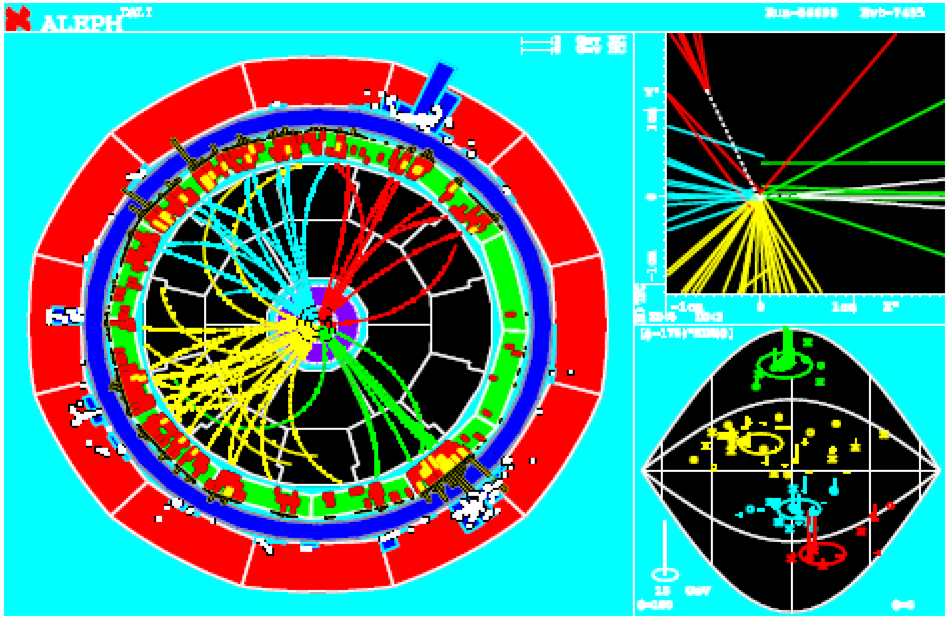
Statistics and Data Analysis

Back to basics



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

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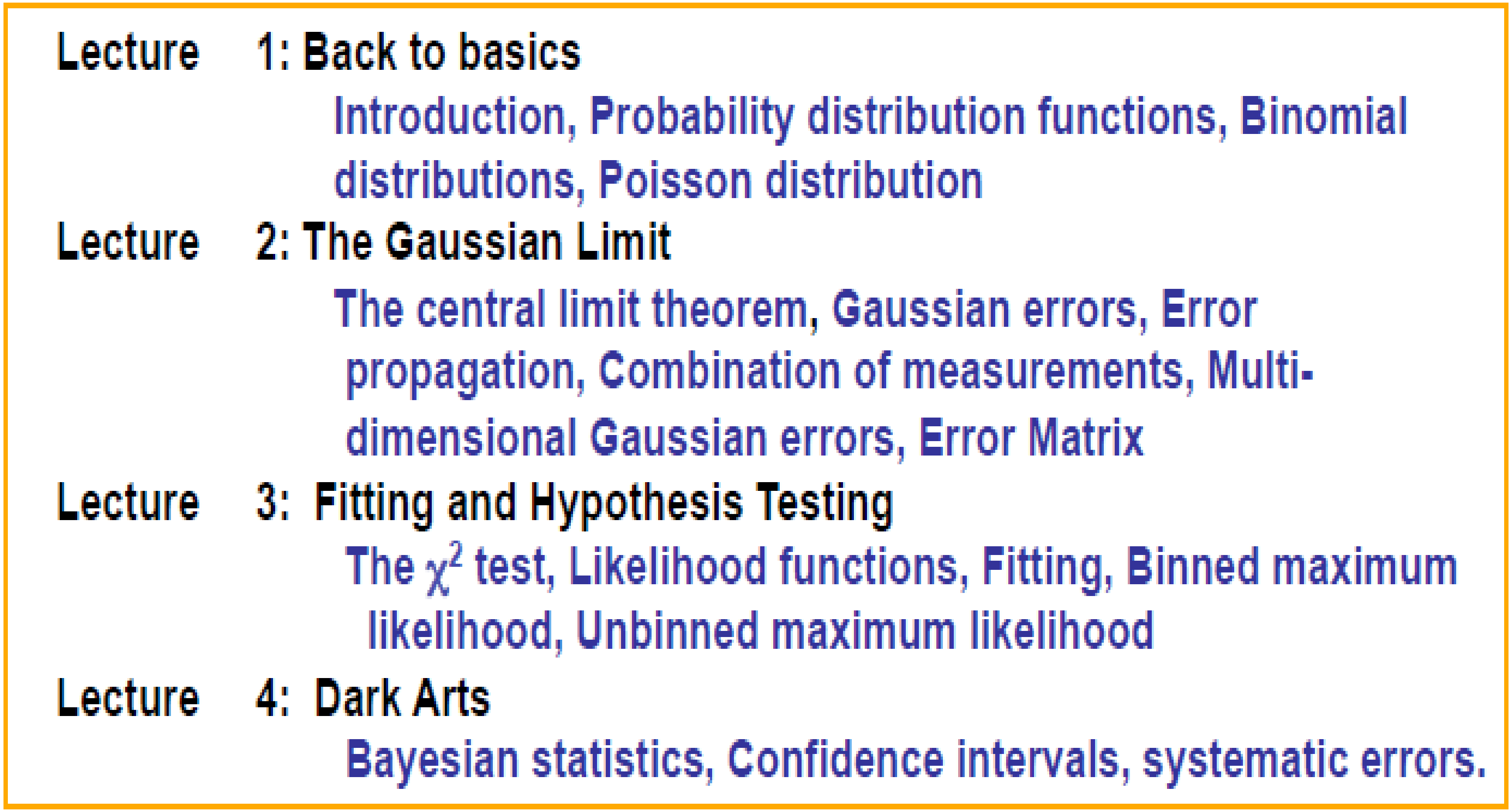
Lectures Synopsis



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.

Experimental Physics

- Experimental science concerned with two types of experimental measurement:
  - Measurement of a quantity : *parameter estimation*
  - Tests of a theory/model : *hypothesis testing*

- For parameter estimation we usually have some data (a set of measurements) and from which we want to obtain
  - The best estimate of the true parameter; "the measured value"
  - The best estimate of how well we have measured the parameter; "the uncertainty"

- For hypothesis testing we usually have some data (a set of measurements) and one or more theoretical models, and want
  - A measure of how consistent our data are with the model; "a probability"
  - Which model best describes our data; "a relative probability"

To address the above questions we need to use and understand statistical techniques

- In these 5±1 lectures we will cover most aspects of statistics as applied to experimental high energy physics:
  - Nothing will be stated without proof (or at least justification).
  - Understanding the derivations will help you to understand the basis behind the statistical techniques

The path to enlightenment:

- If you measure something always quote an uncertainty
- Understand what you are doing and why
- Don’t forget that you are usually *estimating* the uncertainty
  - e.g. don’t worry too much about whether an effect is 2.9σ and 3.1σ
    unlikely you can estimate the uncertainty that well
- Don’t worry too much about the difference between Bayesian and Frequentist approaches
  - often give same results
  - if the results are different – usually means data are weak
    – so do another experiment

Three Types of Errors

Statistical Uncertainties:

- ★ Random fluctuations
  - e.g. shot noise, measuring small currents, how many electrons arrive in a fixed time
  - Tossing a coin N times, how many heads

The main topic of these lectures

Systematic Uncertianies:

- ★ Biases
  - e.g. energy calibration wrong
  - Thermal expansion of measuring device
  - Imperfect theoretical predications

Discussed in the last lecture

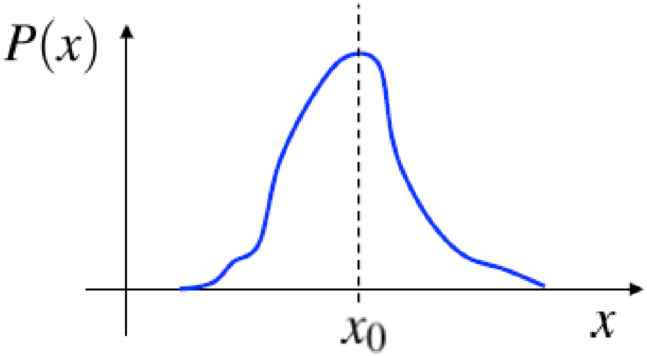
Blunders, i.e. errors:

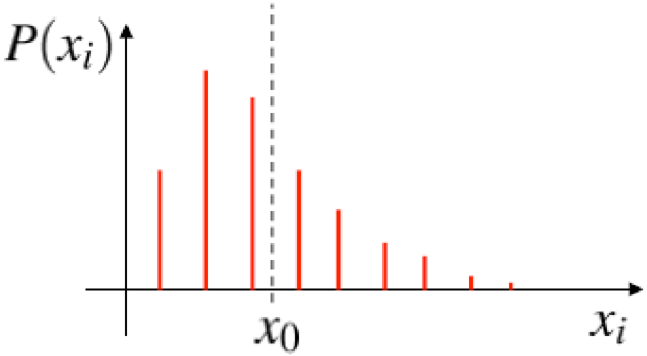
- ★ Mistakes
  - Forgot to include a particular background in analysis
  - Bugs in analysis code

Not discussed, never happen…

Probability Distributions

★ Suppose we are trying to measure some quantity with true value x_0 the result of a single measurement follows a probability density function (**PDF**) which may or may not be of a known form.





★ Normalised:

$$\int_{-\infty}^{+\infty} P(x) = 1 \qquad \sum_{i=0}^{\infty} P(x_i) = 1$$

★ In general, can parameterise the PDF by its moments α_n

$$\alpha_n = \int x^n P(x) \mathrm{d}x \qquad \alpha_n = \sum x^n P_i$$

<u>Note:</u> $\alpha_n \equiv \langle x^n \rangle$

Mean and Variance

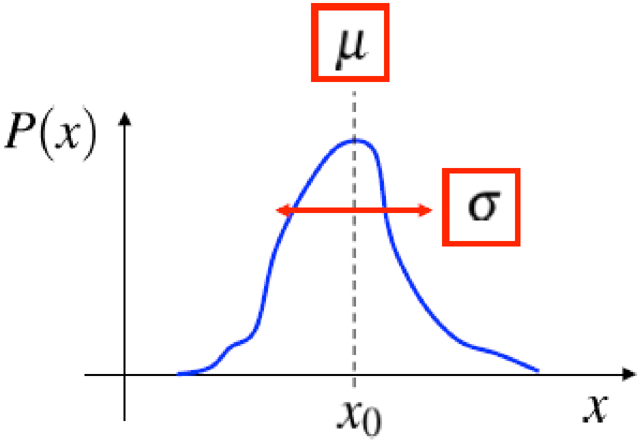
★ Can now define a few important properties of the PDF

Mean: $\mu \equiv \langle x \rangle = \int x P(x)\mathrm{d}x$ "average of many measurements"

Mean of squares: $\langle x^2 \rangle = \int x^2 P(x)\mathrm{d}x$

Variance: $Var(x) \equiv \sigma^2 \equiv \langle (x-\mu)^2 \rangle = \int (x-\mu)^2 P(x)\mathrm{d}x$

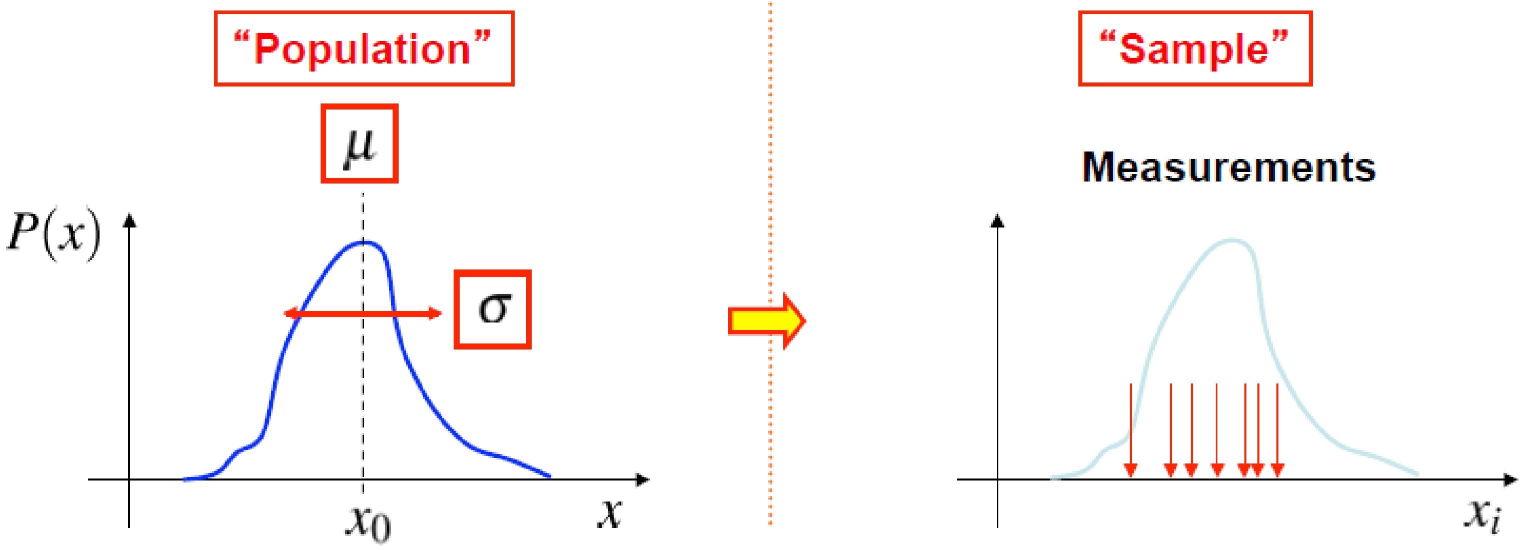
- The variance represents the width of the PDF about the mean
- Convenient to express this in terms of the standard deviation σ
- μ and σ describe the mean and "width" of a PDF
- Sometimes you will see the 3rd and 4th moments used (skewness, kurtosis) (these are not particularly useful)



$$\boxed{\begin{aligned}
\sigma^2 \equiv \langle (x-\mu)^2 \rangle &= \langle x^2 - 2\mu x + \mu^2 \rangle \\
&= \langle x^2 \rangle - 2\mu \langle x \rangle + \mu^2 \\
&= \langle x^2 \rangle - 2\mu^2 + \mu^2 \\
&= \langle x^2 \rangle - \mu^2
\end{aligned}}$$

Estimating the Mean and Variance

- ★ In general do not know the PDF – instead have a number of measurements distributed according to the PDF
- ★ Unless one has a infinite number of measurements cannot fully reconstruct the PDF (not a particularly useful thing to do anyway)
- ★ But can obtain unbiased estimates of the mean and variance



- ★ Best estimate of mean of distribution is the mean of the sample

$$\boxed{\bar{x} = \frac{1}{n}\sum_i x_i}$$

- ★ Can also define **sample** variance

$$\boxed{s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})^2}$$

- ★ How does sample variance s^2 relate to true variance σ^2 ?
- ★ Can calculate average value of variance

$$\begin{aligned}
\langle s^2\rangle &= \langle (x_i - \overline{x})^2\rangle \\
&= \langle x_i^2\rangle - 2\langle x_i \frac{1}{n}\sum_j x_j\rangle + \frac{1}{n^2}\langle [\sum_j x_j]^2\rangle \\
&= \langle x_i^2\rangle - \frac{2}{n}\langle x_i^2 + \sum_{j\neq i} x_i x_j\rangle + \frac{1}{n^2}\left(n\langle x_i^2\rangle + n(n-1)\langle x_i x_j\rangle_{i\neq j}\right) \\
&= \langle x^2\rangle - \frac{1}{n}\langle x^2\rangle + \frac{(n-1)}{n}\langle x_i x_j\rangle_{i\neq j} \\
&= \frac{(n-1)}{n}\left(\langle x^2\rangle - \langle x_i x_j\rangle_{i\neq j}\right) \\
&= \frac{(n-1)}{n}\left(\langle x^2\rangle - \mu^2\right) = \frac{n-1}{n}\sigma^2
\end{aligned}$$

Question 1: prove

$$\boxed{\langle x_i x_j\rangle_{i\neq j} = \mu^2}$$

what assumption have you made?

★ Hence, on average, the sample variance is a factor $\frac{n-1}{n}$ smaller than the true variance

★ For an unbiased estimate of the true variance for a single measurement use:

$$\boxed{s_{n-1}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

★ For the best unbiased estimate of the true mean use the sample mean:

$$\boxed{\bar{x} = \frac{1}{n}\sum_i x_i}$$

★ What is the “error” (i.e. square root of the variance) on the sample mean ?

$$\begin{aligned}
Var(\bar{x}) \equiv \sigma_{\bar{x}}^2 &= \langle(\bar{x}-\mu)^2\rangle \\
&= \langle(\frac{1}{n}\sum_i x_i - \mu)^2\rangle \\
&= \frac{1}{n^2}n\langle x^2\rangle + \frac{n(n-1)}{n^2}\langle x_i x_j\rangle_{i\neq j} - 2\mu\langle\bar{x}\rangle + \mu^2 \\
&= \frac{\langle x^2\rangle}{n} + \frac{n-1}{n}\mu^2 - \mu^2 \\
&= \frac{\langle x^2 - \mu^2\rangle}{n} = \frac{\sigma^2}{n}
\end{aligned}$$

★ Hence the uncertainty on the mean is $\sqrt{n}$ smaller than the uncertainty on a single measurement

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

★ **Note:** this is general result – doesn't rely on distribution

★ Of course we only have an estimate of σ, so our best (unbiased) estimate of the uncertainty on the mean is:

$$\sigma_{\overline{x}} = \frac{1}{\sqrt{n}} s_{n-1}$$

★ There is one final question we can ask… what is the uncertainty on our estimate of the uncertainty. The answer to this question depends on the form of the PDF.

- We'll come back to this in the context of a Gaussian distribution…..

QUESTION 2

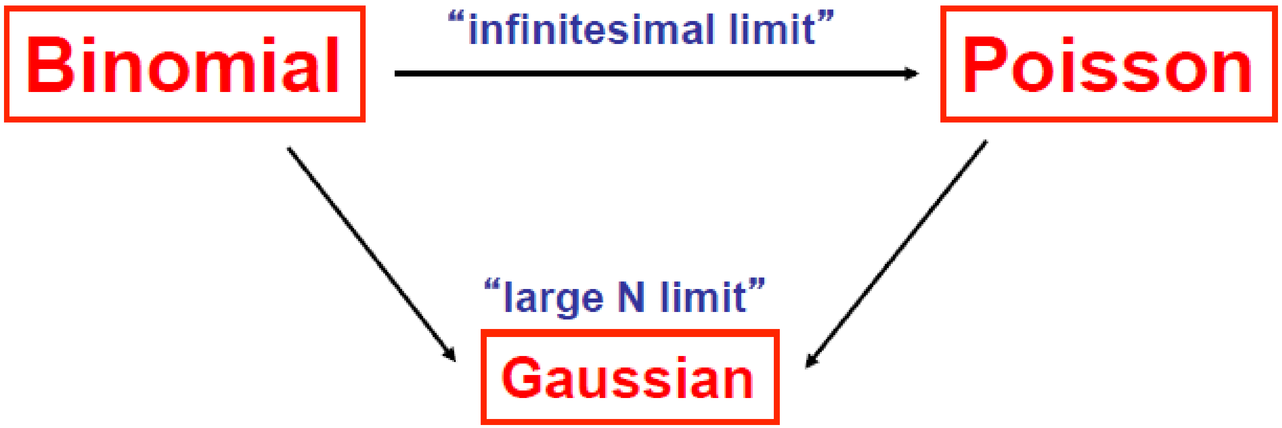
Given 5 measurements of a quantity x: 10.2, 5.5, 6.7, 3.4, 3.5

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

For later, how well do you know the uncertainty?

Special Probability Distributions

- So far, dealt in generalities
- Now consider some special distributions…
- Simplest case "Binomial distribution"
  - Random process with two outcomes with probabilities p and (1-p)
  - Repeat process a fixed number of times ⇨ distribution of outcomes
- Next simplest, "Poisson distribution"
  - Discrete random process with fixed mean
- Then, "Gaussian distribution"
  - Continuous "high statistics" limit



Binomial

"infinitesimal limit"

Poisson

"large N limit"

Gaussian

Binomial Distribution

- Applies for a fixed number of trials when there are two possible outcomes, e.g.
  - Toss an unbiased coin ten times, how many heads ?

$$\boxed{P(r;n) \quad = \quad {}^{n}C_r p^r (1-p)^{n-r}}$$

$$\begin{aligned}
\bar{x} &= \frac{\Sigma_{r=0}^{n} rP(r)}{\Sigma_{0}^{n} P(r)} = \sum_{0}^{n} rP(r) \\
&= \sum_{r=0}^{n} rp^r (1-p)^{n-r} \frac{n!}{r!(n-r)!} \\
&= np \sum_{r=1}^{n} p^{(r-1)} (1-p)^{(n-r)} \frac{(n-1)!}{(r-1)!(n-r)!} && \text{(n=0 term is zero)} \\
&= np \sum_{r'=0}^{n-1} p^{r'} (1-p)^{(n-1-r')} \frac{(n-1)!}{r'!(n-1-r')!} && \text{(let } r' = r\text{-1)} \\
&= np \sum_{r=0}^{n-1} P(r;n-1) \longleftarrow \boxed{\text{normalised to unity}} \\
&= np
\end{aligned}$$

- Hence $\boxed{\bar{x} = np}$ (hardly a surprising result)

Variance of the binomial distribution

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

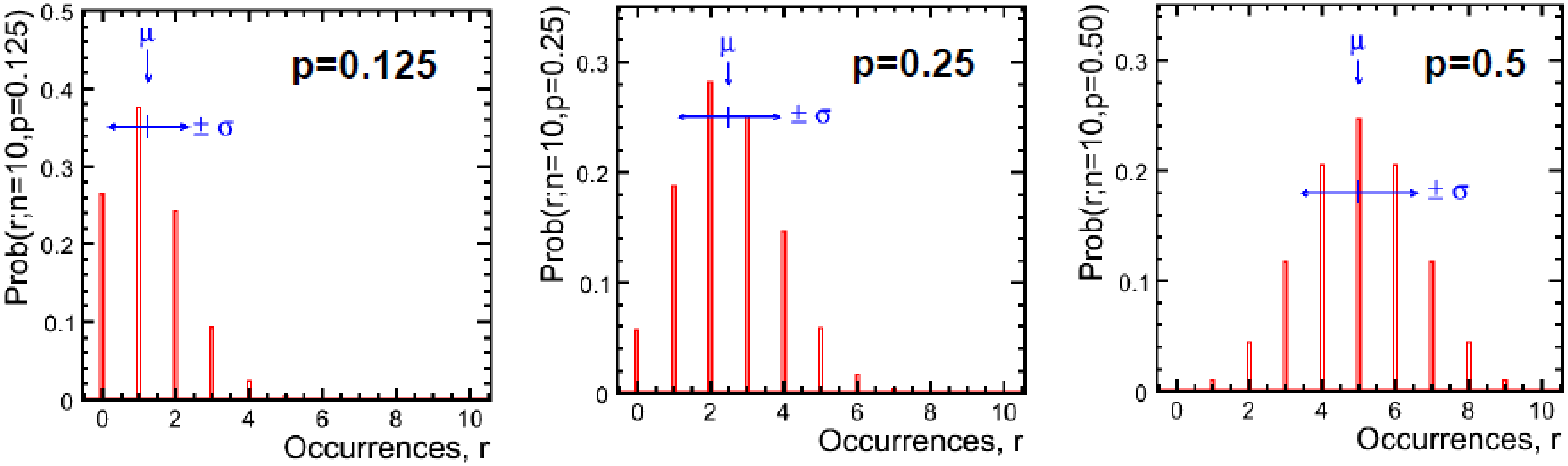
$$\begin{aligned}
\langle r^2 \rangle = \frac{\sum r^2 P(r;n)}{P(r;n)} &= \sum_{r=0}^{n} r^2 p^r (1-p)^{n-r} \frac{n!}{r!(n-r)!} \\
&= np \sum_{r=1}^{n} r p^{r-1} (1-p)^{n-r} \frac{(n-1)!}{(r-1)!(n-r)!} \\
&= np \sum_{r'=0}^{n-1} (r'+1) p^{r'} (1-p)^{n-1-r'} \frac{(n-1)!}{r'!(n-1-r')!} \\
&= np \sum_{r=0}^{n-1} P(r;n-1) + np \sum_{r=0}^{n-1} r P(r;n-1) \\
&= np + np \times (n-1)p \\
\langle r^2 \rangle &= np(np-p+1)
\end{aligned}$$

⇒

$$\begin{aligned}
Var(r) &= \langle r^2 \rangle - \mu^2 = np(np-p+1) + np - (np)^2 \\
&= np(1-p)
\end{aligned}$$

$$\boxed{Var(r) = np(1-p)}$$

e.g. n=10



★ **What is the meaning of σ ?**

- **By definition, σ, is root of the mean square (rms) deviation from the mean**

$$\sigma \equiv \langle (r-\mu)^2 \rangle^{\frac{1}{2}}$$

- **For a binomial distribution** $\sigma = \sqrt{np(1-p)}$
- **It provides a well-defined measure of the spread about the mean**
- **For above values: 62 %, 57 %, and 66 % of distribution within ± 1 σ of mean**
  Answer depends on n and p, but roughly ~55-70%

Example: Efficiency Uncertainty

- Suppose you use MC events to determine a selection efficiency
  - m out n events pass some selection, what is the efficiency and uncertainty
- This is a binomial process (fixed number of trials). Hence the number of events passing the selection will be distributed as:

$$P(m;n) \quad = \quad {}^{n}C_{m}\varepsilon^{m}(1-\varepsilon)^{n-m}$$

- Want to quote *best estimate* of the efficiency and the *best estimate* of the uncertainty (i.e. square root of the variance).
- Best estimate of efficiency is "clearly": $\boxed{\varepsilon_e = \frac{m}{n}}$
- From properties of binomial distribution expect

$$\sigma^2 = \langle\varepsilon^2\rangle \quad = \quad n\varepsilon(1-\varepsilon) \times \frac{1}{n^2}$$

$$\boxed{\sigma^2 \quad = \quad \frac{\varepsilon(1-\varepsilon)}{n}} \qquad \left(= \frac{m(n-m)}{n^3}\right)$$

e.g. 90 out of 100 events pass trigger requirements,

$$\varepsilon = 0.90 \pm 0.03$$

A more advanced analysis

- Asserted that our best estimate of the true efficiency ε is $\varepsilon_e = \frac{m}{n}$

  Suppose we repeated the experiment many times

$$\langle \varepsilon_e \rangle = \frac{\langle m \rangle}{n} = \frac{n\varepsilon}{n} = \varepsilon$$

  so on average this procedure gives an unbiased estimate of ε

GOOD

- What about our estimate for the variance ?

$$\sigma_e^2 = \frac{\varepsilon_e(1-\varepsilon_e)}{n} = \frac{m(n-m)}{n^3}$$

  Again suppose we repeated the experiment many times

$$\begin{aligned} \langle \sigma_e^2 \rangle &= \frac{n\langle m \rangle}{n^3} - \frac{\langle m^2 \rangle}{n^3} \\ &= \frac{n^2\varepsilon}{n^3} - \frac{n^2\varepsilon^2 - n\varepsilon^2 + n\varepsilon}{n^3} \\ &= \frac{\varepsilon(1-\varepsilon)}{n} + \frac{\varepsilon(1-\varepsilon)}{n^2} = \frac{n+1}{n^2}\varepsilon(1-\varepsilon) \\ &= \frac{n+1}{n}\sigma^2 \end{aligned}$$

GOOD ENOUGH

a problem …

$$\boxed{\sigma^2 = \frac{\varepsilon(1-\varepsilon)}{n}}$$

- ★ Suppose you want to estimate a trigger efficiency based on 100 MC events
- ★ If all the MC events pass the trigger selection…
  - ▪ best estimate of efficiency is 100 %
  - ▪ but what about the uncertainty on the efficiency ?
  - ▪ the above equation would suggest zero
  - ▪ this is clearly nonsense
  - ▪ so what’s wrong ?

We’ll come back to this in lecture 4…

The Poisson Distribution

- ★ Probably the most important distribution for experimental particle physicists
- ★ Appropriate for discrete counts at a fixed rate
  - e.g. in time **t**, on average expect μ events

$$\boxed{p(n;\mu) = \frac{\mu^n e^{-\mu}}{n!}}$$

- ★ The form of this equation is not immediately obvious (unlike that of the binomial distribution) – so (for completeness) derive the Poisson Distribution…
- ★ In time **t**, on average expect μ events. Now divide **t** into **N** intervals of **δt**
  - Probability of one event on **δt** is **δp**

$$\boxed{\delta p = \mu\frac{\delta t}{t} = \frac{\mu}{N}}$$

  - Probability of getting two events is negligibly small
  - Hence the problem has been transformed into N trials each with two discrete outcomes, i.e. a binomial distribution

$$p(n;\mu) = \lim_{N\to\infty} \delta p^n (1-\delta p)^{N-n} \frac{N!}{n!(N-n)!}$$

The Poisson Distribution

$$\begin{aligned} P &= (\delta p)^n (1-\delta p)^{N-n} \frac{N!}{n!(N-n)!} \\ \ln P &= n \ln \delta p + (N-n)\underline{\ln(1-\delta p)} + \ln N! - \ln n! - \ln(N-n)! \end{aligned}$$

First consider:

$$\begin{aligned} (N-n)\ln(1-\delta p) &= (N-n)[-\delta p + \cancel{(\delta p)^2/2} + \ldots] \\ &\approx -N\delta p + n\delta p \\ &= -\mu + \frac{n}{N}\mu \end{aligned}$$

hence

$$\lim_{N\to\infty} \{(N-n)\ln(1-\delta p)\} = -\mu$$

Stirling's approx

Now consider:

$$\begin{aligned} \ln \frac{N!}{(N-n)!} &= N\ln N - N - (N-n)\ln(N-n) + (N-n) \\ &= N\ln N + n - (N-n)\ln\left(1-\frac{n}{N}\right) - (N-n)\ln N \\ &\approx n\ln N + n + (N-n)\frac{n}{N} \\ &= \ln N^n + \cancel{\frac{n^2}{N}} \end{aligned}$$

hence

$$\lim_{N\to\infty} \left\{ \frac{N!}{(N-n)!} \right\} = N^n$$

So finally,

$$P(n;N) = (\delta p)^n (1-\delta p)^{N-n} \frac{N!}{n!(N-n)!}$$

becomes:

$$P(n;\mu) = (\delta p)^n e^{-\mu} \frac{N^n}{n!} = \left(\frac{\mu}{N}\right)^n e^{-\mu} \frac{N^n}{n!}$$

$$\boxed{P(n;\mu) = \frac{\mu^n e^{-\mu}}{n!}}$$

★ Check that the Poisson distribution is normalised…

$$\begin{aligned} \sum_{n=0}^{\infty} P(n;\mu) &= e^{-\mu}\left(1+\frac{\mu}{1!}+\frac{\mu^2}{2!}+\ldots\right) \\ &= e^{-\mu}e^{+\mu} = 1 \end{aligned}$$

Properties of the Poisson Distribution

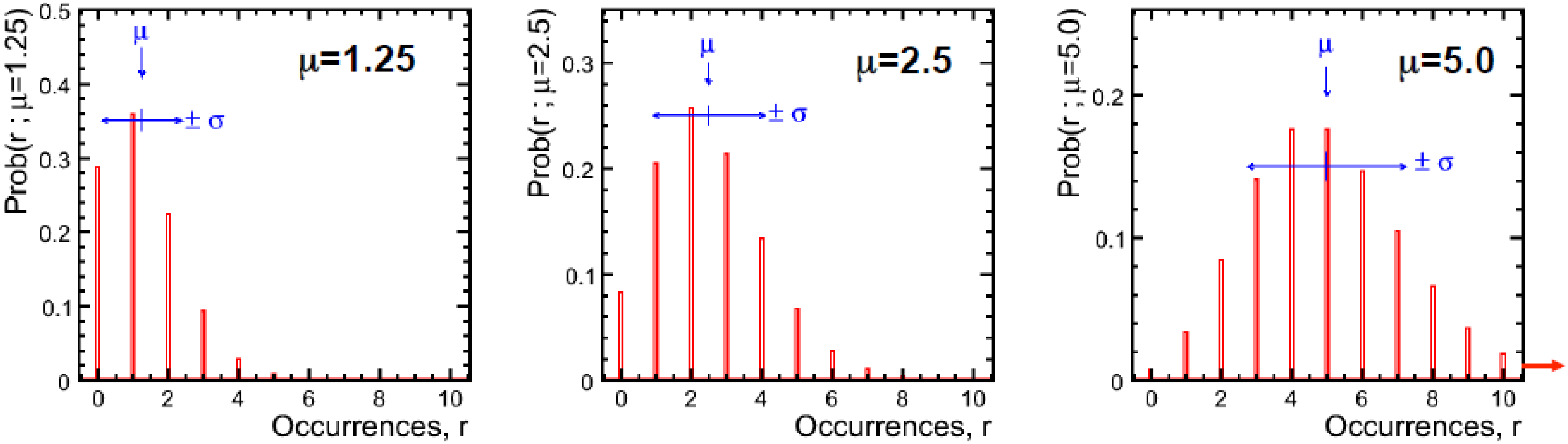
$$
\begin{aligned}
\langle n \rangle = \sum_{n=0}^{\infty} nP(n;\mu) &= \sum_{n=0}^{\infty} n \frac{\mu^n e^{-\mu}}{n!} \\
&= \sum_{n=1}^{\infty} n \frac{\mu^n e^{-\mu}}{n!} \\
&= \mu \sum_{n=1}^{\infty} \frac{\mu^{n-1} e^{-\mu}}{(n-1)!} \\
&= \mu \sum_{n'=0}^{\infty} \frac{\mu^{n'} e^{-\mu}}{n'!} \\
&= \mu \sum_{n=0}^{\infty} P(n;\mu) \\
&= \mu
\end{aligned}
$$

$$\boxed{\langle n \rangle = \mu}$$

$$
\begin{aligned}
\langle n^2 \rangle = \sum_{n=0}^{\infty} nP(n;\mu) &= \sum_{n=0}^{\infty} n^2 \frac{\mu^n e^{-\mu}}{n!} \\
&= \sum_{n=1}^{\infty} n^2 \frac{\mu^n e^{-\mu}}{n!} \\
&= \mu \sum_{n=1}^{\infty} n \frac{\mu^{n-1} e^{-\mu}}{(n-1)!} \\
&= \mu \sum_{n'=0}^{\infty} (n'+1) \frac{\mu^{n'} e^{-\mu}}{n'!} \\
&= \mu \left\{ \sum_{n=0}^{\infty} nP(n;\mu) + \sum_{n=0}^{\infty} P(n;\mu) \right\} \\
&= \mu^2 + \mu \\
\sigma^2 = Var(n) &= \langle n^2 \rangle - \langle n \rangle^2 \\
&= \mu
\end{aligned}
$$

$$\boxed{\sigma^2 = \mu}$$

e.g. μ=1.25, 2.5, 5.0



$$\langle N \rangle = \mu \qquad \sigma = \sqrt{\mu}$$

Example I

★ Suppose I am trying to measure a cross section for a process

- observe N events for an integrated luminosity of $\mathscr{L}$
- for this luminosity the expected number of events is

$$\mu = \sigma \mathscr{L}$$

- observed number of events will be Poisson distributed according to μ
- our best unbiased estimate of μ is simply the number of observed events

$$\mu_e = N$$

- for a Poisson distribution the variance is equal to the mean
- hence we can estimate the uncertainty on the estimated mean as $\sqrt{N}$

$$\mu_e = N \pm \sqrt{N}$$

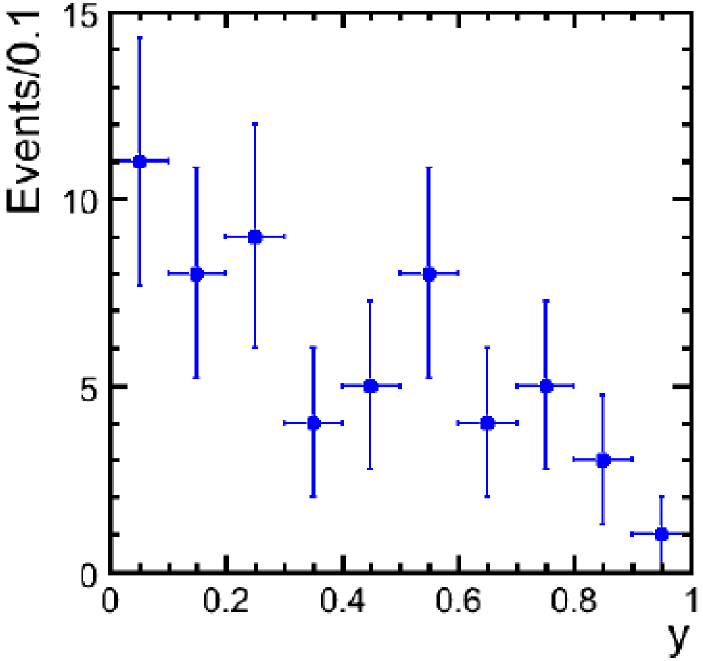
$$\sigma = \frac{1}{\mathscr{L}}(N \pm \sqrt{N})$$

NOTE: if you observe N events, the estimated uncertainty on the mean of the underlying Poisson distribution is $\sqrt{N}$
: it is not the “error” on N – there is no uncertainty on what you counted

★ Poisson fluctuations are the ultimate limit to any counting experiment

Example II

- Suppose a colleague makes a histogram of event counts as a function of y
  - the histogram includes errors bars (made by root)



- How should you interpret the error bars
  - If symmetric then probably $\sqrt{N}$
  - i.e. they indicate the expected "spread" assuming the mean expected counts in that bin are equal to the observed value
  - For large N this is not unreasonable
  - But for small N this doesn't make much sense…

High Statistics Limit of Poisson Distribution

$$P(n;\mu) = \frac{\mu^n e^{-\mu}}{n!}$$

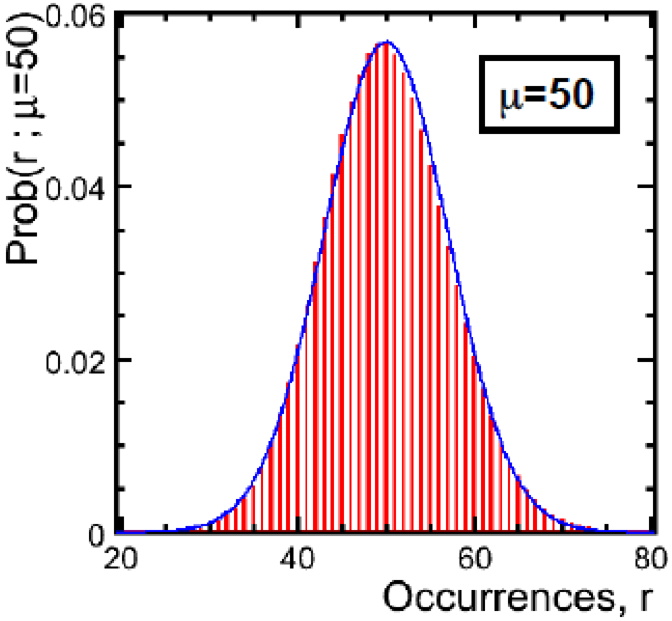
$$\begin{aligned}
\text{let}\quad f(x) &= \ln P(x;\mu) \\
&= -\mu - \ln x! + x\ln\mu \\
&\approx -\mu + x\ln x - x + x\ln\mu \\
\text{hence}\quad f'(x) &= \ln\mu - \ln x \\
f''(x) &= -1/x
\end{aligned}$$

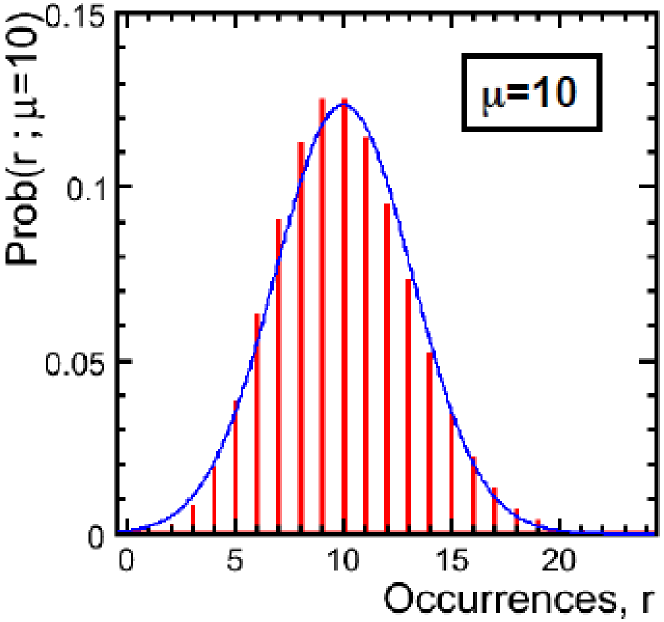
Taylor expansion about mean:

$$\begin{aligned}
f(x) &= f(\mu) + (x-\mu)f'(\mu) + \frac{1}{2!}(x-\mu)^2 f''(\mu) + \frac{1}{3!}(x-\mu)^3 f'''(\mu).. \\
&= f(\mu) - \frac{(x-\mu)^2}{2\mu} + \frac{(x-\mu)^3}{6\mu^2} + \ldots
\end{aligned}$$

$$\boxed{P(x;\mu) \approx k e^{-\frac{(x-\mu)^2}{2\mu}}}$$

$$P(x;\mu) \approx k e^{-\frac{(x-\mu)^2}{2\mu}}$$





★ Even for relatively small μ, (apart from in the extreme tails), a **Gaussian Distribution** is a pretty good approximation

▪Problem 3: for "fun" show that the high statistics limit of a binomial distribution is a Gaussian of width σ^2=np(1-p)

Next time

★ Investigate the treatment of statistics in the Gaussian Limit

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