Statistical Data Analysis 2020/21
Lecture Week 2

London Postgraduate Lectures on Particle Physics

University of London MSc/MSci course PH4515

Glen Cowan
Physics Department
Royal Holloway, University of London
g.cowan@rhul.ac.uk
www.pp.rhul.ac.uk/~cowan

Course web page via RHUL moodle (PH4515) and also

www.pp.rhul.ac.uk/~cowan/stat_course.html

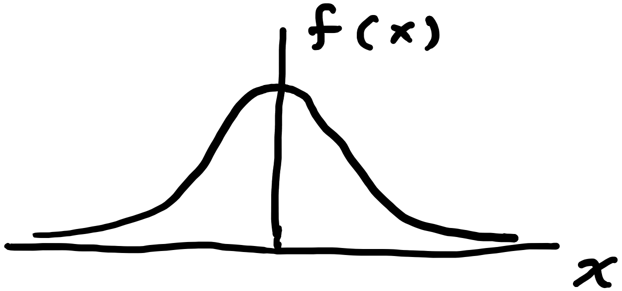
Statistical Data Analysis
Lecture 2-1

- Functions of random variables
  - Single variable, unique inverse
  - Function without unique inverse
  - Functions of several random variables

Functions of a random variable

A function of a random variable ***is itself*** a random variable.

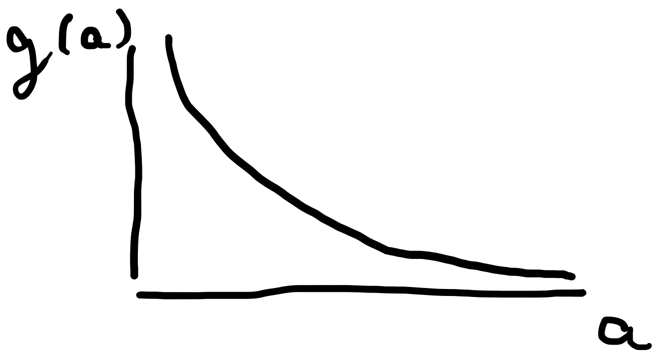
Suppose x follows a pdf $f(x)$



Consider a function $a(x)$

e.g. $a = x^2$

What is the pdf $g(a)$?

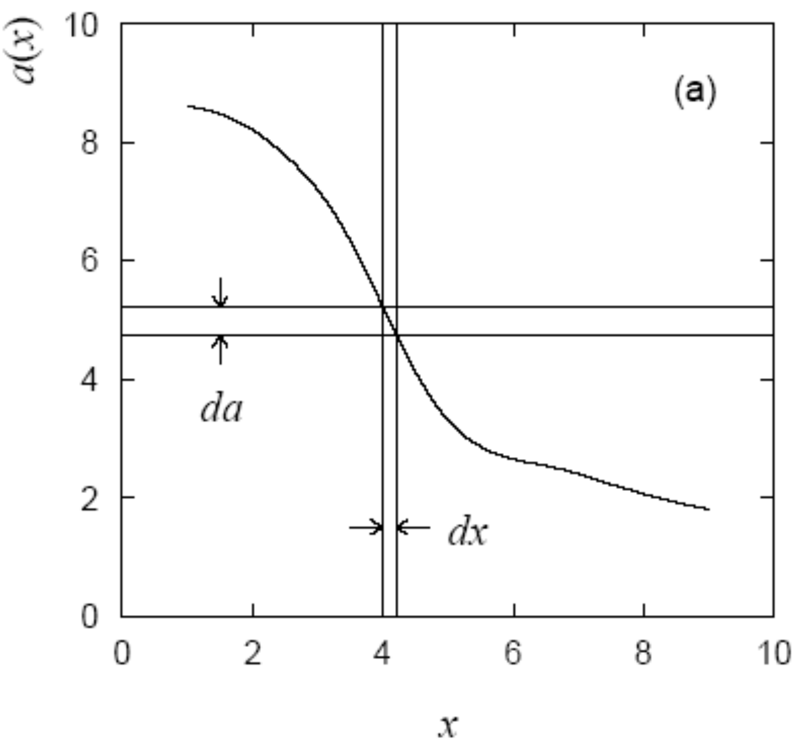


Function of a single random variable

General prescription:

$$g(a)\,da = \int_{dS} f(x)\,dx$$

dS = region of x space for which a is in $[a, a+da]$.



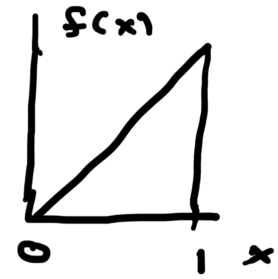
For one-variable case with unique inverse this is simply

$$g(a)\,da = f(x)\,dx$$

$$\rightarrow \quad g(a) = f(x(a)) \left| \frac{dx}{da} \right|$$

Example: function with unique inverse

$$f(x) = 2x , \quad 0 < x \le 1$$



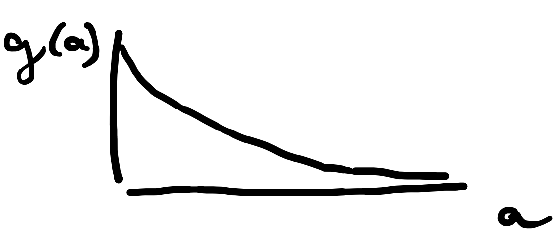
$$a = -\ln x$$

$$x = e^{-a} , \quad \frac{dx}{da} = -e^{-a}$$

$$g(a) = f(x(a)) \left| \frac{dx}{da} \right| = 2e^{-a} \cdot \left| -e^{-a} \right|$$

$$= 2e^{-2a}$$

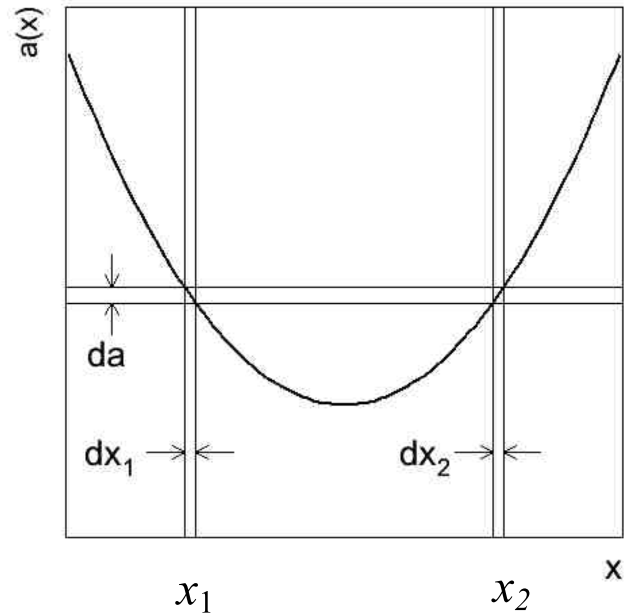
$$0 \le a < \infty$$



Functions without unique inverse

If inverse of $a(x)$ not unique, include all dx intervals in dS which correspond to da:

$$g(a) = \sum_i f(x_i(a)) \left| \frac{dx}{da} \right|_{x_i(a)}$$



Example: $a(x) = x^2, \quad x_1(a) = -\sqrt{a}, \quad x_2(a) = \sqrt{a}, \quad \frac{dx_{1,2}}{da} = \mp \frac{1}{2\sqrt{a}}$

$$dS = [x_1, x_1 + dx_1] \cup [x_2, x_2 + dx_2]$$

$$g(a) = f(x_1(a)) \left| \frac{dx}{da} \right|_{x_1(a)} + f(x_2(a)) \left| \frac{dx}{da} \right|_{x_2(a)} = \frac{f(-\sqrt{a})}{2\sqrt{a}} + \frac{f(\sqrt{a})}{2\sqrt{a}}$$

Change of variable example (cont.)

Suppose the pdf of x is $f(x) = \frac{x+1}{2}, \quad -1 \le x \le 1$

and we consider the function $a(x) = x^2$ (so $0 \le a \le 1$)

and the inverse has two parts: $x = \pm\sqrt{a}$

To get the pdf of a we include the contributions from both parts:

$$g(a) = \frac{-\sqrt{a}+1}{2 \cdot 2\sqrt{a}} + \frac{\sqrt{a}+1}{2 \cdot 2\sqrt{a}} = \frac{1}{2\sqrt{a}}, \quad 0 \le a \le 1$$

Functions of more than one random variable

Consider a vector r.v. $\boldsymbol{x} = (x_1, ..., x_n)$ that follows $f(x_1, ..., x_n)$ and consider a scalar function $a(\boldsymbol{x})$.

The pdf of a is found from

$$g(a')da' = \int \dots \int_{dS} f(x_1, \dots, x_n) dx_1 \dots dx_n$$

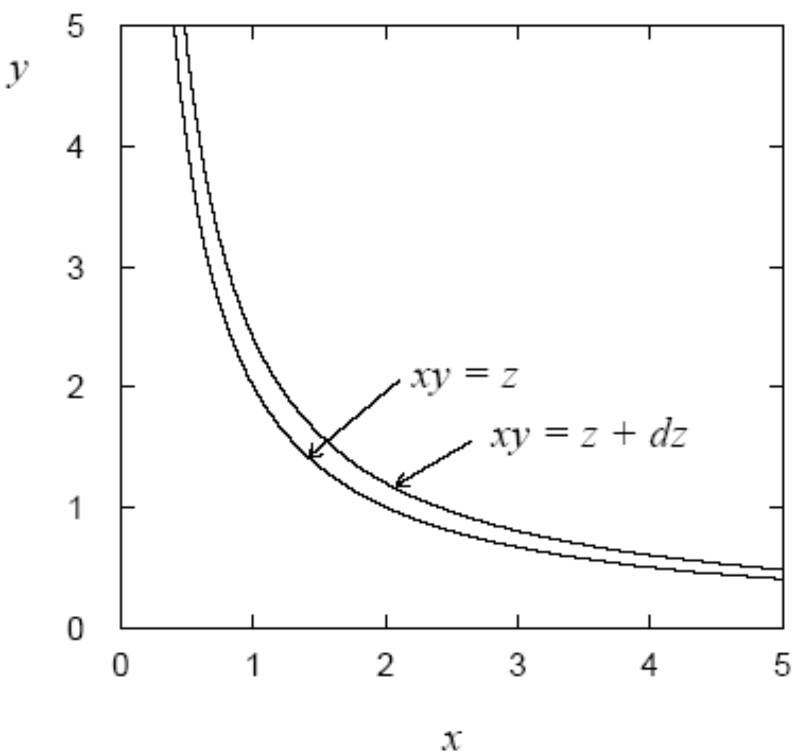
dS = region of $\boldsymbol{x}$-space between (hyper)surfaces defined by

$$a(\vec{x}) = a', \; a(\vec{x}) = a' + da'$$

Functions of more than one r.v. (2)

Example: r.v.s $x, y > 0$ follow joint pdf $f(x,y)$,

consider the function $z = xy$. What is $g(z)$?



$$g(z)\,dz = \int \ldots \int_{dS} f(x,y)\,dx\,dy$$

$$= \int_0^\infty dx \int_{z/x}^{(z+dz)/x} f(x,y)\,dy$$

$$\rightarrow \quad g(z) = \int_0^\infty f(x, \frac{z}{x}) \frac{dx}{x}$$

$$= \int_0^\infty f(\frac{z}{y}, y) \frac{dy}{y}$$

(Mellin convolution)

More on transformation of variables

Consider a random vector $\vec{x} = (x_1, \ldots, x_n)$ with joint pdf $f(\vec{x})$.

Form n linearly independent functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_n(\vec{x}))$

for which the inverse functions $x_1(\vec{y}), \ldots, x_n(\vec{y})$

Then the joint pdf of the vector of functions is $g(\vec{y}) = |J| f(\vec{x})$

where J is the Jacobian determinant:

$$J = \begin{vmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \ldots & \frac{\partial x_1}{\partial y_n} \\ \frac{\partial x_2}{\partial y_1} & \frac{\partial x_2}{\partial y_2} & \ldots & \frac{\partial x_2}{\partial y_n} \\ \vdots & & & \vdots \\ & & \ldots & \frac{\partial x_n}{\partial y_n} \end{vmatrix}$$

For e.g. $g_1(y_1)$ integrate $g(\vec{y})$ over the unwanted components.

Statistical Data Analysis
Lecture 2-2

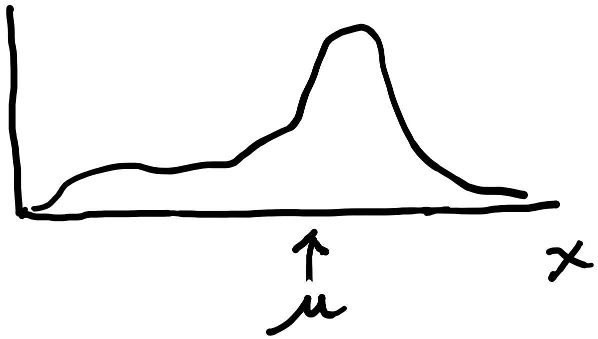
- Expectation values
- Covariance and correlation

Expectation values

Consider continuous r.v. x with pdf $f(x)$.

Define expectation (mean) value as $E[x] = \int x \, f(x) \, dx$

Notation (often): $E[x] = \mu$ ~ "centre of gravity" of pdf.



For discrete r.v.s, replace integral by sum: $E[x] = \sum_{x_i \in S} x_i P(x_i)$

For a function $y(x)$ with pdf $g(y)$,

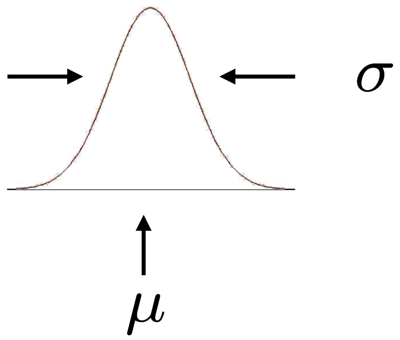
$$E[y] = \int y \, g(y) \, dy = \int y(x) f(x) \, dx$$ (equivalent)

Variance, standard deviation

Variance: $V[x] = E[x^2] - \mu^2 = E[(x-\mu)^2]$

Notation: $V[x] = \sigma^2$

Standard deviation: $\sigma = \sqrt{\sigma^2}$



$\sigma \sim$ width of pdf, same units as x.

Relation between σ and other measures of width, e.g., Full Width at Half Max (FWHM) depend on the pdf, e.g., FWHM = 2.35σ for Gaussian.

Moments of a distribution

Can characterize shape of a pdf with its moments:

$$E[x^n] = \int x^n f(x)\, dx \equiv \mu'_n$$

= nth algebraic moment, e.g., $\mu'_1 = \mu$ (the mean)

$$E[(x - E[x])^n] = \int (x-\mu)^n f(x)\, dx \equiv \mu_n$$

= nth central moment, e.g., $\mu_2 = \sigma^2$

Zeroth moment = 1 (always). Higher moments may not exist.

3rd moment is a measure of "skewness": $\tilde{\mu}^3 = E\left[\left(\frac{x-\mu}{\sigma}\right)^3\right]$

Expectation values – multivariate case

Suppose we have a 2-D joint pdf $f(x,y)$.

By "expectation value of x" we mean:

$$E[x] = \int \int x f(x,y)\, dx\, dy = \int x f_x(x)\, dx = \mu_x$$

Sometimes it is useful to consider e.g. the conditional expectation value of x given y,

$$E[x|y] = \int x f(x|y)\, dx$$

$$f(x|y) = \frac{f(x,y)}{f_y(y)}$$

Covariance and correlation

Define covariance $\mathrm{cov}[x,y]$ (also use matrix notation V_{xy}) as

$$\mathrm{cov}[x,y] = E[xy] - \mu_x \mu_y = E[(x-\mu_x)(y-\mu_y)]$$

Correlation coefficient (dimensionless) defined as

$$\rho_{xy} = \frac{\mathrm{cov}[x,y]}{\sigma_x \sigma_y}$$

Can show $-1 \le \rho \le 1$.

If x, y, independent, i.e., $f(x,y) = f_x(x) f_y(y)$

$$E[xy] = \int \int xy \, f(x,y) \, dx dy = \mu_x \mu_y$$

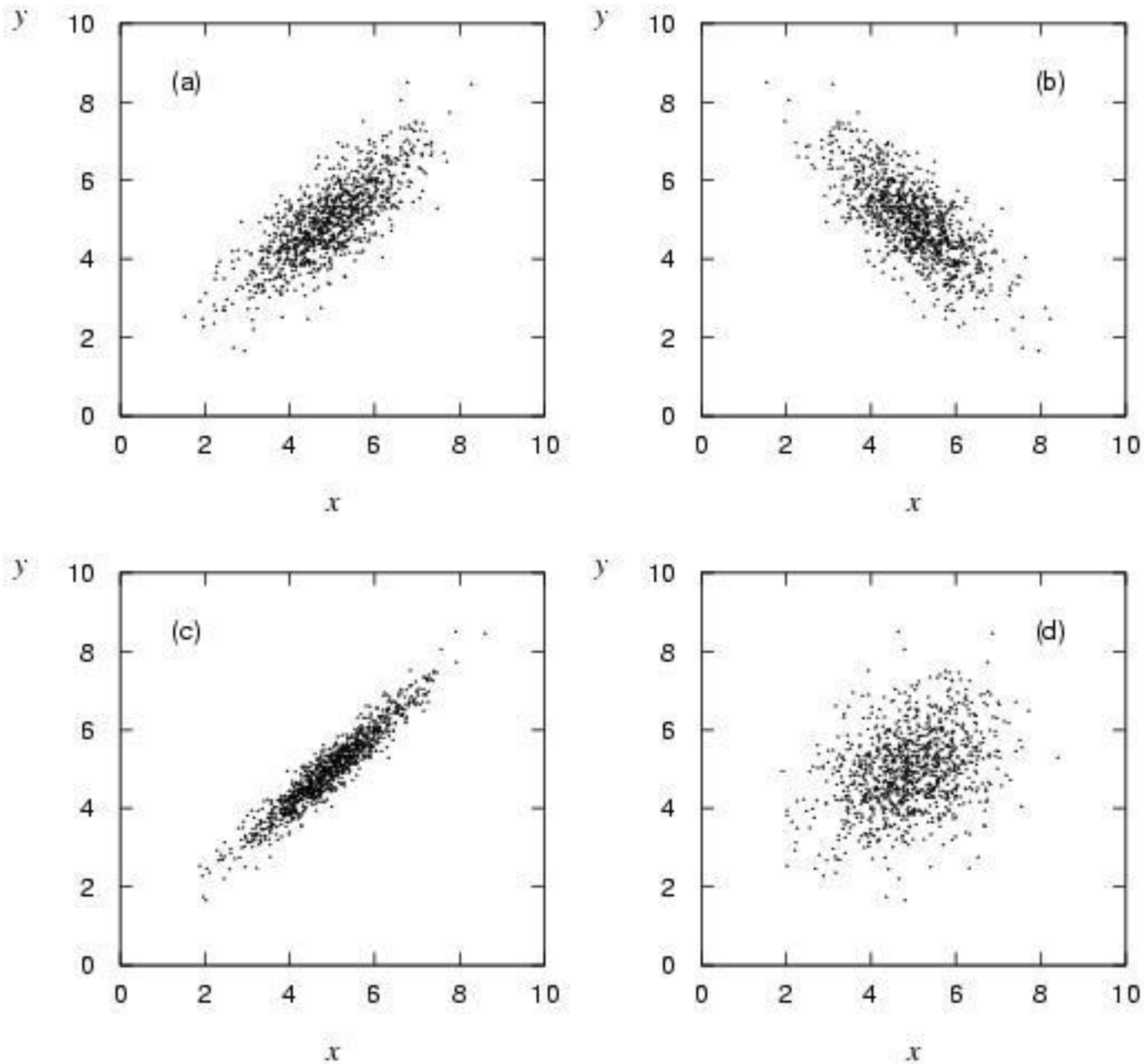
$\rightarrow$ $\mathrm{cov}[x,y] = 0$

N.B. converse not always true.

Correlation (cont.)

$\rho = 0.75$

$\rho = -0.75$



$\rho = 0.95$

$\rho = 0.25$

Covariance matrix

Suppose we have a set of n random variables, say, $x_1,\ldots, x_n$.

We can write the covariance of each pair as an n x n matrix:

$$V_{ij} = \mathrm{cov}[x_i, x_j] = \rho_{ij}\sigma_i\sigma_j$$

$$V = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \cdots & \rho_{1n}\sigma_1\sigma_n \\ \rho_{21}\sigma_2\sigma_1 & \sigma_2^2 & \cdots & \rho_{2n}\sigma_2\sigma_n \\ \vdots & & \ddots & \vdots \\ \rho_{n1}\sigma_n\sigma_1 & \rho_{n2}\sigma_n\sigma_2 & \cdots & \sigma_n^2 \end{pmatrix}$$

Covariance matrix is:

symmetric,

diagonal = variances,

positive semi-definite:

$$z^T V z \geq 0 \text{ for all } z \in \mathbb{R}^n$$

Correlation matrix

Closely related to the covariance matrix is the n x n matrix of correlation coefficients:

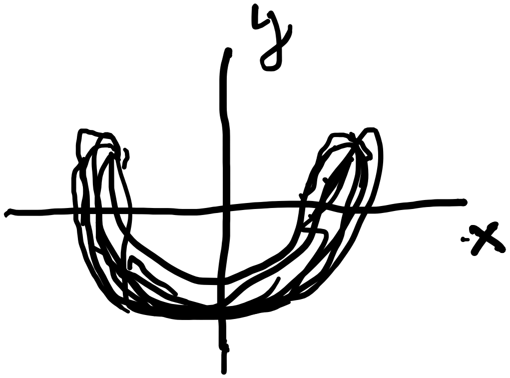
$$\rho_{ij} = \frac{\mathrm{cov}[x_i, x_j]}{\sigma_i \sigma_j}$$

$$\rho = \begin{pmatrix} 1 & \rho_{12} & \dots & \rho_{1n} \\ \rho_{21} & 1 & \dots & \rho_{2n} \\ \vdots & & \ddots & \vdots \\ \rho_{n1} & \rho_{n2} & \dots & 1 \end{pmatrix}$$

By construction, diagonal elements are $\rho_{ii} = 1$

Correlation vs. independence

Consider a joint pdf such as:



I.e. here $f(-x,y) = f(x,y)$

Because of the symmetry, we have $E[x] = 0$ and also

$$E[xy] = \int_{-\infty}^{\infty} \int_{-\infty}^{0} xy f(x,y)\, dx\, dy + \int_{-\infty}^{\infty} \int_{0}^{\infty} xy f(x,y)\, dx\, dy = 0$$

and so $\rho = 0$, the two variables x and y are uncorrelated.

But $f(y|x)$ clearly depends on x, so x and y are not independent.

Uncorrelated: the joint density of x and y is not tilted.

Independent: imposing x does not affect conditional pdf of y.

Statistical Data Analysis
Lecture 2-3

- Error propagation
  - goal: find variance of a function
  - derivation of formula
  - limitations
  - special cases

Error propagation

Suppose we measure a set of values $\vec{x} = (x_1, \ldots, x_n)$

and we have the covariances $V_{ij} = \mathrm{cov}[x_i, x_j]$

which quantify the measurement errors in the x_i.

Now consider a function $y(\vec{x})$.

What is the variance of $y(\vec{x})$?

The hard way: use joint pdf $f(\vec{x})$ to find the pdf $g(y)$,

then from $g(y)$ find $V[y] = E[y^2] - (E[y])^2$.

Often not practical, $f(\vec{x})$ may not even be fully known.

Error propagation formula (1)

Suppose we had $\vec{\mu} = E[\vec{x}]$

in practice only estimates given by the measured $\vec{x}$

Expand $y(\vec{x})$ to 1st order in a Taylor series about $\vec{\mu}$

$$y(\vec{x}) \approx y(\vec{\mu}) + \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i)$$

To find $V[y]$ we need $E[y^2]$ and $E[y]$.

$$E[y(\vec{x})] \approx y(\vec{\mu}) \quad \text{since} \quad E[x_i - \mu_i] = 0$$

Error propagation formula (2)

$$E[y^2(\vec{x})] \approx y^2(\vec{\mu}) \; + \; 2y(\vec{\mu}) \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} E[x_i - \mu_i]$$

$$+E \left[\left(\sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]_{\vec{x}=\vec{\mu}} (x_i - \mu_i) \right) \left(\sum_{j=1}^{n} \left[\frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} (x_j - \mu_j) \right) \right]$$

$$= y^2(\vec{\mu}) + \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}$$

Putting the ingredients together gives the variance of $y(\vec{x})$

$$\sigma_y^2 \approx \sum_{i,j=1}^{n} \left[\frac{\partial y}{\partial x_i} \frac{\partial y}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}$$

Error propagation formula (3)

If the x_i are uncorrelated, i.e., $V_{ij} = \sigma_i^2 \delta_{ij}$, then this becomes

$$\sigma_y^2 \approx \sum_{i=1}^{n} \left[\frac{\partial y}{\partial x_i} \right]^2_{\vec{x}=\vec{\mu}} \sigma_i^2$$

Similar for a set of m functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_m(\vec{x}))$

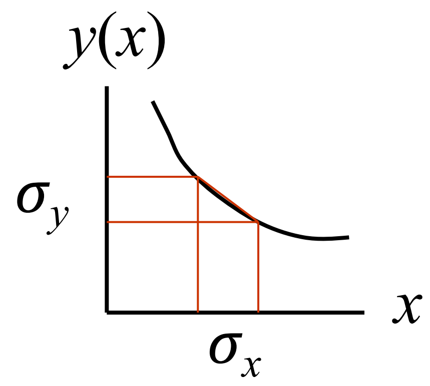
$$U_{kl} = \mathrm{cov}[y_k, y_l] \approx \sum_{i,j=1}^{n} \left[\frac{\partial y_k}{\partial x_i} \frac{\partial y_l}{\partial x_j} \right]_{\vec{x}=\vec{\mu}} V_{ij}$$

or in matrix notation $U = AVA^T$, where

$$A_{ij} = \left[\frac{\partial y_i}{\partial x_j} \right]_{\vec{x}=\vec{\mu}}$$

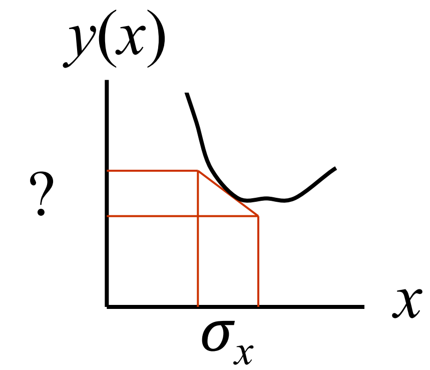
Error propagation – limitations

The 'error propagation' formulae tell us the covariances of a set of functions $\vec{y}(\vec{x}) = (y_1(\vec{x}), \ldots, y_m(\vec{x}))$ terms of the covariances of the original variables.



Limitations: exact only if $\vec{y}(\vec{x})$ linear.

Approximation breaks down if function nonlinear over a region comparable in size to the σ_i.



N.B. We have said nothing about the exact pdf of the x_i, e.g., it doesn't have to be Gaussian.

Error propagation – special cases

$$y = x_1 + x_2 \quad \rightarrow \quad \sigma_y^2 = \sigma_1^2 + \sigma_2^2 + 2\text{cov}[x_1, x_2]$$

$$y = x_1 x_2 \quad \rightarrow \quad \frac{\sigma_y^2}{y^2} = \frac{\sigma_1^2}{x_1^2} + \frac{\sigma_2^2}{x_2^2} + 2\frac{\text{cov}[x_1, x_2]}{x_1 x_2}$$

That is, if the x_i are uncorrelated:

add errors quadratically for the sum (or difference),

add relative errors quadratically for product (or ratio).

But correlations can change this completely...

Error propagation – special cases (2)

Consider $y = x_1 - x_2$ with

$$\mu_1 = \mu_2 = 10, \quad \sigma_1 = \sigma_2 = 1, \quad \rho = \frac{\mathrm{cov}[x_1, x_2]}{\sigma_1 \sigma_2} = 0 \, .$$

$$V[y] = 1^2 + 1^2 = 2, \rightarrow \sigma_y = 1.4$$

Now suppose $\rho = 1$. Then

$$V[y] = 1^2 + 1^2 - 2 = 0, \rightarrow \sigma_y = 0$$

i.e. for 100% correlation, error in difference $\rightarrow$ 0.

Statistical Data Analysis
Lectures 2-4 through 3-2 intro

We will now run through a short catalog of probability functions and pdfs.

For each (usually) show expectation value, variance, a plot and discuss some properties and applications.

See also chapter on probability from **`pdg.lbl.gov`**

For a more complete catalogue see e.g. the handbook on statistical distributions by Christian Walck from
`staff.fysik.su.se/~walck/suf9601.pdf`

Some distributions

Distribution/pdf	Example use in Particle Physics
Binomial	Branching ratio
Multinomial	Histogram with fixed N
Poisson	Number of events found
Uniform	Monte Carlo method
Exponential	Decay time
Gaussian	Measurement error
Chi-square	Goodness-of-fit
Cauchy	Mass of resonance
Landau	Ionization energy loss
Beta	Prior pdf for efficiency
Gamma	Sum of exponential variables
Student's t	Resolution function with adjustable tails

Statistical Data Analysis
Lecture 2-4

- Discrete probability distributions
  - binomial
  - multinomial
  - Poisson

Binomial distribution

Consider N independent experiments (Bernoulli trials):

outcome of each is 'success' or 'failure',

probability of success on any given trial is p.

Define discrete r.v. n = number of successes ($0 \leq n \leq N$).

Probability of a specific outcome (in order), e.g. 'ssfsf' is

$$pp(1-p)p(1-p) = p^n(1-p)^{N-n}$$

But order not important; there are $\dfrac{N!}{n!(N-n)!}$

ways (permutations) to get n successes in N trials, total probability for n is sum of probabilities for each permutation.

Binomial distribution (2)

The binomial distribution is therefore

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

random variable

parameters

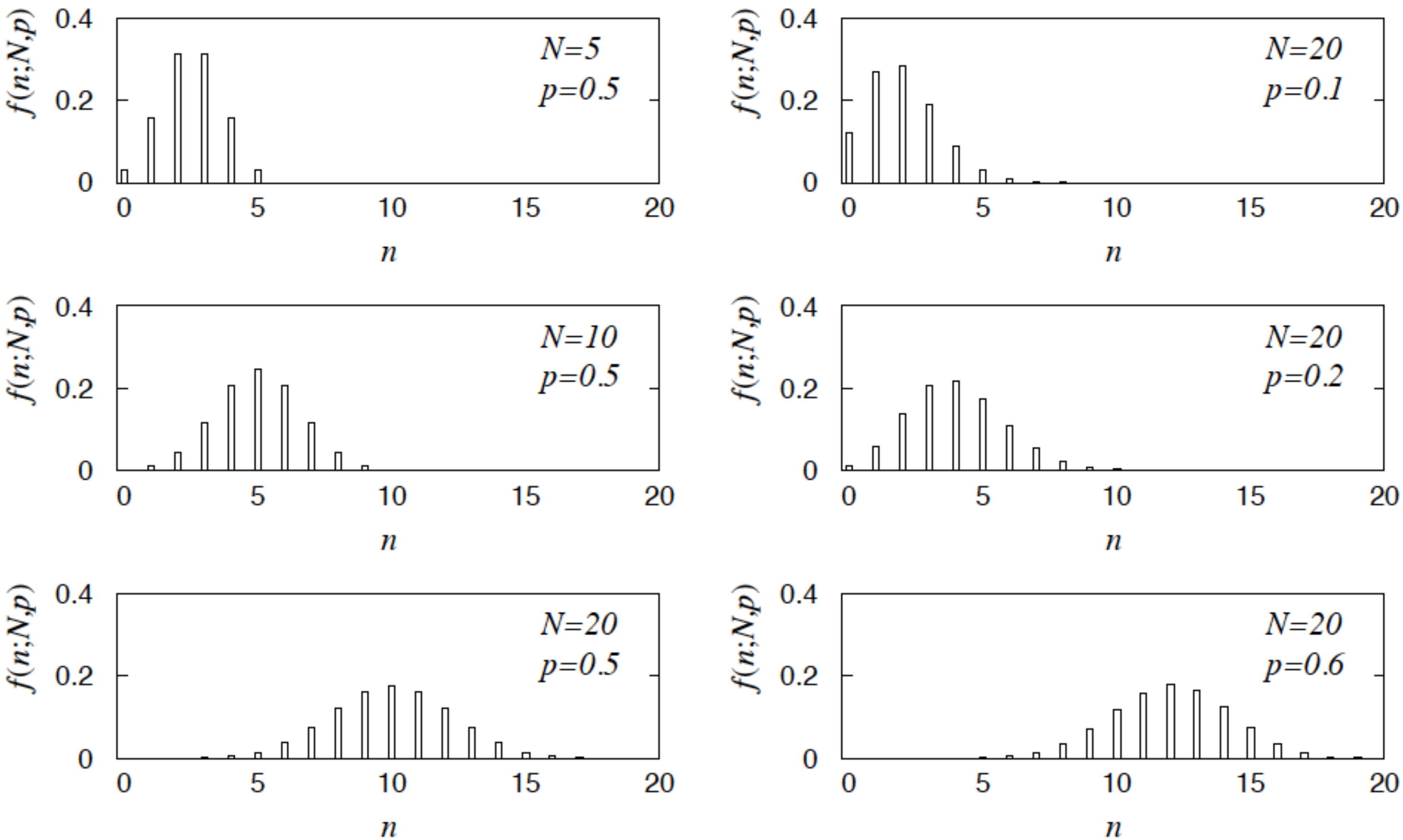
For the expectation value and variance we find:

$$E[n] = \sum_{n=0}^{N} n f(n; N, p) = Np$$

$$V[n] = E[n^2] - (E[n])^2 = Np(1-p)$$

Binomial distribution (3)

Binomial distribution for several values of the parameters:



Example: observe N decays of $W^{\pm}$, the number n of which are $W\to\mu\nu$ is a binomial r.v., p = branching ratio.

Multinomial distribution

Like binomial but now m outcomes instead of two, probabilities are

$$\vec{p} = (p_1, \ldots, p_m)\,, \quad \text{with} \sum_{i=1}^{m} p_i = 1\,.$$

For N trials we want the probability to obtain:

n_1 of outcome 1,
n_2 of outcome 2,
⋮
n_m of outcome m.

This is the multinomial distribution for $\vec{n} = (n_1, \ldots, n_m)$

$$f(\vec{n}; N, \vec{p}) = \frac{N!}{n_1! n_2! \cdots n_m!} p_1^{n_1} p_2^{n_2} \cdots p_m^{n_m}$$

Multinomial distribution (2)

Now consider outcome i as 'success', all others as 'failure'.

→ all n_i individually binomial with parameters N, p_i

$$E[n_i] = Np_i, \quad V[n_i] = Np_i(1 - p_i) \quad \text{for all } i$$

One can also find the covariance to be

$$V_{ij} = Np_i(\delta_{ij} - p_j)$$

Example: $\vec{n} = (n_1, \ldots, n_m)$ represents a histogram

with m bins, N total entries, all entries independent.

Poisson distribution

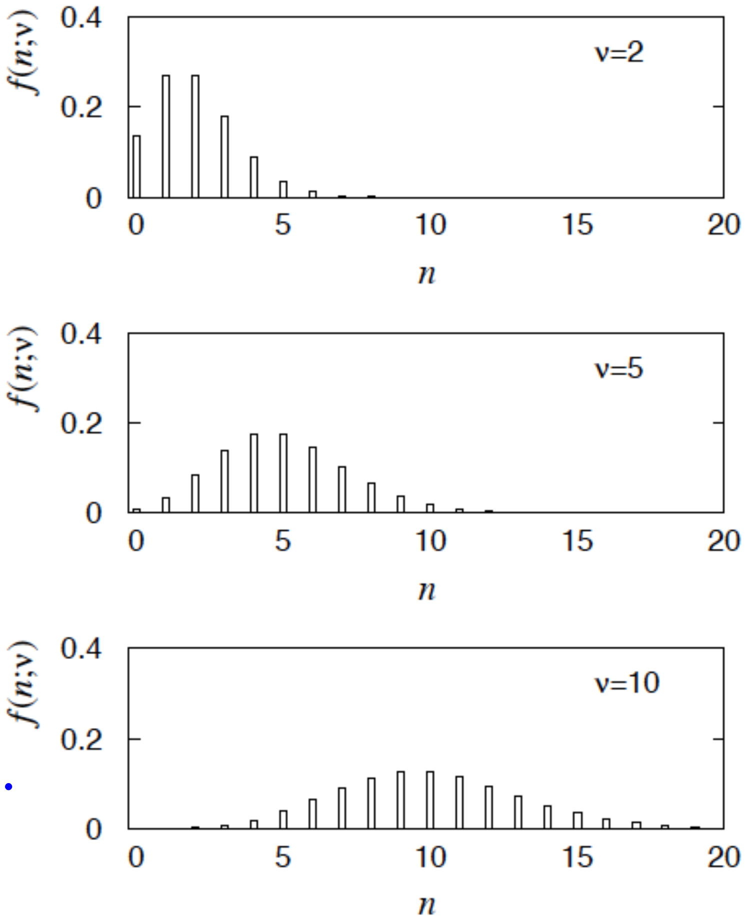
Consider binomial n in the limit

$$N \to \infty, \qquad p \to 0, \qquad E[n] = Np \to \nu \ .$$

$\to$ n follows the Poisson distribution:

$$f(n;\nu) = \frac{\nu^n}{n!} e^{-\nu} \qquad (n \geq 0)$$

$$E[n] = \nu \,, \qquad V[n] = \nu \ .$$



Example: number of scattering events n with cross section σ found for a fixed integrated luminosity, with $\nu = \sigma \int L \, dt$.