Lecture 4 outline

Statistical tests (part I)

1. **Hypotheses, test statistics, significance level, power**
2. **An example with particle selection**
3. **The Neyman-Pearson lemma**
4. **Constructing a test statistic:**

   Fisher discriminant function

   Neural networks

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. $e^+e^- \to q\bar{q}$, $e^+e^- \to WW$, 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, …not r.v.s.)

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), $t(\vec{x})$:

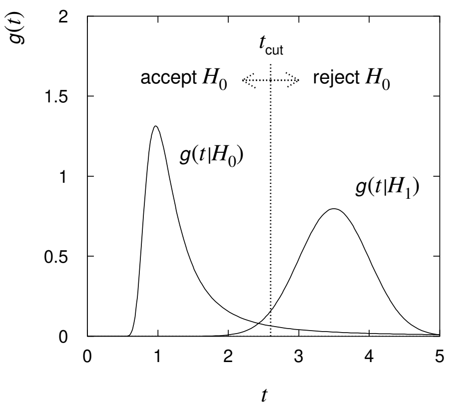
compactify data,

try not to lose ability to discriminate bewteen hypotheses.

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

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, $t \geq t_{\mathrm{cut}}$.

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):

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

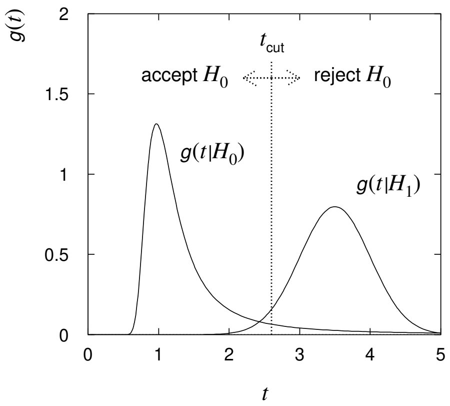
Probability to accept H_0 if H_1 is true (error of 2nd kind):

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

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 $t < t_{\mathrm{cut}}$. The selection efficiencies are:

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

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

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

$$f(t; a_{\mathrm{e}}) = a_{\mathrm{e}} g(t|e) + (1 - a_{\mathrm{e}}) g(t|\pi)$$

$\rightarrow$ estimate a_{e} (for now assume a_{e}, $a_\pi = 1 - a_{\mathrm{e}}$ known)

Purity of selected sample

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

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

(Bayes' theorem)

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

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

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

$\rightarrow$ here both approaches make sense

Often want purity of selected sample:

$$p_\mathrm{e} = \frac{\text{number of electrons with } t < t_\mathrm{cut}}{\text{number of all particles with } t < t_\mathrm{cut}}$$

$$= \frac{\int_{-\infty}^{t_\mathrm{cut}} a_\mathrm{e} g(t|\mathrm{e})dt}{\int_{-\infty}^{t_\mathrm{cut}} (a_\mathrm{e} g(t|\mathrm{e}) + (1 - a_\mathrm{e}) g(t|\pi))dt}$$

$$= \frac{\int_{-\infty}^{t_\mathrm{cut}} h(\mathrm{e}|t)\, f(t)\, dt}{\int_{-\infty}^{t_\mathrm{cut}} f(t)\, dt}$$

$$= \text{electron probability averaged over interval } (-\infty, t_\mathrm{cut}]$$

Sometimes $h(e|t)$ is reinterpreted as the test statistic;

in principle OK, but but you need to know electron fraction a_e.

The Neyman–Pearson lemma

Consider a multidimensional test statistic $\vec{t} = (t_1, \ldots, t_m)$;

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 = 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: $H_0 = \mathrm{e^+e^-} \to \mathrm{WW} \to$ hadrons (usually four jets)

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

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

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!

$\Rightarrow$ 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 $g(t|H_0)$, $g(t|H_1)$.

$\rightarrow$ Must define 'separation'.

We have the expectation values and covariances,

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

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

$k = 0, 1$ (hypothesis),

$i, j = 1, \ldots, n$ (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:

large $|\tau_0 - \tau_1|$,

small Σ_0^2, Σ_1^2 (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

$$(\tau_0 - \tau_1)^2 = \sum_{i,j=1}^{n} a_i a_j (\mu_0 - \mu_1)_i (\mu_0 - \mu_1)_j$$

$$= \sum_{i,j=1}^{n} a_i a_j B_{ij} = \vec{a}^T\, B\, \vec{a}\,.$$

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 $J(\vec{a}) = \dfrac{\vec{a}^T\, B\, \vec{a}}{\vec{a}^T\, W\, \vec{a}} = \dfrac{\text{separation between classes}}{\text{separation within classes}}$

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

This defines Fisher's linear discriminant function,

determined up to a scale factor for $\vec{a}$.

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

The Fisher discriminant (continued)

We can generalize $t(\vec{x})$ to be

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

Use the arbitrary scale and the offset a_0 to fix τ_0, τ_1.

Then maximizing $J(\vec{a}) = \dfrac{(\tau_0 - \tau_1)^2}{\Sigma_0^2 + \Sigma_1^2}$ means minimizing

$$\Sigma_0^2 + \Sigma_1^2 = E_0[(t - \tau_0)^2] + E_1[(t - \tau_1)^2]$$

(index shows hypothesis for expectation value)

$\rightarrow$ Maximizing Fisher's $J(\vec{a})$ is a type of least squares principle.

G. Cowan – Computing and Statistical Data Analysis – University of London Postgraduate Lectures

The Fisher discriminant for Gaussian $\vec{x}$

Suppose $f(\vec{x}|H_k)$ is multivariate Gaussian with mean values

$$\vec{\mu}_0 \text{ for } H_0,$$
$$\vec{\mu}_1 \text{ for } H_1,$$

and covariance matrices $V_0 = V_1 \equiv V$ for both.

The Fisher discriminant (with an offset) is

$$t(\vec{x}) = a_0 + (\vec{\mu}_0 - \vec{\mu}_1)^T V^{-1} \vec{x} \,.$$

Recall the likelihood ratio (maximum purity for given efficiency):

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

$$= \exp\left[-\tfrac{1}{2}(\vec{x}-\vec{\mu}_0)^T V^{-1}(\vec{x}-\vec{\mu}_0) + \tfrac{1}{2}(\vec{x}-\vec{\mu}_1)^T V^{-1}(\vec{x}-\vec{\mu}_1)\right]$$

$$\propto e^t$$

That is, $t \propto \log r + \text{const.}$ (monotonic) so for this case,

$\Rightarrow$ Fisher discriminant equivalent to likelihood ratio.

N.B. for $\vec{x}$ following other pdfs, this no longer holds.

The Fisher discriminant for Gaussian $\vec{x}$ (continued)

Multivariate Gaussian $\vec{x}$ with equal covariance matrices also gives a simple expression for posterior probabilities, e.g.

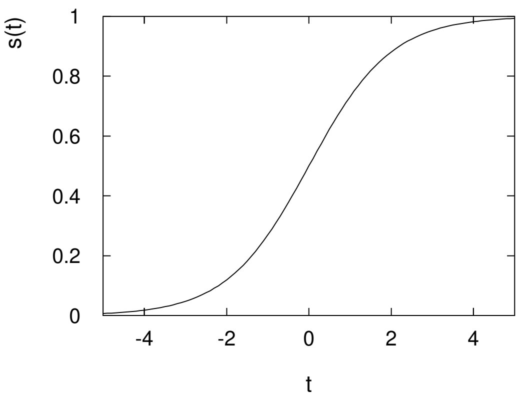
$$P(H_0|\vec{x}) = \frac{f(\vec{x}|H_0)\pi_0}{f(\vec{x}|H_0)\pi_0 + f(\vec{x}|H_1)\pi_1} \quad \leftarrow \text{Bayes' theorem}$$

$$= \frac{1}{1 + \frac{\pi_1}{\pi_0 r}}$$

For a particular choice of the offset a_0 this can be written as

$$P(H_0|\vec{x}) = \frac{1}{1 + e^{-t}} \equiv s(t)\,,$$

which is the logistic sigmoid function:



Neural networks (1)

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

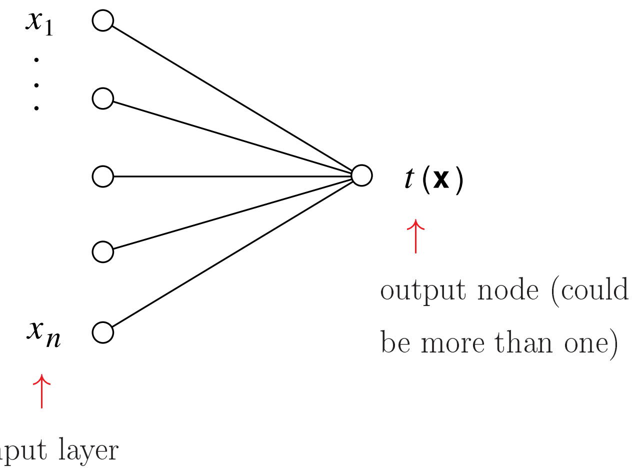
Suppose we take $t(\vec{x})$ to have the form

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

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

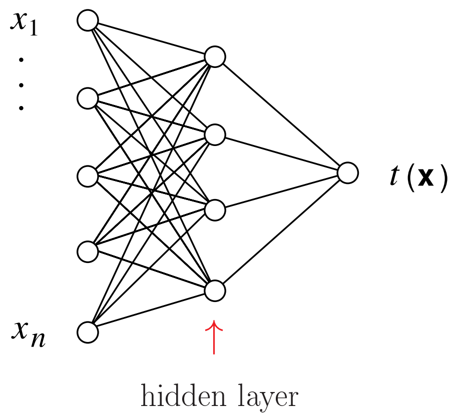
This is the single-layer perceptron.

$s(\cdot)$ is monotic $\Rightarrow$ 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-propogation'.

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)

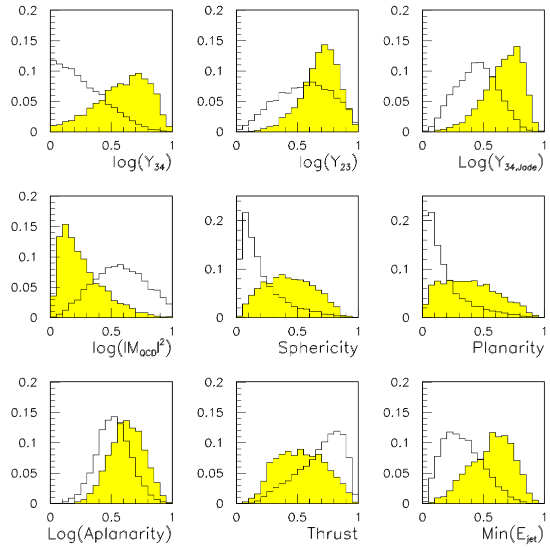
An example with WW event selection

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

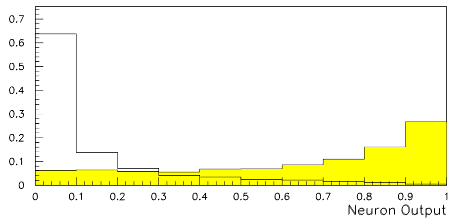
The input variables:

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 → fewer parameters to be adjusted,

→ parameters better determined for finite training data.

Some inputs may be highly correlated → drop all but one.

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

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

→ 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).

⇒ 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.)

Lecture 4 summary

- **Statistical tests:** test to what extent data stand in agreement with predicted probabilities, i.e. hypotheses.
- **Test statistics:** reduce vector $\vec{x}$ to a single (or few) component function $t(\vec{x})$.
- **The ingredients of a test:** critical region, significance level, power, (related to efficiency, purity).
- **The Neyman-Pearson lemma:** gives cut region with maximum purity for a given efficiency.
- **Constructing a test statistic:** likelihood ratio best, but usually need to determine too many parameters.
- **Alternative Ansätze for statistics:**

  Fisher discriminant function (linear)

  Neural network (nonlinear)