sqrt{2\nu}$ is LARGE

e.g. $S_{min} = 2200$ for $\nu = 2000$?



Cf: Area in tails of Gaussian

χ^2 with ν degrees of freedom?

ν = data – free parameters ?

Why asymptotic (apart from Poisson → Gaussian) ?

a) Fit flatish histogram with

$y = N\,\{1 + 10^{-6}\cos(x-x_0)\}$ $\quad x_0$ = free param

b) Neutrino oscillations: almost degenerate parameters

$y \sim 1 - A\sin^2(1.27\,\Delta m^2\,L/E)$ 2 parameters

$\xrightarrow{\text{Small }\Delta m^2} 1 - A\,(1.27\,\Delta m^2\,L/E)^2$ 1 parameter

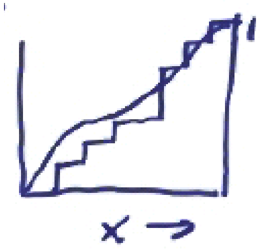
Goodness of Fit

.

$\chi 2$ Very general
Needs binning
Not sensitive to sign of deviation

Run Test

Kolmogorov-Smirnov



Aslan and Zech
PHYSTAT at Durham IPPP (2003)

etc

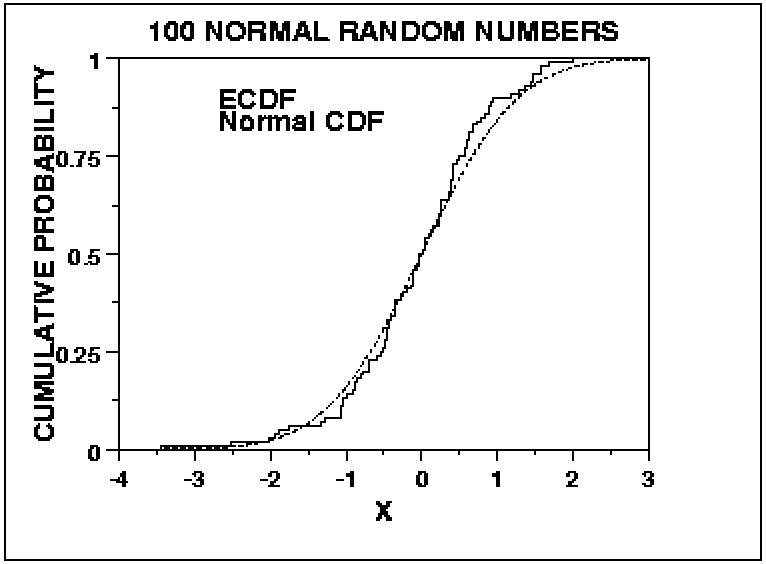
Goodness of Fit: Kolmogorov-Smirnov

Compares data and model cumulative plots

(or 2 sets of data)

Uses largest discrepancy between dists.

Model can be analytic or MC sample



Uses individual data points

Not so sensitive to deviations in tails

(so variants of K-S exist)

Not readily extendible to more dimensions

Distribution-free conversion to p; depends on n

(but not when free parameters involved – needs MC)

Wrong Decisions

Error of First Kind

Reject H0 when true (Loss of efficiency)

Should happen x% of tests

Errors of Second Kind

Accept H0 when something else is true (Contamination)

Frequency depends on ………

i) How similar other hypotheses are

e.g. H0 = μ

Alternatives are: e π K p

ii) Relative frequencies: 10^{-4} 10^{-4} 1 0.1 0.1

Aim for maximum efficiency ← Low error of 1st kind

maximum purity ← Low error of 2nd kind

As χ^2 cut tightens, efficiency ↑ and purity ↓

Choose compromise

How serious are errors of 1st and 2nd kind?

1) Result of experiment

e.g Is spin of resonance = 2?

Get answer WRONG

Where to set cut?

Small cut ⇒ Reject when correct

Large cut ⇒ Never reject anything

Depends on nature of H0 e.g.

Does answer agree with previous expt?

Is expt consistent with special relativity?

2) Class selector e.g. b-quark / galaxy type / γ-induced cosmic shower

Error of 1st kind: Loss of efficiency

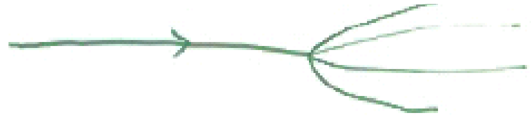
Error of 2nd kind: More background

Usually easier to allow for 1st than for 2nd

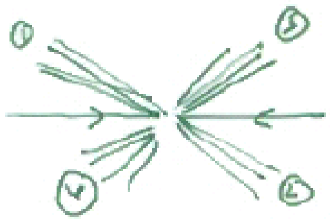
3) Track finding

KINEMATIC FITTING

Tests whether observed event is consistent with specified reaction

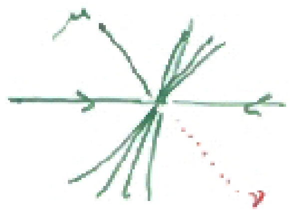
e.g. 

$\bar{p}p \to \bar{p}p\pi^+\pi^-$?



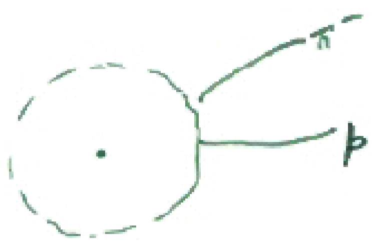
$e^+e^- \to W^+W^-$, $W^+ \to j_1 j_2$, $W^- \to j_3 j_4$

M_W, jet pairings



$e^+e^- \to W^+W^-$, $W^+ \to j_1 j_2$, $W^- \to \mu\nu$

$\Lambda \to p\pi^-$ from prodn vertex



$p + \pi^-$ intersect & $\Lambda \to p\pi^-$ from prodn vert.

Kinematic Fitting: Why do it?

1) Check whether event consistent with hypothesis [Goodness of Fit]

2) Can calculate missing quantities [Param detn.]

3) Good to have tracks conserving E-P [Param detn.]

4) Reduces uncertainties [Param detn.]

Kinematic Fitting: Why do it?

1) Check whether event consistent with hypothesis [Goodness of Fit]
Use S_{min} and ndf

2) Can calculate missing quantities [Param detn.]
e.g. Can obtain |P| for short/straight track, neutral beam; p_x,p_y,p_z of outgoing ν, n, K^0

3) Good to have tracks conserving E-P [Param detn.]
e.g. identical values for resonance mass from prodn or decay

4) Reduces uncertainties [Param detn.]
Example of "Including theoretical input reduces uncertainties"

How we perform Kinematic Fitting ?

Observed event: 4 outgoing charged tracks
Assumed reaction: $pp \rightarrow pp\pi^+\pi^-$

Measured variables: 4-momenta of each track, v_i^{meas}
(i.e. 3-momenta & assumed mass)
Then test hypothesis:
Observed event = example of assumed reaction

i.e. Can tracks be wiggled “a bit” to do so?

Tested by:

$$S_{min} = \Sigma(v_i^{fitted} - v_i^{meas})^2 / \sigma^2$$

where v_i^{fitted} conserve 4-momenta
(Σ over 4 components of each track)
N.B. Really need to take correlations into account

i.e. Minimisation subject to constraints (involves Lagrange Multipliers)

Toy example of Kinematic Fit

$\bar{p} p \to \bar{p} p$

Fixed target experiment

4 constraints:

1) Coplanar
2) p_1 at θ_1
3) p_2 at θ_2
4) θ_1 at θ_2 ⟸ Non-relativistic equal mass elastic scatter : $\theta_1 + \theta_2 = \pi/2$

Measured	$\theta_1^m \pm \sigma$	$\theta_2^m \pm \sigma$
Fitted	θ_1	θ_2

Minimise $S(\theta_1, \theta_2) = \frac{(\theta_1 - \theta_1^m)^2}{\sigma^2} + \frac{(\theta_2 - \theta_2^m)^2}{\sigma^2}$

subject to $C(\theta_1, \theta_2) = \theta_1 + \theta_2 - \pi/2 = 0$

Lagrange : $\frac{\partial S}{\partial \theta_1} + \lambda \frac{\partial C}{\partial \theta_1} = \frac{\partial S}{\partial \theta_2} + \lambda \frac{\partial C}{\partial \theta_2} = 0$

⇒ 3 eqns for θ_1 θ_2 λ

Eqns simple to solve because

$c(\theta_1, \theta_2)$ linear in θ_1, θ_2

$$\Rightarrow \theta_1 = \theta_1^m + \frac{1}{2}\left(\pi/2 - \theta_1^m - \theta_2^m\right)$$

$$\theta_2 = \theta_2^m + \frac{1}{2}\left(\pi/2 - \theta_1^m - \theta_2^m\right)$$

$$\sigma(\theta_1) = \sigma(\theta_2) = \sigma/\sqrt{2}$$

i.e. KINEMATIC FIT →
REDUCED UNCERTAINTIES

THE PARADOX

Histogram with 100 bins

Fit with 1 parameter

S_{min}: χ^2 with NDF = 99 (Expected $\chi^2 = 99 \pm 14$)

For our data, $S_{min}(p_0) = 90$

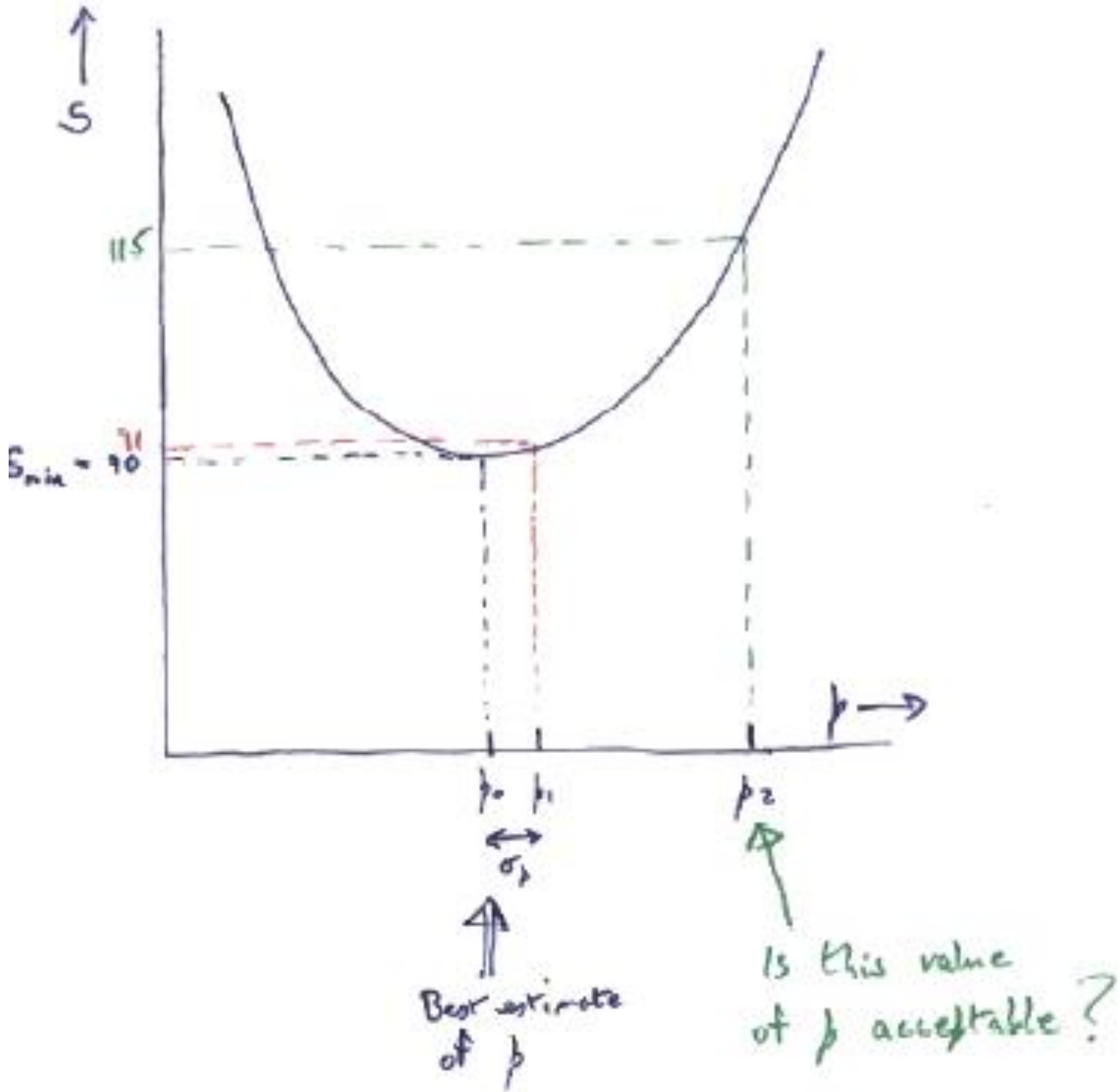
Is p_2 acceptable if $S(p_2) = 115$?

1) YES. Very acceptable χ^2 probability

2) NO. σ_p from $S(p_0 + \sigma_p) = S_{min} + 1 = 91$

But $S(p_2) - S(p_0) = 25$

So p_2 is 5σ away from best value



S
115
91
S_{min} = 90
p
p_0
p_1
p_2
σ_p
Best estimate of p
Is this value of p acceptable?