

Lecture 1

1. Probability
2. Random variables, probability densities, etc.
3. Brief catalogue of probability densities
4. The Monte Carlo method

Lecture 2

1. Statistical tests
2. Fisher discriminants, neural networks, etc.
3. Goodness-of-fit tests
4. The significance of a signal
5. Introduction to parameter estimation

Lecture 3

1. The method of maximum likelihood (ML)
2. Variance of ML estimators
3. The method of least squares (LS)
4. Interval estimation, setting limits

[Hypotheses, test statistics](#)

Suppose the result of a measurement is $\vec{x} = (x_1, \dots, x_n)$

e.g. events from e^+e^- collisions; for each event measure

$x_1 =$ number of charged particles produced

$x_2 =$ mean p_\perp of particles

$x_3 =$ number of 'jets' (according to some algorithm)

$x_4 = \dots$

\vec{x} follows some joint pdf in an n -dimensional space, which depends on the type of event produced, i.e. $e^+e^- \rightarrow q\bar{q}$, $e^+e^- \rightarrow WW$, etc.

That is, the joint pdf $f(\vec{x})$ is specified by a certain

HYPOTHESIS

i.e. predicted probability densities $f(\vec{x}|H_0)$, $f(\vec{x}|H_1)$, etc.

(Note sloppy but traditional notation: usually H_0, H_1, \dots not r.v.)

Simple hypothesis: $f(\vec{x})$ completely specified,

Composite hypothesis: form of $f(\vec{x}; \theta)$ given, parameter θ unknown

Usually awkward to work with multidimensional \vec{x} ,

\Rightarrow construct **test statistic** of lower dimension (e.g. scalar), $t(\vec{x})$:

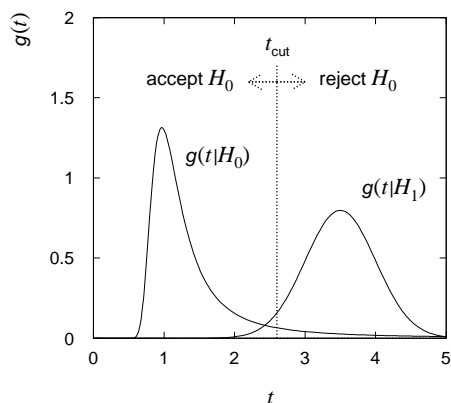
compactify data,

try not to lose ability to discriminate between hypotheses.

The statistic t then has pdfs $g(t|H_0)$, $g(t|H_1)$, \dots

Critical region, errors of 1st and 2nd kind

Consider a test statistic t following $g(t|H_0)$, $g(t|H_1)$, ...



Define a **critical region** where t is not likely to occur if H_0 is true,

e.g. for the case above, $t \geq t_{\text{cut}}$.

If observed value t_{obs} is in critical region, reject H_0 , otherwise 'accept'.

Probability to reject H_0 if it is true (error of 1st kind):

$$\alpha = \int_{t_{\text{cut}}}^{\infty} g(t|H_0) dt \quad (\text{significance level})$$

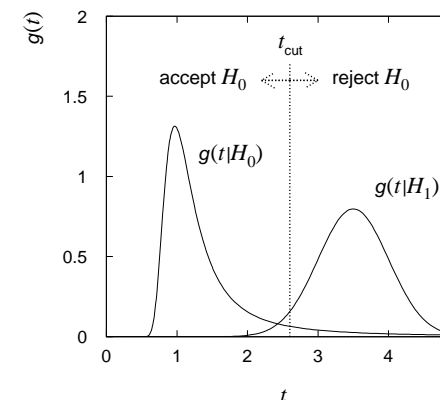
Probability to accept H_0 if H_1 is true (error of 2nd kind):

$$\beta = \int_{-\infty}^{t_{\text{cut}}} g(t|H_1) dt \quad (1 - \beta = \text{power})$$

An example with particle selection

Suppose we obtain n energy loss measurements for a particle in a drift chamber, construct $t =$ truncated mean of the measurements and suppose we know the particles are either electrons or pions:

$H_0 =$ electron (signal)
 $H_1 =$ pion (background)



Select electrons by requiring $t < t_{\text{cut}}$. The selection **efficiencies**:

$$\varepsilon_e = \int_{-\infty}^{t_{\text{cut}}} g(t|e) dt = 1 - \alpha$$

$$\varepsilon_\pi = \int_{-\infty}^{t_{\text{cut}}} g(t|\pi) dt = \beta$$

Loose cut: most e accepted, lots of π background

Tight cut: low signal efficiency, pure sample

Fractions of e, π may be unknown; t follows

$$f(t; a_e) = a_e g(t|e) + (1 - a_e) g(t|\pi)$$

→ estimate a_e (for now assume a_e , $a_\pi = 1 - a_e$ known)

Purity of selected sample

For a measured value t , what is the probability to be e/π ?

$$h(e|t) = \frac{a_e g(t|e)}{a_e g(t|e) + a_\pi g(t|\pi)} \quad (\text{Bayes' theorem})$$

$$h(\pi|t) = \frac{a_\pi g(t|\pi)}{a_e g(t|e) + a_\pi g(t|\pi)}$$

Bayesian: degree of belief that this particle is e or π

Frequentist: fraction of particles at given t which are e/π

→ here both approaches make sense

Often want purity of selected sample:

$$\begin{aligned} p_e &= P(e | t < t_{\text{cut}}) \\ &= \frac{\text{number of electrons with } t < t_{\text{cut}}}{\text{number of all particles with } t < t_{\text{cut}}} \\ &= \frac{\int_{-\infty}^{t_{\text{cut}}} a_e g(t|e) dt}{\int_{-\infty}^{t_{\text{cut}}} (a_e g(t|e) + (1 - a_e) g(t|\pi)) dt} \\ &= \frac{\int_{-\infty}^{t_{\text{cut}}} h(e|t) f(t) dt}{\int_{-\infty}^{t_{\text{cut}}} f(t) dt} \\ &= \text{electron probability averaged over interval } (-\infty, t_{\text{cut}}] \end{aligned}$$

The Neyman–Pearson lemma

Consider a multidimensional test statistic $\vec{t} = (t_1, \dots, t_m)$; hypotheses H_0 ('signal') and H_1 ('background').

What is the optimal choice of the critical region (i.e. cuts)?

The **Neyman–Pearson lemma** states: to get the highest purity for a given efficiency, (i.e. highest power for a given significance level) choose the acceptance region such that

$$\frac{g(\vec{t}|H_0)}{g(\vec{t}|H_1)} > c,$$

where $c = \text{constant}$ which determines the efficiency.

(For a proof see Brandt Chapter 8.) Value of c left open; choose this depending on what efficiency you want.

Equivalently, the optimal scalar test statistic is

$$r = \frac{g(\vec{t}|H_0)}{g(\vec{t}|H_1)},$$

called the likelihood ratio for simple hypotheses H_0 and H_1 .

Requiring $r > c$ gives maximum purity for a given efficiency.

N.B. any monotonic function of r is just as good.

Constructing a test statistic

Example: $H_0 = e^+e^- \rightarrow WW \rightarrow \text{hadrons}$ (usually four jets)

$H_1 = e^+e^- \rightarrow q\bar{q} \rightarrow \text{hadrons}$ (usually two jets)

For each event measure $\vec{x} = (x_1, \dots, x_n)$.

According to Neyman–Pearson, to select WWs we should cut on

$$t(\vec{x}) = \frac{f(\vec{x}|H_0)}{f(\vec{x}|H_1)},$$

but we need to know $f(\vec{x}|H_0)$ and $f(\vec{x}|H_1)$.

In practice, get these from Monte Carlo event generator:

Generate events, for each, obtain \vec{x} and enter into
 n -dimensional histogram. If e.g. M bins per component,
total number of cells in \vec{x} -space = M^n

Approximate $f(\vec{x}|H)$ by probability to be in corresponding cell,
i.e. determine M^n parameters. But n is potentially large!

⇒ prohibitively large number of cells to populate with MC data.

Compromise solution:

Make Ansatz for form of $t(\vec{x})$ with fewer parameters;
determine the parameters (e.g. using MC) to give best
discrimination between H_0 and H_1 .

Linear test statistic

Ansatz: $t(\vec{x}) = \sum_{i=1}^n a_i x_i = \vec{a}^T \vec{x}$

A choice of \vec{a} gives certain pdfs $g(t|H_0)$, $g(t|H_1)$.

Choose the a_i to maximize ‘separation’ between $g(t|H_0)$, $g(t|H_1)$.

→ Must define ‘separation’.

We have the expectation values and covariances,

$$(\mu_k)_i = \int x_i f(\vec{x}|H_k) d\vec{x},$$

$$(V_k)_{ij} = \int (x_i - \mu_k)_i (x_j - \mu_k)_j f(\vec{x}|H_k) d\vec{x},$$

$$k = 0, 1 \quad (\text{hypothesis}),$$

$$i, j = 1, \dots, n \quad (\text{component of } \vec{x}).$$

Similarly for mean and variance of $t(\vec{x})$,

$$\tau_k = \int t(\vec{x}) f(\vec{x}|H_k) d\vec{x} = \vec{a}^T \vec{\mu}_k,$$

$$\Sigma_k^2 = \int (t(\vec{x}) - \tau_k)^2 f(\vec{x}|H_k) d\vec{x} = \vec{a}^T V_k \vec{a}.$$

We should require:

$$\text{large } |\tau_0 - \tau_1|,$$

$$\text{small } \Sigma_0^2, \Sigma_1^2 \quad (\text{pdfs tightly concentrated about their means})$$

Linear test statistic (continued)

Fisher defines as a measure of separation

$$J(\vec{a}) = \frac{(\tau_0 - \tau_1)^2}{\Sigma_0^2 + \Sigma_1^2}.$$

The numerator of $J(\vec{a})$ is

$$\begin{aligned} (\tau_0 - \tau_1)^2 &= \sum_{i,j=1}^n a_i a_j (\mu_0 - \mu_1)_i (\mu_0 - \mu_1)_j \\ &= \sum_{i,j=1}^n a_i a_j B_{ij} = \vec{a}^T B \vec{a}. \end{aligned}$$

The denominator is

$$\Sigma_0^2 + \Sigma_1^2 = \sum_{i,j=1}^n a_i a_j (V_0 + V_1)_{ij} = \vec{a}^T W \vec{a}.$$

This gives $J(\vec{a}) = \frac{\vec{a}^T B \vec{a}}{\vec{a}^T W \vec{a}} = \frac{\text{separation between classes}}{\text{separation within classes}}$

Set $\frac{\partial J}{\partial a_i} = 0 \Rightarrow \vec{a} \propto W^{-1}(\vec{\mu}_0 - \vec{\mu}_1)$

This defines **Fisher's linear discriminant function**,
determined up to a scale factor for \vec{a} .

R.A. Fisher, *Ann. Eugen.* 7 (1936) 179.

Neural networks (1)

Used in neurobiology, pattern recognition, financial forecasting . . .
here, neural nets are just a type of test statistic.

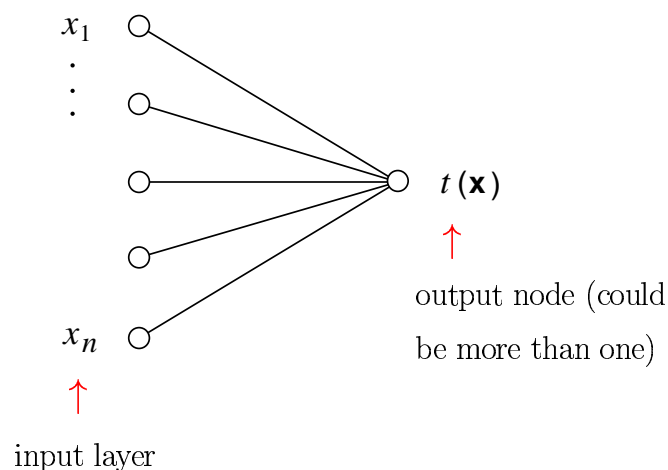
Suppose we take $t(\vec{x})$ to have the form

$$t(\vec{x}) = s \left(a_0 + \sum_{i=1}^n a_i x_i \right)$$

where $s(u) = (1 + e^{-u})^{-1}$ (the 'activation function')

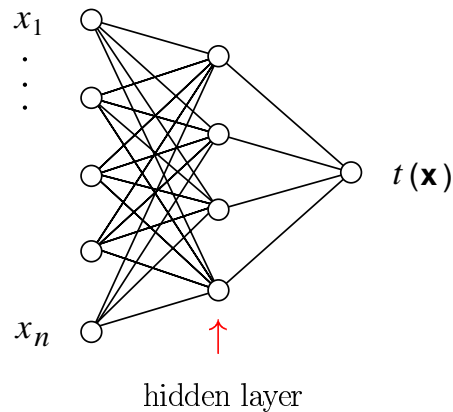
This is the **single-layer perceptron**.

$s(\cdot)$ is monotonic \Rightarrow equivalent to linear $t(\vec{x})$.



Neural networks (2)

Generalize this to the **multilayer perceptron**:



The output is defined by $t(\vec{x}) = s\left(a_0 + \sum_{i=1}^m a_i h_i(\vec{x})\right)$,

where the h_i are functions of the nodes in the previous layer,

$$h_i(\vec{x}) = s\left(w_{i0} + \sum_{j=1}^n w_{ij} x_j\right).$$

a_i, w_{ij} = weights (connection strengths)

Easy to generalize to arbitrary number of layers.

Feed-forward net: values of a node depend only on earlier layers, usually only on previous layer \rightarrow ‘network architecture’

More nodes \rightarrow neural net gets closer to optimal $t(\vec{x})$, but more parameters need to be determined.

Neural networks (3)

Parameters usually determined by minimizing an error function,

$$\mathcal{E} = E_0[(t - t^{(0)})^2] + E_1[(t - t^{(1)})^2],$$

where $t^{(0)}, t^{(1)}$ are **target values**, e.g. 0 and 1 for logistic sigmoid cf. least squares principle with Fisher discriminant.

In practice, replace expectation values by averages of **training data** from Monte Carlo. (Adjusting parameters = network ‘learning’.)

In general this can be tricky; fortunately, programs like **JETNET** do it for you, e.g. with ‘error back-propagation’.

For more information see

- L. Lönnblad et al., *Comput. Phys. Commun.* 70 (1992) 167;
- C. Peterson, et al., *Comput. Phys. Commun.* **81** (1994) 185;
- C.M. Bishop, *Neural Networks for Pattern Recognition*, Clarendon Press, Oxford (1995);
- John Hertz, et al., *Introduction to the Theory of Neural Computation*, Addison-Wesley, New York (1991);
- B. Müller et al., *Neural Networks: an Introduction*, 2nd edition, Springer, Berlin (1995).

Neural networks (4)

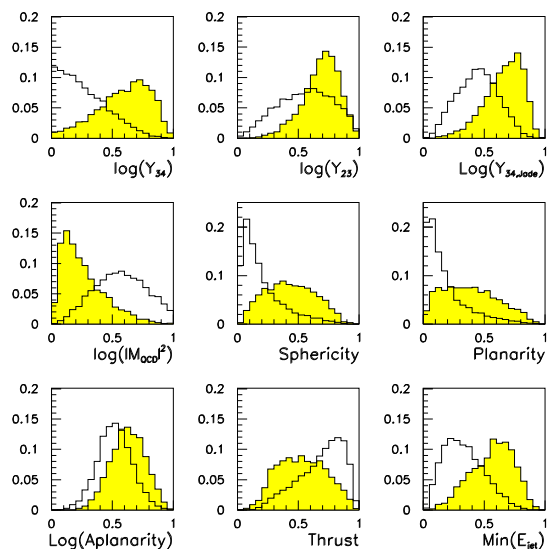
An example with WW event selection

(Garrido, Juste and Martinez, ALEPH 96-144)

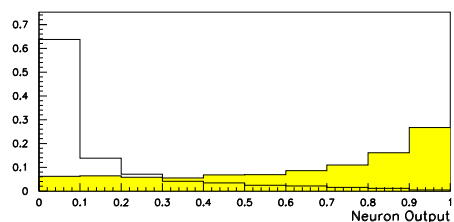
The input variables:

Shaded histograms: WW (signal)

Open histograms: $q\bar{q}$ (background)



The neural network output:



Choosing the input variables

Why not use all of the available input variables?

Fewer inputs \rightarrow fewer parameters to be adjusted,
 \rightarrow parameters better determined for finite training data.

Some inputs may be highly correlated \rightarrow drop all but one.

Some inputs may contain little or no discriminating power between the hypotheses \rightarrow drop them.

NN exploits higher moments of joint pdf $f(\vec{x}|H)$, but these may not be well modeled in training data.

\rightarrow better to have simpler $t(\vec{x})$ where you can 'understand what it's doing'.

Recall that the purpose of the statistical test is usually to select objects for further study; e.g. select WW events, then measure their properties (e.g. particle multiplicity).

\Rightarrow avoid input variables that are correlated with the properties of the selected objects which you want to study. (Not always easy; correlations may not be well known.)

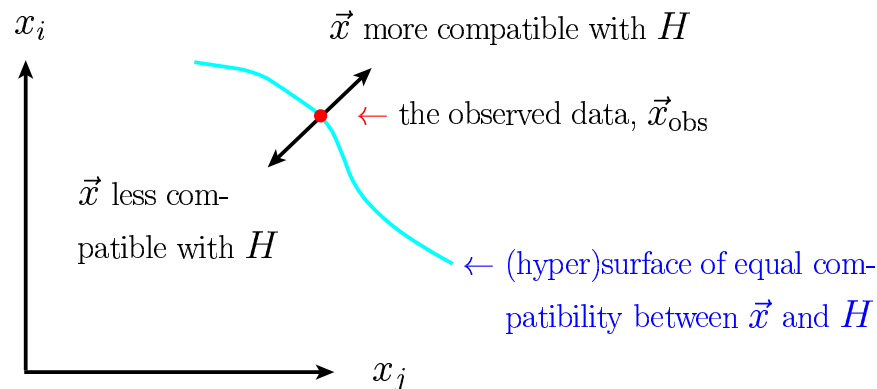
Testing goodness-of-fit

Suppose hypothesis H predicts $f(\vec{x}|H)$ for some vector of data $\vec{x} = (x_1, \dots, x_n)$.

We observe a single point in \vec{x} -space: \vec{x}_{obs} .

What can we say about the validity of H in light of the data?

→ Decide what part of \vec{x} -space represents less compatibility with H than does the observed point \vec{x}_{obs} . (Not unique!)



Usually construct test statistic $t(\vec{x})$ whose value reflects level compatibility between \vec{x} and H , e.g.

low $t \rightarrow$ data more compatible with H ;

high $t \rightarrow$ data less compatible with H .

Since pdf $f(\vec{x}|H)$ known, the pdf $g(t|H)$ can be determined.

P-values

Express ‘goodness-of-fit’ by giving the P -value (also called observed significance level or confidence level):

$P =$ probability to observe data \vec{x} (or $t(\vec{x})$) having equal or lesser compatibility with H as \vec{x}_{obs} (or $t(\vec{x}_{\text{obs}})$)

This is not the ‘probability’ that H is true!

In classical statistics we never talk about $P(H)$.

In Bayesian statistics, treat H as a random variable; use Bayes’ theorem (here symbolically) to obtain

$$P(H|t) = \frac{P(t|H)\pi(H)}{\int P(t|H)\pi(H)dH}$$

where $\pi(H)$ is the prior probability for H ; normalize by integrating (or summing) over all possible hypotheses. For now stick with classical approach, i.e. our final answer is the P -value.

N.B. No alternative hypotheses mentioned.

N.B. P -value is a random variable. Previously considered significance level was a **constant**, specified before the test.

If H true, then (for continuous \vec{x}) P is uniform in $[0, 1]$.

If H not true, then pdf of P is (usually) peaked closer to 0.

An example of a goodness-of-fit test

Probability to observe n_h heads in N coin tosses is:

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

Hypothesis H : the coin is fair ($p_h = p_t = 0.5$)

Take as goodness-of-fit statistic $t = |n_h - \frac{N}{2}|$.

We toss the coin $N = 20$ times and get 17 heads, i.e. $t_{\text{obs}} = 7$.

Region of t -space with equal or lesser compatibility:

$$t \geq 7$$

$$P\text{-value} = P(n_h = 0, 1, 2, 3, 17, 18, 19 \text{ or } 20) = 0.0026$$

So does this mean H is false? P -value does not answer this question; it only gives the probability of obtaining such a level of discrepancy (or higher) with H as that observed.

P -value = probability of obtaining such a bizarre result ‘by chance’.

A philosophical objection (but not a real problem):

Could have defined experiment to end after at least 3 heads and tails; in ours this happened to occur after 20 tosses. In such an experiment, the P -value is 0.00072!

Pragmatist’s solution: ‘repetition of experiment’ taken to mean repetition with same number of trials per experiment.

The significance of an observed signal

Suppose we observe n events; these can consist of:

n_b events from known processes (background)

n_s events from new processes (signal)

If n_b, n_s are Poisson r.v.s with means ν_b, ν_s , $\Rightarrow n = n_s + n_b$

is also Poisson, mean $\nu = \nu_s + \nu_b$ (cf. SDA Chapter 10):

$$P(n; \nu_s, \nu_b) = \frac{(\nu_s + \nu_b)^n}{n!} e^{-(\nu_s + \nu_b)}$$

Suppose $\nu_b = 0.5$ and we observe $n_{\text{obs}} = 5$.

Should we claim evidence for a new discovery?

Hypothesis H : $\nu_s = 0$, i.e. only background present.

$$P\text{-value} = P(n \geq n_{\text{obs}})$$

$$= \sum_{n=n_{\text{obs}}}^{\infty} P(n; \nu_s = 0, \nu_b)$$

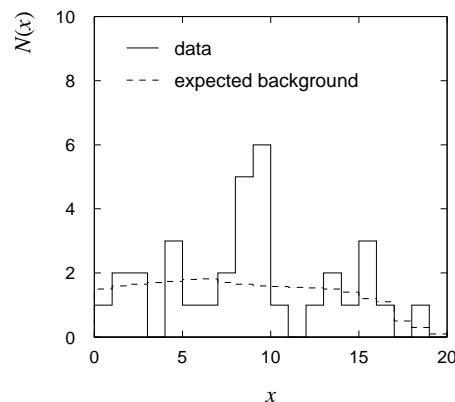
$$= 1 - \sum_{n=0}^{n_{\text{obs}}-1} \frac{\nu_b^n}{n!} e^{-\nu_b}$$

$$= 1.7 \times 10^{-4}$$

$$(\neq P(\nu_s = 0)!)$$

The significance of a peak

Suppose in addition to counting events, we measure x for each.



← Histogram of observed and expected data. Each bin is a Poisson variable.

In the 2 bins with peak, 11 entries found, $\nu_b = 3.2$,

$$P(n \geq 11; \nu_b = 3.2; \nu_s = 0) = 5.0 \times 10^{-4}$$

But... did we know where to look for the peak?

→ give $P(n \geq 11)$ in any 2 adjacent bins.

Is the observed width consistent with the expected x resolution?

→ take x window several times expected resolution

How many bins \times distributions have we looked at?

→ look at a thousand of them, you'll find a 10^{-3} effect.

Did we adjust the cuts to 'enhance' the peak?

→ freeze cuts, repeat analysis with new data.

How about the bins to the sides of the peak ... (too low!)

Should we publish???

Pearson's χ^2 test

Test statistic for comparing observed data $\vec{n} = (n_1, \dots, n_N)$ to predicted expectation values $\vec{\nu} = (\nu_1, \dots, \nu_N)$:

$$\chi^2 = \sum_{i=1}^N \frac{(n_i - \nu_i)^2}{\nu_i}$$

If n_i are independent Poisson r.v.s with means ν_i , and all ν_i not too small (rule of thumb: all $\nu_i \geq 5$), then χ^2 will follow the chi-square pdf for N dof.

The observed χ^2 then gives a P -value:

$$P = \int_{\chi^2}^{\infty} f(z; N) dz$$

where $f(z; N)$ is the chi-square pdf for N degrees of freedom.

Recall for chi-square pdf, $E[z] = N$,

→ often give χ^2/N as measure of level of agreement

Better to give χ^2 , N separately ...

$$\chi^2 = 15, N = 10 \rightarrow P\text{-value} = 0.13$$

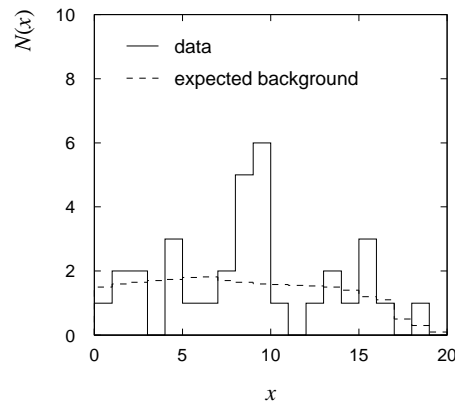
$$\chi^2 = 150, N = 100 \rightarrow P\text{-value} = 9.0 \times 10^{-4}$$

If $n_{\text{tot}} = \sum_{i=1}^N n_i$ is fixed, n_i are binomial, $p_i = \nu_i/n_{\text{tot}}$,

$$\chi^2 = \sum_{i=1}^N \frac{(n_i - p_i n_{\text{tot}})^2}{p_i n_{\text{tot}}}$$

will follow chi-square for $N - 1$ dof (all $p_i n_{\text{tot}} \gg 1$).

Example of χ^2 test



← This gives

$$\chi^2 = \sum_{i=1}^N \frac{(n_i - \nu_i)^2}{\nu_i}$$

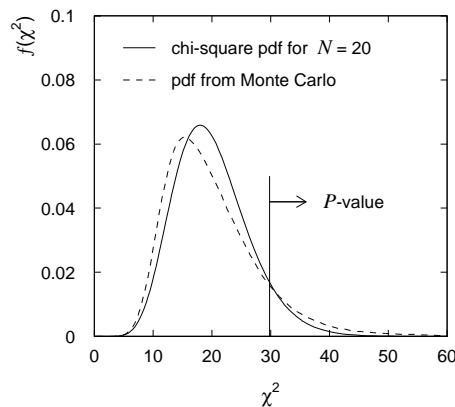
$$= 29.8 \text{ for } N = 20 \text{ dof.}$$

But... many bins have few (or no) entries,

→ here χ^2 will not follow chi-square pdf.

Pearson's χ^2 still usable as a test statistic, but to compute P -value first get $f(\chi^2)$ from Monte Carlo:

Generate n_i from Poisson, mean ν_i , $i = 1, \dots, N$,
compute χ^2 , record in histogram,
repeat experiment many times (here 10^6).



Using pdf from MC gives

$$P = 0.11$$

Chi-square pdf would give

$$P = 0.073$$

Parameter estimation: general concepts

Consider n independent observations of an r.v. x ,

→ sample of size n

Equivalently, single observation of an n -dimensional vector:

$$\vec{x} = (x_1, \dots, x_n)$$

The x_i are independent \Rightarrow joint pdf for the sample is

$$f_{\text{sample}}(\vec{x}) = f(x_1)f(x_2) \cdots f(x_n)$$

Task: given a data sample, infer properties of $f(x)$.

→ construct functions of the data to estimate various properties of $f(x)$ (mean, variance, ...)

Often, form of $f(x)$ hypothesized, value of parameter(s) unknown

→ given form of $f(x; \theta)$ and data sample, estimate θ

Statistic = function of the data

Estimator = statistic used to estimate some property of a pdf

notation: estimator for θ is $\hat{\theta}$ (hat means estimator)

Estimate = an observed value of an estimator (often: $\hat{\theta}_{\text{obs}}$)

N.B. $\hat{\theta}(\vec{x})$ is a function of a (vector) random variable,

\Rightarrow it is itself a random variable, characterized by a pdf $g(\hat{\theta})$
with an expectation value (mean), variance, etc.

Estimators

How do we construct an estimator $\hat{\theta}(\vec{x})$?

There is no golden rule on how
to construct an estimator.

Construct estimators to satisfy (in general conflicting) criteria.

As a start, require **consistency**: $\lim_{n \rightarrow \infty} \hat{\theta} = \theta$

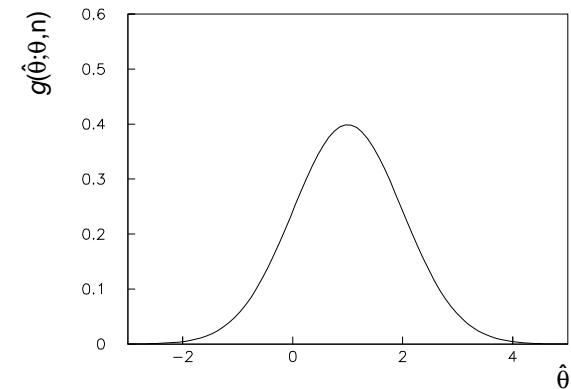
i.e. as size of sample increases, estimate converges to true value:

$$\text{for any } \epsilon > 0, \lim_{n \rightarrow \infty} P(|\hat{\theta} - \theta| > \epsilon) = 0.$$

N.B. convergence in the sense of probability, i.e. no guaranty that any particular $\hat{\theta}_{\text{obs}}$ will be within any given distance of θ .

Properties of estimators

Consider the pdf of $\hat{\theta}$ for a fixed sample size n :



N.B. $g(\hat{\theta}; \theta, n)$ depends on true (unknown!) parameter θ .

We don't know θ , just a single value $\hat{\theta}_{\text{obs}}$.

Properties of $g(\hat{\theta}; \theta, n)$:

$$\text{variance } V[\hat{\theta}] = \sigma_{\hat{\theta}}^2. \quad (\sigma_{\hat{\theta}} = \text{'statistical error'})$$

$$\text{bias } b = E[\hat{\theta}] - \theta \quad (\text{'systematic error', depends on } n)$$

For many estimators we will have $\sigma_{\hat{\theta}} \propto \frac{1}{\sqrt{n}}$, $b \propto \frac{1}{n}$.

Sometimes consider **mean squared error**:

$$\text{MSE} = V[\hat{\theta}] + b^2$$

In general, there is a trade-off between bias and variance,

\rightarrow often require minimum variance among estimators with 0 bias

Estimator for the mean (expectation value)

Consider n measurements of r.v. x , x_1, \dots, x_n , we want an estimator for $\mu = E[x]$. Try arithmetic mean of the x_i :

$$\hat{\mu} = \bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad (\text{the sample mean})$$

If $V[x]$ finite, \bar{x} is a consistent estimator for μ , i.e.

$$\text{for any } \epsilon > 0, \lim_{n \rightarrow \infty} P \left(\left| \frac{1}{n} \sum_{i=1}^n x_i - \mu \right| \geq \epsilon \right) = 0.$$

This is the **Weak Law of Large Numbers**. Compute expectation value:

$$E[\bar{x}] = E \left[\frac{1}{n} \sum_{i=1}^n x_i \right] = \frac{1}{n} \sum_{i=1}^n E[x_i] = \frac{1}{n} \sum_{i=1}^n \mu = \mu$$

$\rightarrow \bar{x}$ is an unbiased estimator for μ . Compute variance:

$$\begin{aligned} V[\bar{x}] &= E[\bar{x}^2] - (E[\bar{x}])^2 = E \left[\left(\frac{1}{n} \sum_{i=1}^n x_i \right) \left(\frac{1}{n} \sum_{j=1}^n x_j \right) \right] - \mu^2 \\ &= \frac{1}{n^2} \sum_{i,j=1}^n E[x_i x_j] - \mu^2 \\ &= \frac{1}{n^2} [(n^2 - n)\mu^2 + n(\mu^2 + \sigma^2)] - \mu^2 = \frac{\sigma^2}{n} \end{aligned}$$

where σ^2 is the variance of x , and we used

$$E[x_i x_j] = \mu^2 \text{ for } i \neq j \text{ and } E[x_i^2] = \mu^2 + \sigma^2.$$

Estimator for the variance

Suppose mean μ and variance $V[x] = \sigma^2$ both unknown.

Estimate σ^2 with the **sample variance**:

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

Factor of $1/(n-1)$ included so that $E[s^2] = \sigma^2$ (i.e. no bias)

If $\mu = E[x]$ is known a priori,

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

is an unbiased estimator for σ^2 .

Computing the variance of s^2 (long calculation!) gives

$$V[s^2] = \frac{1}{n} \left(\mu_4 - \frac{n-3}{n-1} \mu_2^2 \right)$$

where μ_k is k th central moment (e.g. $\mu_2 = \sigma^2$).

The μ_k can be estimated using

$$m_k = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^k$$

Estimator for covariance and correlation coefficient

To estimate the covariance $V_{xy} = \text{cov}[x, y]$, use

$$\widehat{V}_{xy} = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) = \frac{n}{n-1} (\overline{xy} - \bar{x}\bar{y})$$

which is unbiased.

For the correlation coefficient $\rho = \frac{V_{xy}}{\sigma_x \sigma_y}$, use

$$\begin{aligned} r &= \frac{\widehat{V}_{xy}}{s_x s_y} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\left(\sum_{j=1}^n (x_j - \bar{x})^2 \cdot \sum_{k=1}^n (y_k - \bar{y})^2\right)^{1/2}} \\ &= \frac{\overline{xy} - \bar{x}\bar{y}}{\sqrt{(\overline{x^2} - \bar{x}^2)(\overline{y^2} - \bar{y}^2)}}. \end{aligned}$$

r has a bias which goes to zero as $n \rightarrow \infty$.

In general, pdf $g(r; \rho, n)$ is complicated; for Gaussian x, y ,

$$E[r] = \rho - \frac{\rho(1 - \rho^2)}{2n} + O(n^{-2})$$

$$V[r] = \frac{1}{n} (1 - \rho^2)^2 + O(n^{-2})$$

(cf. R.J. Muirhead, *Aspects of Multivariate Statistical Theory*, Wiley, New York, 1982.)

Lecture 2 summary

- **Statistical tests:** test whether data stand in agreement with predicted probabilities, i.e., hypotheses. Critical region, significance level, power, (related to efficiency, purity).
- **Fisher discriminants, neural networks, etc.:** reduce data vector \vec{x} to a single (or few) component function $t(\vec{x})$. Compact data while retaining ability to discriminate between hypotheses.
- **Goodness-of-fit tests:** quantify level of agreement between data and hypothesis with P -value.
- **The significance of a signal:** often give P -value of hypothesis that only background present.
- **Introduction to parameter estimation:** try to minimize bias and variance. Simple estimators for mean, variance, covariance.