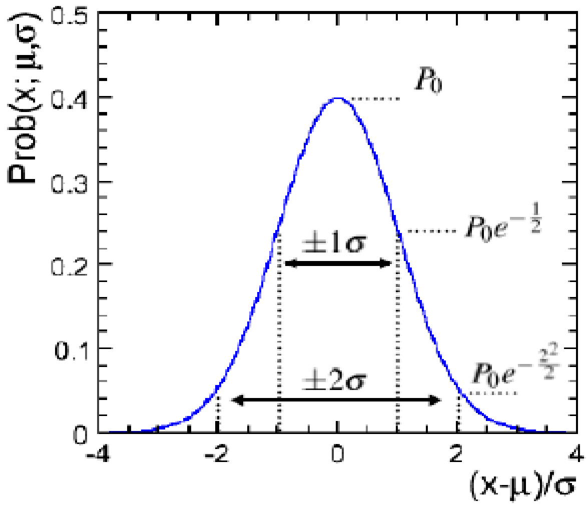
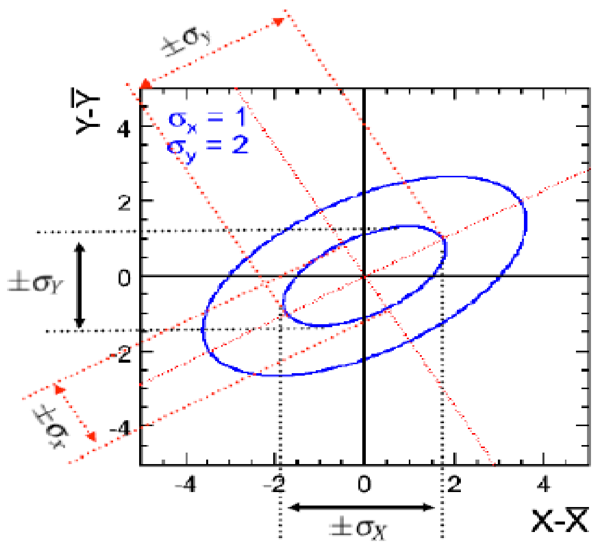
Statistics and Data Analysis (HEP)

The Gaussian Limit

- The central limit theorem,
- Gaussian errors,
- Error propagation,
- Combination of measurements,
- Multidimensional Gaussian errors,
- Error Matrix





Following the course/slides from M. A. Thomson lectures at Cambridge University

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Lecture 1: Back to basics

Introduction, Probability distribution functions, Binomial distributions, Poisson distribution

Lecture 2: The Gaussian Limit

The central limit theorem, Gaussian errors, Error propagation, Combination of measurements, Multi-dimensional Gaussian errors, Error Matrix

Lecture 3: Fitting and Hypothesis Testing

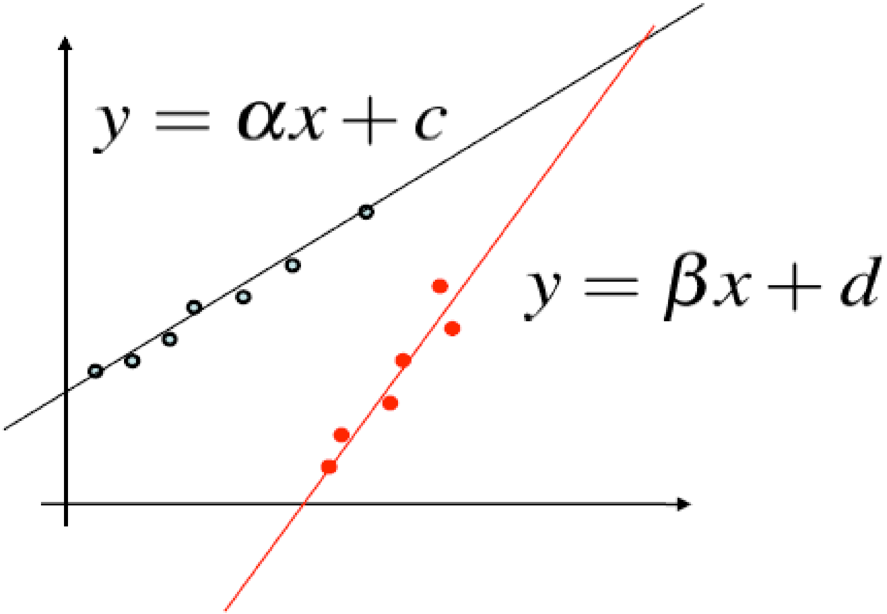
The χ^2 test, Likelihood functions, Fitting, Binned maximum likelihood, Unbinned maximum likelihood

Lecture 4: Dark Arts

Bayesian statistics, Confidence intervals, systematic errors.

How to calculate uncertainties?

- Problem: given the results of two straight line fits with errors, calculate the uncertainty on the intersection



- Solution: first learn about
  - Gaussian errors
  - Correlations
  - Error propagation

The Central Limit Theorem

- ★ We have already shown that for large μ that a Poisson distribution tends to a Gaussian
- ★ This is one example of a more general theorem, the "Central Limit Theorem"*

> If n random variables, x_i, each distributed according to any PDF, are combined then the sum $y = \Sigma\, x_i$ will have a PDF which, for large n, tends to a Gaussian

- ★ For this reason the Gaussian distribution plays an important role in statistics

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

which by make a suitable coordinate transformation, $x \rightarrow \sigma x + \mu$, gives the Normal distribution

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

Mean = zero
Rms = 1

* The proof of the central limit theorem is non-trivial

A useful integral relationship

- ★ We will often take averages of functions of Gaussian distributed quantities $\langle x^2 \rangle, \langle x^4 \rangle$
- ★ Hence interested in integrals of the form

$$\langle (x-\mu)^n \rangle = \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty}(x-\mu)^n e^{-\frac{(x-\mu)^2}{2\sigma^2}}\,\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\sigma^n\int_{-\infty}^{+\infty} y^n e^{-\frac{y^2}{2}}\,\mathrm{d}y$$

- ★ Define

$$I_n = \int_{-\infty}^{+\infty} x^n e^{-\frac{x^2}{2}}\,\mathrm{d}x$$

For n odd, $I_n = 0$

For even n:

$$= \int_{-\infty}^{+\infty} \mathrm{d}(-x^{n-1}e^{-\frac{x^2}{2}}) + (n-1)\int_{-\infty}^{+\infty} x^{n-2}e^{-\frac{x^2}{2}}\,\mathrm{d}x$$

$$= \left[-x^{n-1}e^{-\frac{x^2}{2}}\right]_{-\infty}^{+\infty} + (n-1)I_{n-2}$$

- ★ Hence

$$\frac{I_n}{I_{n-2}} = (n-1) \qquad n > 1$$

- ★ By writing

$$\langle (x-\mu)^n \rangle = \frac{\frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty}(x-\mu)^n e^{-\frac{(x-\mu)^2}{2\sigma^2}}\,\mathrm{d}x}{\frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty} e^{-\frac{(x-\mu)^2}{2\sigma^2}}\,\mathrm{d}x} \Rightarrow \langle (x-\mu)^n \rangle = \frac{I_n}{I_0}\sigma^n$$

e.g.

$$\langle (x-\mu)^4 \rangle = \frac{I_4}{I_0}\sigma^4 = \frac{I_4}{I_2}\frac{I_2}{I_0}\sigma^4 = (4-1)(2-1)\frac{I_0}{I_0}\sigma^4 = 3\sigma^4$$

Properties of Gaussian Distribution

★ Normalised to unity (it's a PDF)

$$\int_{-\infty}^{+\infty} G(x;\mu,\sigma)\mathrm{d}x = 1$$

Proof:

$$\begin{aligned}\int_{-\infty}^{+\infty} G(x;\mu,\sigma)\mathrm{d}x &= \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty} e^{-\frac{(x-\mu)^2}{2\sigma^2}}\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}\sigma}\cdot\sqrt{2}\sigma\cdot\int_{-\infty}^{+\infty} e^{-y^2}\mathrm{d}y \\ &= \frac{1}{\sqrt{2\pi}\sigma}\cdot\sqrt{2}\sigma\cdot\sqrt{\pi} = 1\end{aligned}$$

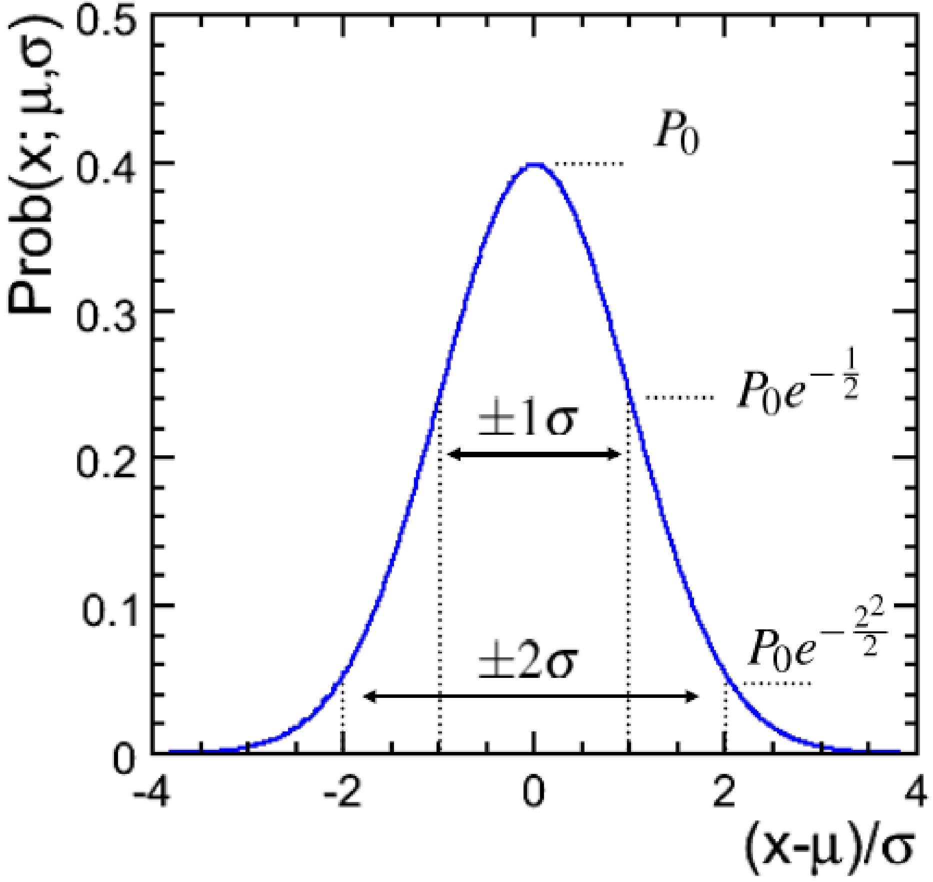
★ Variance

$$Var(x) = \langle (x-\mu)^2\rangle = \sigma^2$$

Proof:

$$\begin{aligned}Var(x) = \int_{-\infty}^{+\infty}(x-\mu)^2 G(x;\mu,\sigma)\mathrm{d}x &= \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{+\infty}(x-\mu)^2 e^{-\frac{(x-\mu)^2}{2\sigma^2}}\mathrm{d}x \\ &= \frac{I_2}{I_0}\sigma^2 \\ &= \sigma^2\end{aligned}$$

Properties of the 1D Gaussian Distribution, cont.



$$G(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

★ Natural to introduce $\chi^2(x)$

$$\chi^2 = \frac{(x-\mu)^2}{\sigma^2}$$

"squared deviation from mean in terms of standard error"

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

★ Fractions of events

$68.3\,\%$	:	$\lvert x-\mu \rvert < 1\sigma$	$(\chi^2 < 1)$
$95.5\,\%$	:	$\lvert x-\mu \rvert < 2\sigma$	$(\chi^2 < 4)$
$99.7\,\%$	:	$\lvert x-\mu \rvert < 3\sigma$	$(\chi^2 < 9)$
6×10^{-7}	:	$\lvert x-\mu \rvert > 5\sigma$	$(\chi^2 > 25)$

Averaging Gaussian Measurements

★ Suppose we have two independent measurements of a quantity, e.g. the W boson mass:

$$x_1 \pm \sigma_1 \quad \text{and} \quad x_2 \pm \sigma_2$$

there are two questions we can ask:

- Are the measurements compatible? [Hypothesis test – we'll return to this]
- What is our best estimate of the parameter x? (i.e. how to average)

★ In principle can take any linear combination as an unbiased estimator of x

$$x_{12} = \omega_1 x_1 + \omega_2 x_2 \qquad \text{provided} \qquad \omega_1 + \omega_2 = 1$$

since $\langle x_{12} \rangle = \omega_1 \langle x_1 \rangle + \omega_2 \langle x_2 \rangle = \omega_1 \mu + \omega_2 \mu = \mu$

★ Clearly want to give the highest weight to the more precise measurements… e.g. two undergraduate measurements of $g\,[\mathrm{m\,s^{-2}}]$

$$10.1 \pm 0.3 \qquad 5 \pm 5$$

★ **Method I:** choose the weights to minimise the uncertainty on

$$\sigma_x^2 = \sum_i \omega_i^2 \sigma_i^2$$

subject to constraint $f(\omega_1, \omega_2, \ldots) = 1 - \sum_i \omega_i = 0$

$$\frac{\partial(\sigma_x^2 + \lambda f)}{\partial \omega_i} = 0$$

$$\Rightarrow \quad 2\omega_i \sigma_i^2 - \lambda = 0$$

$$\omega_i \propto \frac{1}{\sigma_i^2}$$

★ Therefore, since the weights sum to unity:

$$\omega_i = \frac{1/\sigma_i^2}{\sum_j 1/\sigma_j^2}$$

★ Hence for two measurements

$$\bar{x} = \frac{\frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

with

$$\sigma_{\bar{x}}^2 = \frac{1}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

Problem: derive this.

(just error propagation as described later)

Averaging Gaussian Measurements II

★ Can obtain the same expression using a natural probability based approach

- We can interpret the first measurement in terms of a probability distribution for the true value of x, i.e. a Gaussian centred on x_1

$$P(x) = P(x; x_1) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(x-x_1)^2}{2\sigma_1^2}\right\}$$

- Bayes' theorem then tells us how to modify this in the light of a new measurement

$$P(x; data) \propto P(data; x) P(x)$$

$$P(x; data) \propto \exp\left\{-\frac{(x-x_2)^2}{2\sigma_2^2}\right\} \exp\left\{-\frac{(x-x_1)^2}{2\sigma_1^2}\right\}$$

- So our new expression for the knowledge of x is:

$$P(x) \propto \exp -\frac{1}{2}\left\{\frac{(x-x_1)^2}{\sigma_1^2} + \frac{(x-x_2)^2}{\sigma_2^2}\right\}$$

- Completing the square gives plus a little algebra gives

$$P(x) \propto \exp\left\{-\frac{(x-\bar{x})^2}{2\sigma^2}\right\} \quad \text{with} \quad \bar{x} = \frac{\frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}} \quad \text{and} \quad \sigma^2 = \frac{1}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

- Product of n Gaussians is a Gaussian

Error Propagation I

- Suppose measure a quantity x with a Gaussian uncertainty σ_x; what is the uncertainty on a derived quantity

$$y = f(x)$$

  - Expand $f(x)$ about $\bar{x}$

$$f(x) = f(\bar{x}) + (x - \bar{x}) \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}} + \ldots$$

  - Define estimate of y: $\bar{y} = f(\bar{x})$

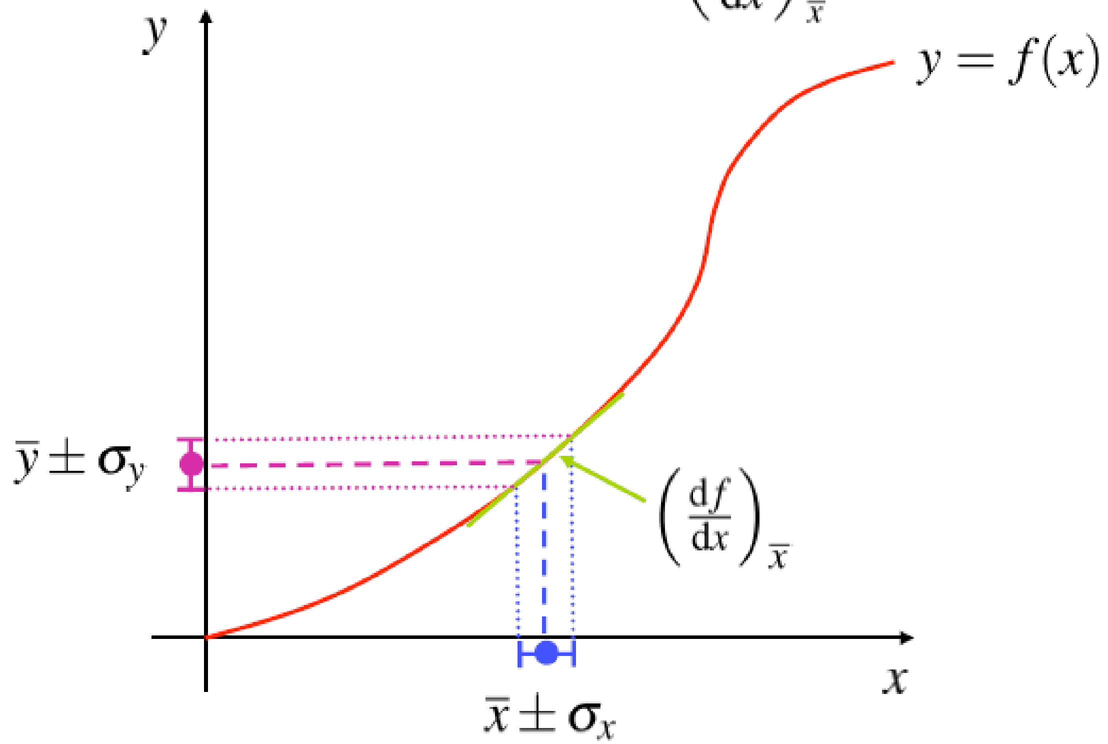
so $$y - \bar{y} = f(x) - f(\bar{x}) \approx (x - \bar{x}) \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}}$$

$$\langle (y - \bar{y})^2 \rangle = \langle (x - \bar{x})^2 \rangle \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}}^2$$

$$\sigma_y^2 = \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}}^2 \sigma_x^2$$

$$\boxed{\sigma_y = \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}} \sigma_x}$$

★ It is easy to understand the origin of $\sigma_y = \left(\frac{df}{dx}\right)_{\bar{x}} \sigma_x$

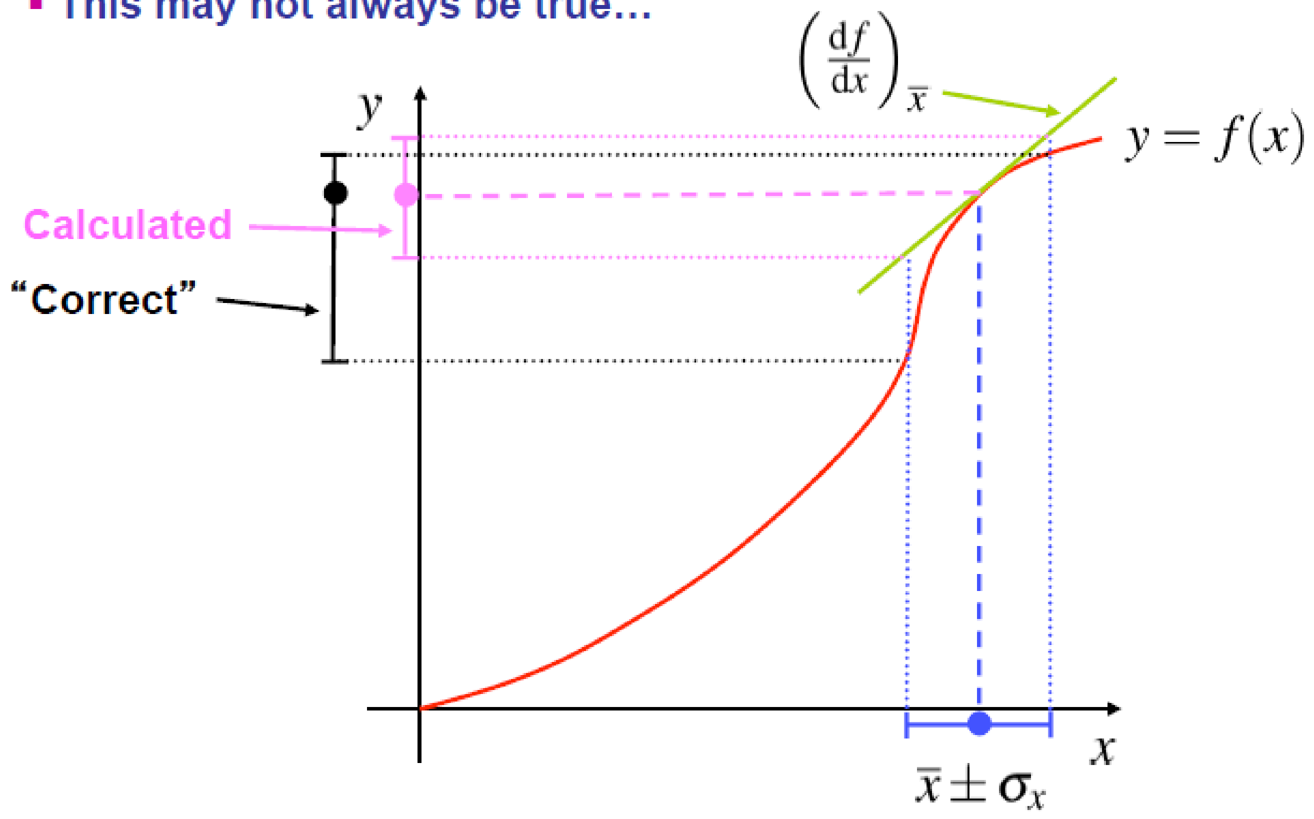


★ How does a "small" change in x, i.e. σ_x, propagate to a small change in y, σ_y

$$\frac{\sigma_y}{\sigma_x} \approx \left(\frac{dy}{dx}\right)_{\bar{x}}$$

★ A word of warning…

- In deriving the error propagation equation → $\sigma_y = \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_{\bar{x}} \sigma_x$
- Neglected second order terms in the Taylor expansion
- This is equivalent to saying that the derivative is constant in region of interest
- This may not always be true…



Error on Error

★ Recall question 2:

Given 5 measurements of a quantity x: 10.2, 5.5, 6.7, 3.4, 3.5

What is the best estimate of x and what is the estimated uncertainty?

$$\bar{x} = 5.86; \quad s_{n-1} = 2.80; \quad \sigma_{\bar{x}} = \frac{s_{n-1}}{\sqrt{5}} = 1.25$$

So our best estimate of x is: $x = 5.9 \pm 1.3$

★ But how good is our estimate of the error – *i.e.* what is the "error on the error" ?

- It can be shown (see Appendix)

$$Var(s^2) = \frac{1}{n}\left(\langle (x-\mu)^4\rangle - \frac{n-3}{n-1}\langle (x-\mu)^2\rangle^2\right)$$

- For a Gaussian distribution $\langle (x-\mu)^4\rangle = 3\sigma^4$

so $$Var(s^2) = \frac{\sigma^4}{n}\left(3 - \frac{n-3}{n-1}\right) = \frac{2\sigma^4}{n-1}$$

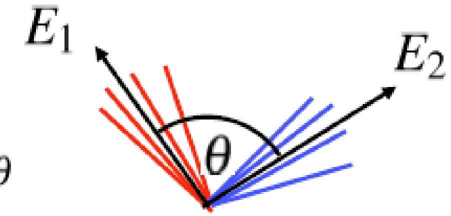
- Hence (by error propagation – show this) the error on the error estimate is

$$\sigma_s = \frac{\sigma}{\sqrt{2(n-1)}}$$

- To obtain a 10% estimate of σ; need rms of 51 measurements !

Combining Gaussian Errors

- There are many cases where we want to combine measurements to extract a single quantity, e.g. di-jet invariant mass



$$m^2 = E_1 E_2 (1 - \cos\theta)$$

  - What is the uncertainty on the mass given $\sigma_{E_1}, \sigma_{E_2}, \sigma_\theta$

- Start by considering a simple example

$$a = x + y$$

  - Mean of a is $\quad \overline{a} = \overline{x} + \overline{y}$
  - Variance of a is given by:

$$\begin{aligned}
\langle (a - \overline{a})^2 \rangle &= \langle (x + y - (\overline{x} + \overline{y}))^2 \rangle \\
\sigma_a^2 &= \langle ([x - \overline{x}] + [y - \overline{y}])^2 \rangle \\
&= \langle (x - \overline{x})^2 \rangle + \langle (y - \overline{y})^2 \rangle + 2\langle (x - \overline{x})(y - \overline{y}) \rangle \\
&= \sigma_x^2 + \sigma_y^2 + 2\langle (x - \overline{x})(y - \overline{y}) \rangle
\end{aligned}$$

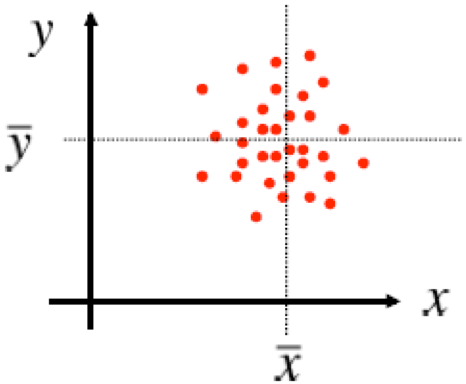
- Two important points:
  - Errors add in quadrature (*i.e.* sum the squares)
  - The appearance of a new term, the covariance of x and y

$$\boxed{\mathrm{cov}(x, y) = \langle (x - \overline{x})(y - \overline{y}) \rangle}$$

Correlated errors: covariance

★ Consider $\mathrm{cov}(x,y) = \langle (x-\bar{x})(y-\bar{y}) \rangle$

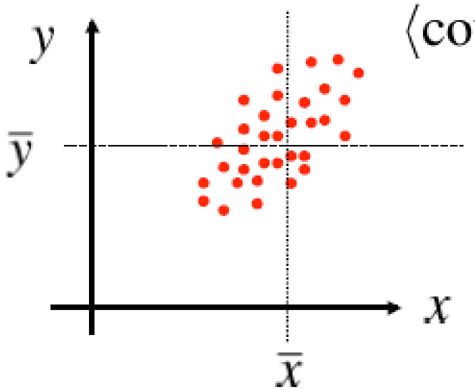
- Suppose in a single experiment measure a value of x and y
- Imagine repeating the measurement multiple times ⇨ $\{x_i, y_i\}$
- If the measurements of x and y are uncorrelated, i.e. **INDEPENDENT**



$$\langle \mathrm{cov}(x,y) \rangle = 0$$

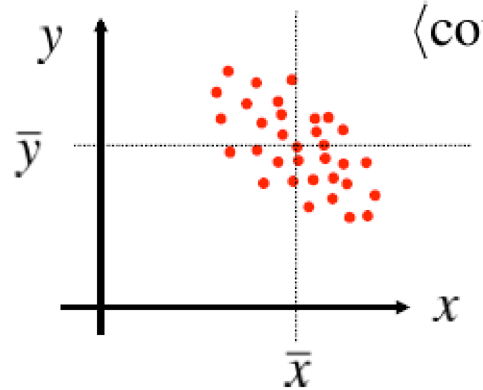
- If x and y are correlated

$$\langle \mathrm{cov}(x,y) \rangle > 0$$



- If x and y are anti-correlated

$$\langle \mathrm{cov}(x,y) \rangle < 0$$

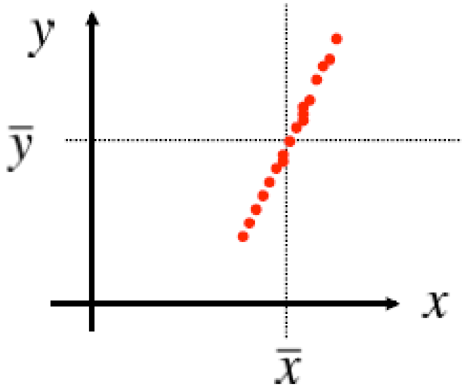


★ Often convenient to express covariance in terms of the correlation coefficient

$$\rho = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y}$$

$$\mathrm{cov}(x,y) = \langle (x-\bar{x})(y-\bar{y}) \rangle$$
$$\sigma_x = \langle (x-\bar{x})^2 \rangle^{\frac{1}{2}}$$

- Consider an experiment which returns two values x and y; where $y\text{-}\bar{y} = 2(x\text{-}\bar{x})$



$$\begin{aligned} \mathrm{cov}(x,y) &= \langle (x-\bar{x})(2x-2\bar{x}) \rangle \\ &= 2\langle (x-\bar{x})^2 \rangle \\ &= 2\sigma_x^2 = \sigma_x \sigma_y \\ \Rightarrow \quad \rho &= +1 \end{aligned}$$

★ Hence (unsurprisingly) the correlation coefficient expresses the degree of correlation with

$$|\rho| \leq 1$$

★ Going back to $a = x + y$

$$\Rightarrow \qquad \sigma_a^2 = \sigma_x^2 + \sigma_y^2 + 2\rho\sigma_x\sigma_y$$

Error propagation II: the general case

- We can now consider the more general case

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

$$\begin{aligned}
a &= f(x,y) = f(\bar{x},\bar{y}) + \frac{\partial f}{\partial x}(x-\bar{x}) + \frac{\partial f}{\partial y}(y-\bar{y}) + \ldots \\
(a-\bar{a})^2 &= (f(x,y) - f(\bar{x},\bar{y}))^2 \\
&\approx \left(\frac{\partial f}{\partial x}\right)^2 (x-\bar{x})^2 + \left(\frac{\partial f}{\partial y}\right)^2 (y-\bar{y})^2 + 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}(x-\bar{x})(y-\bar{y}) \\
\langle (a-\bar{a})^2 \rangle &= \left(\frac{\partial f}{\partial x}\right)^2 \langle (x-\bar{x})^2 \rangle + \left(\frac{\partial f}{\partial y}\right)^2 \langle (y-\bar{y})^2 \rangle + 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\langle (x-\bar{x})(y-\bar{y}) \rangle \\
\sigma_a^2 &= \left(\frac{\partial f}{\partial x}\right)^2 \sigma_x^2 + \left(\frac{\partial f}{\partial y}\right)^2 \sigma_y^2 + 2\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\mathrm{cov}(x,y)
\end{aligned}$$

$$\boxed{\sigma_a^2 = \left(\frac{\partial f}{\partial x}\right)^2 \sigma_x^2 + \left(\frac{\partial f}{\partial y}\right)^2 \sigma_y^2 + 2\rho\frac{\partial f}{\partial x}\frac{\partial f}{\partial y}\sigma_x\sigma_y}$$

- In order to estimate the error on a derived quantity need to know correlations

Example continued

★Back to the original problem $m = \{E_1 E_2 (1-\cos\theta)\}^{\frac{1}{2}}$

$$\sigma_m^2 = \left(\frac{\partial m}{\partial E_1}\right)^2 \sigma_{E_1}^2 + \left(\frac{\partial m}{\partial E_2}\right)^2 \sigma_{E_2}^2 + \left(\frac{\partial m}{\partial \theta}\right)^2 \sigma_\theta^2 + $$
$$2\rho_{12}\frac{\partial m}{\partial E_1}\frac{\partial m}{\partial E_2}\sigma_{E_1}\sigma_{E_2} + 2\rho_{1\theta}\frac{\partial m}{\partial E_1}\frac{\partial m}{\partial \theta}\sigma_{E_1}\sigma_\theta + 2\rho_{2\theta}\frac{\partial m}{\partial E_2}\frac{\partial m}{\partial \theta}\sigma_{E_2}\sigma_\theta$$

★First assume independent errors on E_1, E_2, θ and for simplicity neglect σ_θ term

$$\frac{\partial m}{\partial E_1} = \frac{1}{2}\left\{\frac{E_2}{E_1}(1-\cos\theta)\right\}^{\frac{1}{2}} \qquad \frac{\partial m}{\partial E_2} = \frac{1}{2}\left\{\frac{E_1}{E_2}(1-\cos\theta)\right\}^{\frac{1}{2}}$$

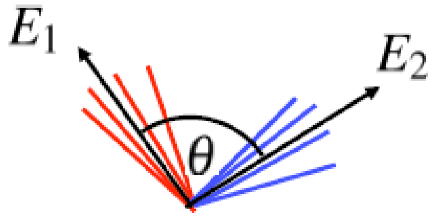
giving: $$\sigma_m^2 = \frac{1}{4}\left\{\frac{E_2}{E_1}(1-\cos\theta)\right\}\sigma_{E_1}^2 + \frac{1}{4}\left\{\frac{E_1}{E_2}(1-\cos\theta)\right\}\sigma_{E_2}^2$$

$$\frac{\sigma_m}{m} = \frac{1}{2}\left\{\frac{\sigma_{E_1}^2}{E_1^2} + \frac{\sigma_{E_2}^2}{E_2^2}\right\}^{\frac{1}{2}}$$

★EXERCISE: by first considering σ_{m^2}, calculate $\frac{\sigma_m}{m}$, including the σ_θ term

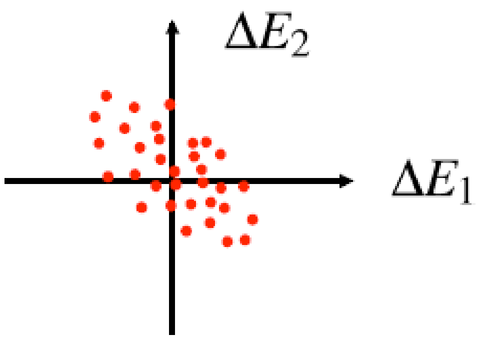
ANS: $$\frac{\sigma_m}{m} = \frac{1}{2}\left\{\frac{\sigma_{E_1}^2}{E_1^2} + \frac{\sigma_{E_2}^2}{E_2^2} + \cot^2\left(\frac{\theta}{2}\right)\sigma_\theta^2\right\}^{\frac{1}{2}}$$

Estimating the Correlation Coefficient



- Correlations can arise from physical effects, e.g.
  - Would expect E_1 and E_2 to be (slightly) anti-correlated why ?
  - Can always check (in MC) by plotting

$$\Delta E_1 = E_1 - E_1^{MC} \quad \text{against} \quad \Delta E_2 = E_2 - E_2^{MC}$$



$$\rho = \frac{\mathrm{cov}(x,y)}{\sigma_x \sigma_y}$$

$$\mathrm{cov}(x,y) = \langle (x-\overline{x})(y-\overline{y}) \rangle$$
$$\sigma_x = \langle (x-\overline{x})^2 \rangle^{\frac{1}{2}}$$

NOTE: uncertainty on correlation coefficient $s_\rho \approx \frac{(1-\rho^2)}{\sqrt{n-2}}$

- Correlations also arise when calculating derived quantities from uncorrelated measurements
  - e.g. $x = a + b \quad y = a - b$
  - this type of correlation can be handled mathematically (see later)

Properties of the 2D Gaussian Distribution

- ★ For two independent variables (x,y) the joint probability distribution $P(x,y)$ is simply the product of the two distributions

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

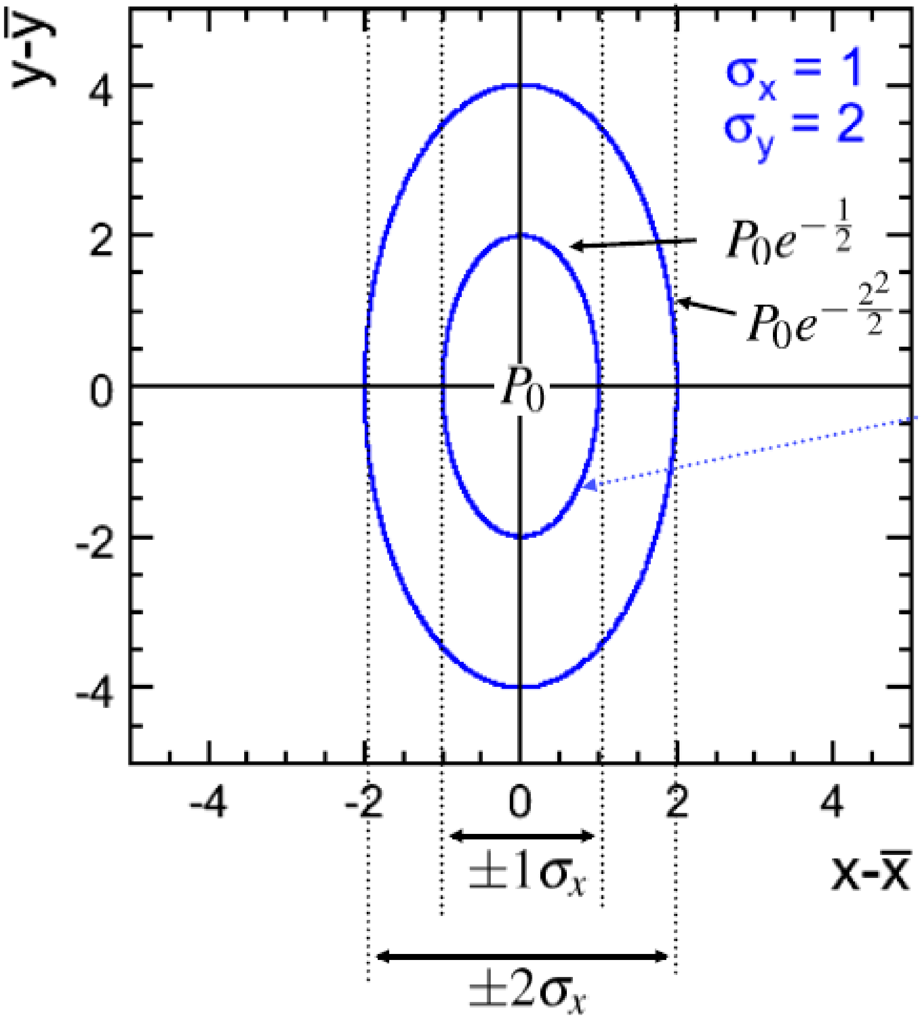
$$P(x,y) = \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{1}{2}\left[\frac{(x-\bar{x})^2}{\sigma_x^2}+\frac{(y-\bar{y})^2}{\sigma_y^2}\right]\right\}$$

NOTE:

$$\int_{-\infty}^{+\infty} P(x,y)\mathrm{d}y = \frac{1}{\sqrt{2\pi}\sigma_x}\exp\left\{-\frac{(x-\bar{x})^2}{2\sigma_x^2}\right\} = P(x)$$

- ★ Can write in terms of χ^2 with

$$P(x,y) = \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{\chi^2}{2}\right\} \qquad \chi^2 = \chi_x^2+\chi_y^2 = \frac{(x-\bar{x})^2}{\sigma_x^2}+\frac{(y-\bar{y})^2}{\sigma_y^2}$$



- 68 % of events within ±1 σ_x
- 68 % of events within ±1 σ_y
- Now consider contours of

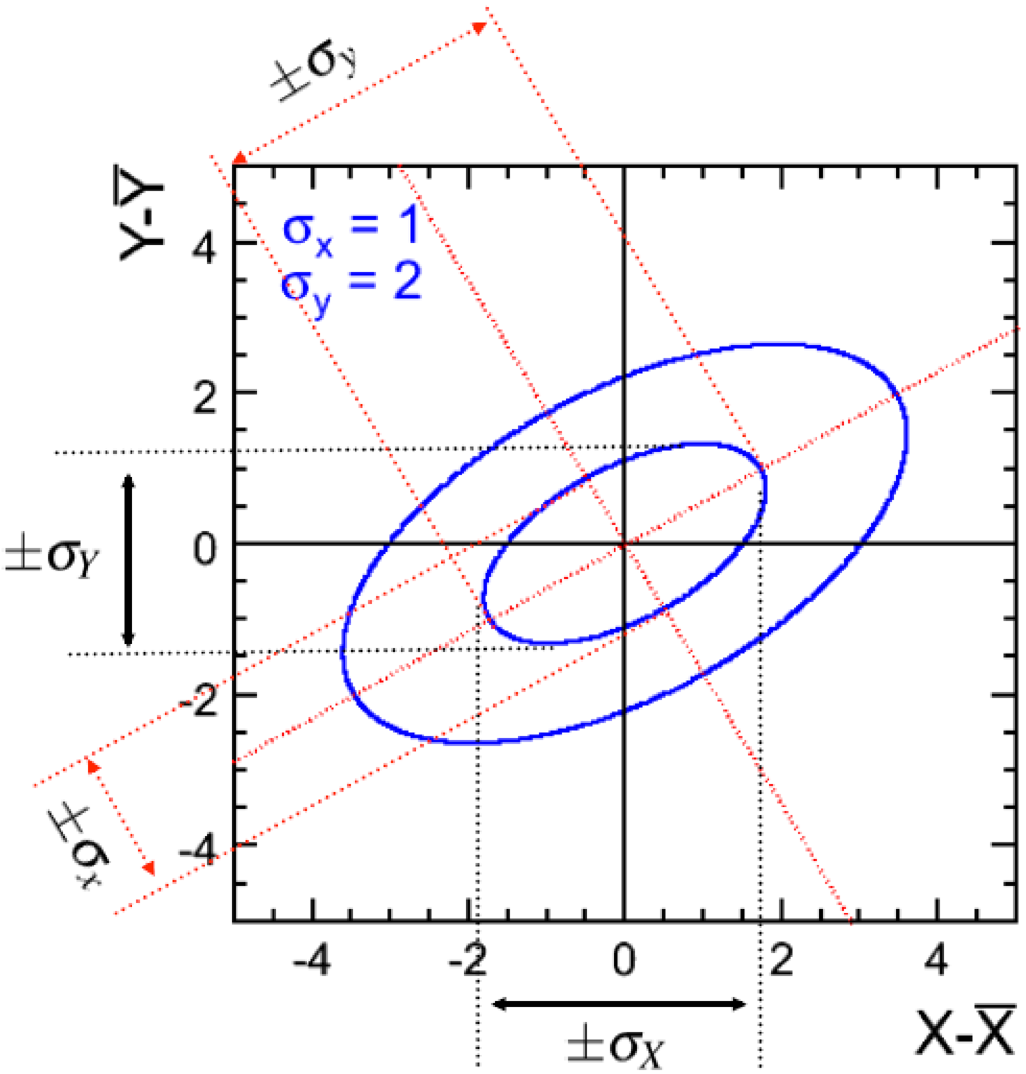
$$\chi^2 = \frac{(x-\bar{x})^2}{\sigma_x^2} + \frac{(y-\bar{y})^2}{\sigma_y^2}$$

- $\chi^2 = 1$ corresponds to contour where PDF falls to $e^{-\frac{1}{2}}$ of peak
- Only 39% of events within $\chi^2 < 1$
- Only 86% of events within $\chi^2 < 4$

Now to introduce correlations… rotate the ellipse

$$\begin{pmatrix} X-\bar{X} \\ Y-\bar{Y} \end{pmatrix} = \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} x-\bar{x} \\ y-\bar{y} \end{pmatrix}$$

$$s = \sin\theta; \quad c = \cos\theta$$



- Same PDF, but now w.r.t. different axes
- Simple to derive the general error ellipse with correlations…

Let
$$\begin{aligned} X &= +cx + sy \\ Y &= -sx + cy \end{aligned}$$

To find the equivalent correlation coefficient, evaluate

$$\langle XY \rangle = \langle scy^2 - scx^2 + (c^2 - s^2)xy \rangle = sc(\sigma_y^2 - \sigma_x^2)$$

hence

$$\rho_{XY}\sigma_X\sigma_Y = sc(\sigma_y^2 - \sigma_x^2)$$

To eliminate the rotation angle, write

$$\sigma_X^2 = \langle X^2 \rangle = \langle c^2x^2 + s^2y^2 + 2csxy \rangle = c^2\sigma_x^2 + s^2\sigma_y^2$$

$$\sigma_Y^2 = \langle Y^2 \rangle = \langle c^2y^2 + s^2x^2 - 2csxy \rangle = c^2\sigma_y^2 + s^2\sigma_x^2$$

giving

$$\sigma_X^2\sigma_Y^2 = s^2c^2(\sigma_x^4 + \sigma_y^4) + (c^4 + s^4)\sigma_x^2\sigma_y^2$$

Compare to:

$$\rho^2\sigma_X^2\sigma_Y^2 = s^2c^2(\sigma_y^4 + \sigma_x^4 - 2\sigma_x^2\sigma_y^2)$$

gives

$$\sigma_X^2\sigma_Y^2 = \rho^2\sigma_X\sigma_Y + (c^4 + 2s^2c^2 + s^4)\sigma_x^2\sigma_y^2$$

hence

$$(1 - \rho^2)\sigma_X^2\sigma_Y^2 = \sigma_x^2\sigma_y^2$$

Properties of 2D Gaussian Distribution

- Start from uncorrelated 2D Gaussian:

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

- Make the coordinate transformation

$$x = cX - sY; \quad y = sX + cY \qquad P(x,y)\mathrm{d}x\mathrm{d}y = P(X,Y)\mathrm{d}X\mathrm{d}Y$$

$$\begin{aligned}
P(X,Y) &= \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{(cX-sY)^2}{2\sigma_x^2}-\frac{(cY+sX)^2}{2\sigma_y^2}\right\} \\
&= \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{X^2}{2}\left[\frac{c^2}{\sigma_x^2}+\frac{s^2}{\sigma_y^2}\right]-\frac{Y^2}{2}\left[\frac{c^2}{\sigma_y^2}+\frac{s^2}{\sigma_x^2}\right]+\frac{2XY}{2}sc\left[\frac{1}{\sigma_x^2}-\frac{1}{\sigma_y^2}\right]\right\} \\
&= \frac{1}{2\pi\sigma_x\sigma_y}\exp\left\{-\frac{X^2}{2}\left[\frac{c^2\sigma_y^2+s^2\sigma_x^2}{\sigma_x^2\sigma_y^2}\right]-\frac{Y^2}{2}\left[\frac{c^2\sigma_x^2+s^2\sigma_y^2}{\sigma_x^2\sigma_y^2}\right]+\frac{2XY}{2}sc\left[\frac{\sigma_y^2-\sigma_x^2}{\sigma_x^2\sigma_y^2}\right]\right\}
\end{aligned}$$

- From previous page identify

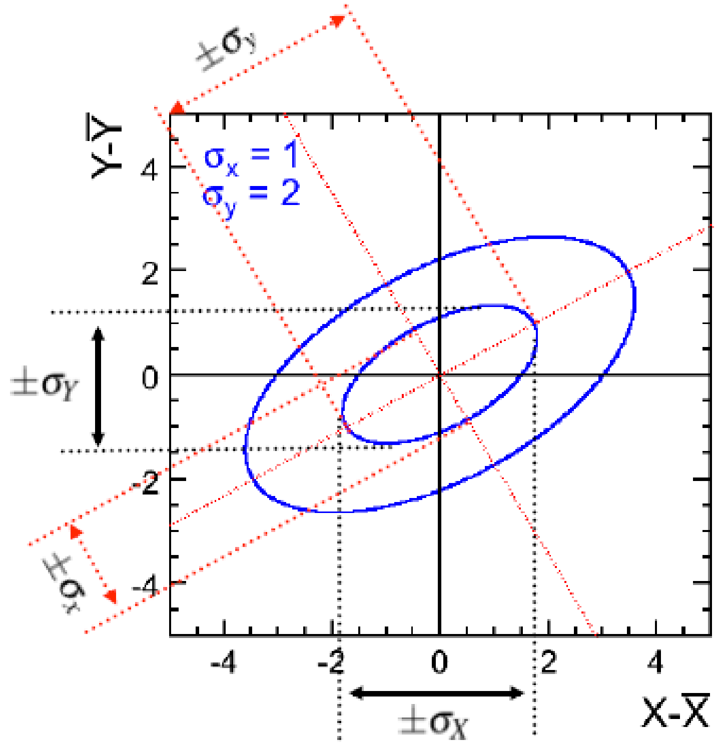
$$\langle X^2\rangle = \sigma_X^2 = c^2\sigma_x^2 + s^2\sigma_y^2 \qquad \langle Y^2\rangle = \sigma_Y^2 = c^2\sigma_y^2 + s^2\sigma_x^2 \qquad (1-\rho^2)\sigma_X^2\sigma_Y^2 = \sigma_x^2\sigma_y^2$$

$$P(X,Y) = \frac{1}{2\pi\sqrt{(1-\rho^2)}\sigma_X\sigma_Y}\exp\left\{-\frac{X^2}{2}\left[\frac{\sigma_Y^2}{(1-\rho^2)\sigma_X^2\sigma_Y^2}\right]-\frac{Y^2}{2}\left[\frac{\sigma_X^2}{(1-\rho^2)\sigma_X^2\sigma_Y^2}\right]+\frac{2\rho XY}{2(1-\rho^2)\sigma_X\sigma_Y}\right\}$$

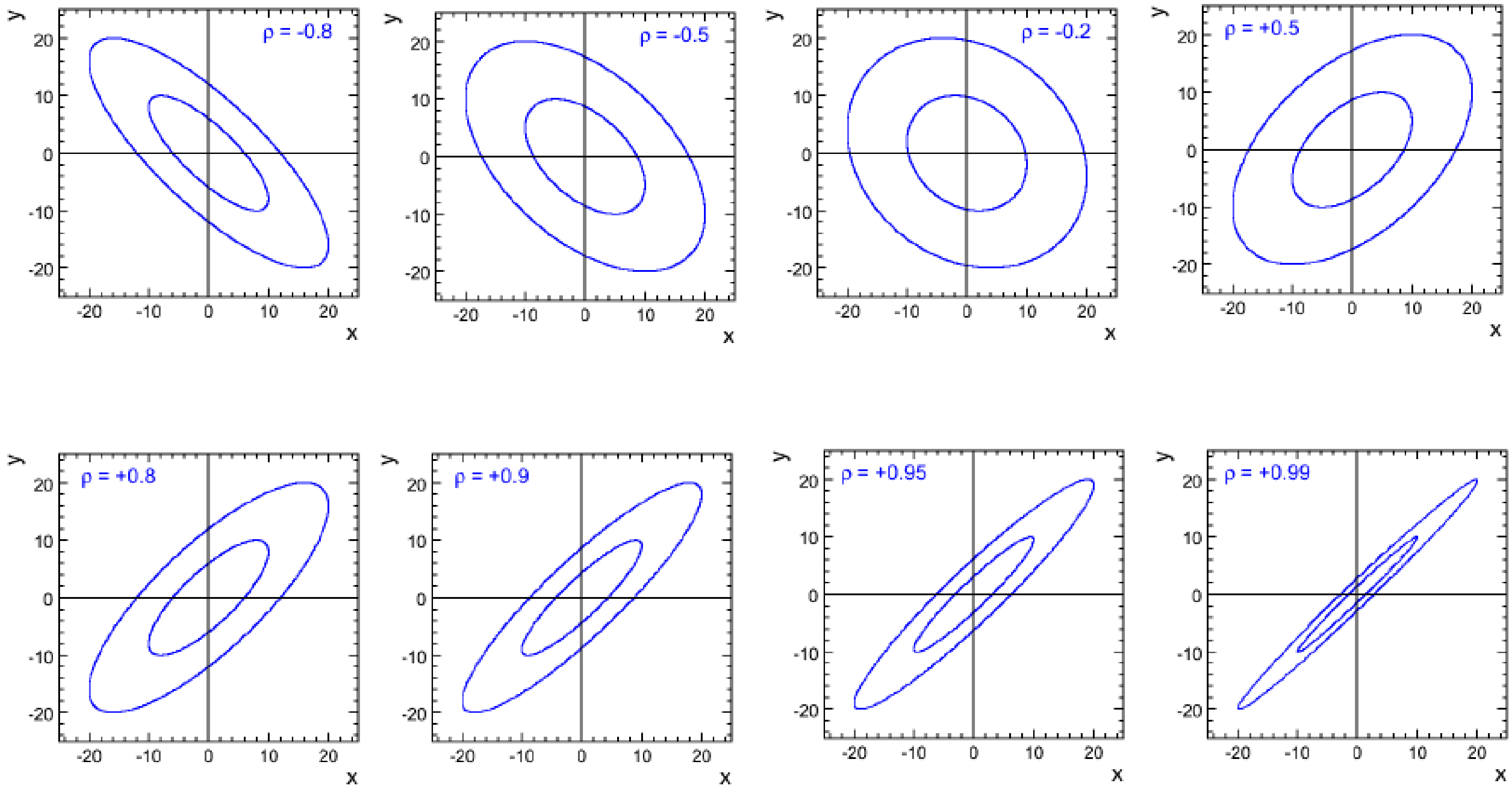
$$= \frac{1}{2\pi\sqrt{(1-\rho^2)}\sigma_X\sigma_Y}\exp\left\{-\frac{1}{2}\frac{1}{1-\rho^2}\left[\frac{X^2}{\sigma_X^2}+\frac{Y^2}{\sigma_Y^2}-\frac{2\rho XY}{\sigma_X\sigma_Y}\right]\right\}$$

- ★ **Note we have now expressed the same ellipse in terms of the new coordinates, where the errors are now correlated.**

- ★ **If dealing with correlated errors can always find a linear combination of variables which are uncorrelated**



★ **Example 2D error ellipses with different correlation coefficients**



The Error Ellipse and Error Matrix

★ Now we have the general equation for two correlated Gaussian distributed quantities

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

★ Defines the error ellipse

★ Ultimately want to generalise this to an N variable hyper-ellipsoid

★ Sounds hard… but is actually rather simple in matrix form

★ Define the ERROR MATRIX

$$\mathbf{M} = \begin{pmatrix} \langle x^2\rangle & \langle xy\rangle \\ \langle xy\rangle & \langle y^2\rangle \end{pmatrix} \quad \text{i.e.} \quad \mathbf{M} = \begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix}$$

★ and define the DISCREPANCY VECTOR

$$\mathbf{x} = \begin{pmatrix} x-\bar{x} \\ y-\bar{y} \end{pmatrix}$$

det**M**

using $\mathbf{M}^{-1} = \frac{1}{1-\rho^2}\begin{pmatrix} \frac{1}{\sigma_x^2} & -\frac{\rho}{\sigma_x\sigma_y} \\ -\frac{\rho}{\sigma_x\sigma_y} & \frac{1}{\sigma_y^2} \end{pmatrix}$ and $|\mathbf{M}| = (1-\rho^2)\sigma_x^2\sigma_y^2$

we can write

$$P(x,y) = \frac{1}{2\pi|\mathbf{M}|^{\frac{1}{2}}}\exp\left\{-\frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{M}^{-1}\mathbf{x}\right\}$$

★ The beauty of this formalism is that it can be extended to any number of correlated Gaussian distributed variables

$$P(x_1, x_2, \ldots, x_n) = \frac{1}{(2\pi)^{\frac{n}{2}} |\mathbf{M}|^{\frac{1}{2}}} \exp\left\{ -\frac{1}{2} \mathbf{x}^{\mathbf{T}} \mathbf{M}^{-\mathbf{1}} \mathbf{x} \right\}$$

with

$$\mathbf{M} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \ldots & \rho_{1n}\sigma_1\sigma_n \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \ldots & \rho_{2n}\sigma_2\sigma_n \\ \ldots & \ldots & \ldots & \ldots \\ \rho_{1n}\sigma_1\sigma_n & \rho_{2n}\sigma_2\sigma_n & \ldots & \sigma_n^2 \end{pmatrix}$$

★ Can write this in terms of the χ^2 for n-variables (including correlations)

$$P(x_1, x_2, \ldots, x_n) = \frac{1}{(2\pi)^{\frac{n}{2}} |\mathbf{M}|^{\frac{1}{2}}} \exp\left\{ -\frac{\chi^2}{2} \right\} = P_0 e^{-\frac{\chi^2}{2}}$$

with $\boxed{\chi^2 = \mathbf{x}^{\mathbf{T}} \mathbf{M}^{-\mathbf{1}} \mathbf{x}}$

General transformation of Errors

- ★ Suppose we have a set of variables, x_i, and the error matrix, **M**, and now wish to transform to a set of variables, y_i, defined by
- ★ Taylor expansion about mean:

$$
\begin{aligned}
y_i &= \bar{y}_i + \sum_k \frac{\partial y_i}{\partial x_k}(x_l - \bar{x}_k) + \mathcal{O}(\Delta x^2) \\
y_i - \bar{y}_i &\approx \sum_k \frac{\partial y_i}{\partial x_k}(x_k - \bar{x}_k) \\
\langle (y_i - \bar{y}_i)(y_j - \bar{y}_j) \rangle &= \left\langle \sum_k \frac{\partial y_i}{\partial x_k}(x_k - \bar{x}_k) \sum_\ell \frac{\partial y_j}{\partial x_\ell}(x_\ell - \bar{x}_\ell) \right\rangle \\
&= \sum_{k\ell} \frac{\partial y_i}{\partial x_k} \frac{\partial y_j}{\partial x_\ell} \langle (x_k - \bar{x}_k)(x_\ell - \bar{x}_\ell) \rangle \\
\mathbf{M}_{\{\mathbf{y}\}}{}^{ij} &= \sum_{k\ell} \frac{\partial y_i}{\partial x_k} \frac{\partial y_j}{\partial x_\ell} \mathbf{M}_{\{\mathbf{x}\}}{}^{k\ell} \\
\mathbf{M}_{\{\mathbf{y}\}} &= \mathbf{T}^{\mathbf{T}} \mathbf{M}_{\{\mathbf{x}\}} \mathbf{T}
\end{aligned}
$$

★ **T** is the error transformation matrix

$$\mathbf{T} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_2} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial y_1}{\partial x_n} & \frac{\partial y_2}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

For Gaussian errors we can now do anything !

★ Can deal with:
- correlated errors
- arbitrary dimensions
- parameter transformations

Examples…

A simple example

★ Measure two uncorrelated variables $a \pm \sigma_a, \; b \pm \sigma_b$

Error matrix $\mathbf{M} = \begin{pmatrix} \sigma_a^2 & 0 \\ 0 & \sigma_b^2 \end{pmatrix} \qquad \mathbf{M}^{-1} = \begin{pmatrix} 1/\sigma_a^2 & 0 \\ 0 & 1/\sigma_b^2 \end{pmatrix}$

★ Calculate two derived quantities

$$x = a + b \qquad y = a - b$$

★ Transformation matrix

$$\mathbf{T} = \begin{pmatrix} \frac{\partial x}{\partial a} & \frac{\partial y}{\partial a} \\ \frac{\partial x}{\partial b} & \frac{\partial y}{\partial b} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

★ Giving

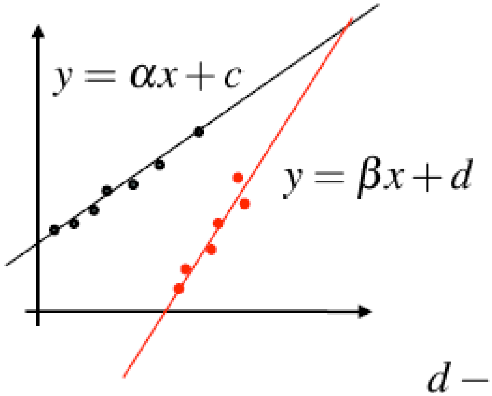
$$\begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix} = \mathbf{T}^{\mathbf{T}}\mathbf{M}\mathbf{T} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \sigma_a^2 & 0 \\ 0 & \sigma_b^2 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_a^2 + \sigma_b^2 & \sigma_a^2 - \sigma_b^2 \\ \sigma_a^2 - \sigma_b^2 & \sigma_a^2 + \sigma_b^2 \end{pmatrix}$$

$$\boxed{\sigma_x^2 = \sigma_y^2 = \sigma_a^2 + \sigma_b^2; \quad \rho = \frac{\sigma_a^2 - \sigma_b^2}{\sigma_a^2 + \sigma_b^2}}$$

A more involved example

★ Given the results of two straight line fits, calculate the uncertainty on the intersection



- With the error matrix (note the results of the two fits are uncorrelated)

$$\mathbf{M} = \begin{pmatrix} \sigma_\alpha^2 & \rho_1\sigma_\alpha\sigma_c & 0 & 0 \\ \rho_1\sigma_\alpha\sigma_c & \sigma_c^2 & 0 & 0 \\ 0 & 0 & \sigma_\beta^2 & \rho_2\sigma_\beta\sigma_d \\ 0 & 0 & \rho_2\sigma_\beta\sigma_d & \sigma_d^2 \end{pmatrix}$$

- Lines Intersect at: $x = \dfrac{d-c}{\alpha-\beta}$ $\quad y = \dfrac{\alpha d - \beta c}{\alpha - \beta}$
- To calculate error on intersection need error transformation matrix, i.e. need the partial derivatives, e.g. $\dfrac{\partial x}{\partial \alpha} = \dfrac{c-d}{(\alpha-\beta)^2}$
- giving

$$\mathbf{T} = \begin{pmatrix} \frac{\partial x}{\partial \alpha} & \frac{\partial y}{\partial \alpha} \\ \frac{\partial x}{\partial c} & \frac{\partial y}{\partial c} \\ \frac{\partial x}{\partial \beta} & \frac{\partial y}{\partial \beta} \\ \frac{\partial x}{\partial d} & \frac{\partial y}{\partial d} \end{pmatrix} = \frac{1}{\alpha-\beta}\begin{pmatrix} -\kappa & -\beta\kappa \\ -1 & -\beta \\ \kappa & \alpha\kappa \\ +1 & \alpha \end{pmatrix}$$

with $\kappa = \dfrac{d-c}{\alpha-\beta}$

- then its just algebra

$$\begin{pmatrix} \sigma_x^2 & \rho\sigma_x\sigma_y \\ \rho\sigma_x\sigma_y & \sigma_y^2 \end{pmatrix} = \mathbf{T}^{\mathrm{T}}\mathbf{M}\mathbf{T}$$

$$= \begin{pmatrix} -\kappa & -1 & \kappa & +1 \\ -\beta\kappa & -\beta & \alpha\kappa & \alpha \end{pmatrix} \begin{pmatrix} \sigma_\alpha^2 & \rho_1\sigma_\alpha\sigma_c & 0 & 0 \\ \rho_1\sigma_\alpha\sigma_c & \sigma_c^2 & 0 & 0 \\ 0 & 0 & \sigma_\beta^2 & \rho_2\sigma_\beta\sigma_d \\ 0 & 0 & \rho_2\sigma_\beta\sigma_d & \sigma_d^2 \end{pmatrix} \begin{pmatrix} -\kappa & -\beta\kappa \\ -1 & -\beta \\ \kappa & \alpha\kappa \\ +1 & \alpha \end{pmatrix}$$

- giving

$$\sigma_x^2 = \frac{1}{(\alpha-\beta)^2}\left[\kappa^2(\sigma_\alpha^2+\sigma_\beta^2)+2\kappa(\rho_1\sigma_\alpha\sigma_c+\rho_2\sigma_\beta\sigma_d)+\sigma_c^2+\sigma_d^2\right]$$

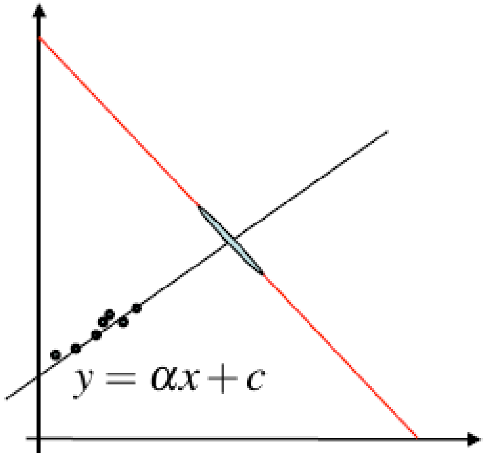
$$\rho\sigma_x\sigma_y = \frac{1}{(\alpha-\beta)^2}\left[\kappa^2(\beta\sigma_\alpha^2+\alpha\sigma_\beta^2)+2\kappa(\rho_1\beta\sigma_\alpha\sigma_c+\rho_2\alpha\sigma_\beta\sigma_d)+\beta\sigma_c^2+\alpha\sigma_d^2\right]$$

$$\sigma_y^2 = \frac{1}{(\alpha-\beta)^2}\left[\kappa^2(\beta^2\sigma_\alpha^2+\alpha^2\sigma_\beta^2)+2\kappa(\rho_1\beta^2\sigma_\alpha\sigma_c+\rho_2\alpha^2\sigma_\beta\sigma_d)+\beta^2\sigma_c^2+\alpha^2\sigma_d^2\right]$$

$$\kappa = \frac{d-c}{\alpha-\beta}$$

★ OK, it is not pretty, but we now have an analytic expression
(i.e. once you have done the calculation, computationally very fast)

- Apply to a special case, intersection with a fixed line $y = 1 - x$



$$\beta = -1;\ d = +1;\ \sigma_\beta = 0;\ \sigma_d = 0$$

$$\sigma_x^2 = \frac{1}{(\alpha-\beta)^2}\left[\kappa^2\sigma_\alpha^2 + 2\kappa\rho_1\sigma_\alpha\sigma_c + \sigma_c^2\right]$$
$$\rho\sigma_x\sigma_y = \frac{1}{(\alpha-\beta)^2}\left[-\kappa^2\sigma_\alpha^2 - 2\kappa\rho_1\sigma_\alpha\sigma_c - \sigma_c^2\right]$$
$$\sigma_y^2 = \frac{1}{(\alpha-\beta)^2}\left[\kappa^2\sigma_\alpha^2 + 2\kappa\rho_1\sigma_\alpha\sigma_c + \sigma_c^2\right]$$

Hence $\sigma_x^2 = \sigma_y^2;\ \rho = -1$ which makes perfect sense

★ The treatment of Gaussian errors via the error matrix is an extremely powerful technique – it is also easy to apply (once you understand the basic ideas)

Summary

- Should now understand:
  - Properties of the Gaussian distribution
  - How to combine errors
  - Propagation simple of 1D errors
  - How to include correlations
  - How to treat multi-dimensional errors
  - How to use the error matrix

- Next up, chi-squared, likelihood fits, …

Appendix: Error on Error - Justification

- Assume mean of distribution is zero (can always make this transformation without affecting the variance)

$$
\begin{aligned}
Var(s^2) &= \langle (s^2-\sigma^2)^2 \rangle \\
&= \langle (\frac{1}{n}\sum x^2 - \sigma^2)^2 \rangle \\
&= \frac{1}{n^2}\langle \sum_i x_i^2 \sum_j x_j^2 \rangle - 2\sigma^2 \langle (\frac{1}{n}\sum x^2) \rangle + \sigma^4 \\
&= \frac{1}{n^2}\left(n\langle x^4\rangle + n(n-1)\langle x_i^2 x_j^2\rangle_{i\neq j}\right) - \sigma^4 \\
&\approx \frac{1}{n}\langle x^4\rangle + \frac{n-1}{n}\sigma^4 - \sigma^4 \\
&= \frac{1}{n}(\langle x^4\rangle - \langle x^2\rangle^2)
\end{aligned}
$$

For large n: $\langle x_i^2 x_j^2\rangle_{i\neq j} \approx \sigma^4$