Truth of a Hypothesis: The χ^2 Test

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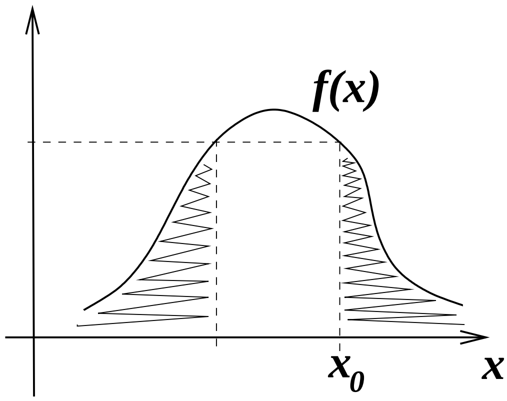
1 The single observable case

x ... a random observable
$f(x)$ ... p.d.f.
x_0 ... the measured value of x



Def: $\boxed{x \text{ is } \textit{worse} \text{ than } x_0 \quad \Leftrightarrow \quad f(x) < f(x_0)}$

Backing of x_0 for the hypothesis $f(x)$:

$$\boxed{\text{support of } x_0 \text{ for } f(x) \quad = \quad \text{probability of obtaining any value worse than } x_0}$$

$$B(x_0; f) = \int_{f(x)<f(x_0)} f(x)\, dx \tag{1}$$

Symmetric p.d.f.:
let $f(x)$ have a peak at $x = X$
let $f(X - \Delta x) = f(X + \Delta x), \forall \Delta x$
then

$$B(x_0; f) = 2 \int_{x_0}^{\infty} f(x)\, dx \tag{2}$$

note that

$$x \text{ is worse than } x_0 \quad \Leftrightarrow \quad |x - X| > |x_0 - X|$$

Gaussian p.d.f.:
let $f(x)$ be a Gaussian, the peak at $X = \mu$,

$$f(x) = \frac{1}{(2\pi)^{1/2}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \tag{3}$$

the backing:

$$B(x_0;\mu,\sigma) = \frac{2}{(2\pi)^{1/2}\sigma} \int_{x_0}^{\infty} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] dx = \sqrt{\frac{2}{\pi}} \int_{\chi_0}^{\infty} e^{-\chi^2/2}\, d\chi,$$

where $\chi \equiv (x-\mu)/\sigma > 0$, $\chi_0 \equiv (x_0-\mu)/\sigma > 0$;
let $z \equiv \chi^2$

$$B(x_0;\mu,\sigma) = \frac{1}{\sqrt{2\pi}} \int_{\chi_0^2}^{\infty} \frac{e^{-z/2}}{\sqrt{z}}\, dz = \int_{\chi_0^2}^{\infty} p_{\chi^2}(z)\, dz \tag{4}$$

$$\boxed{\text{the backing of } x_0 \text{ is equal to the probability that } z > \chi_0^2 \text{ for } z \text{ distributed as } p_{\chi^2}(z)}$$

Def of χ^2-distribution function (a single observable case):

$$p_{\chi^2}(z) = \frac{1}{\sqrt{2\pi}} \frac{e^{-z/2}}{\sqrt{z}} \tag{5}$$

2 The n observables case

$\vec{X} = \{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$ ... independent random observables
$\vec{f} = \{f^{(1)}(x^{(1)}), f^{(2)}(x^{(2)}), \ldots, f^{(n)}(x^{(n)})\}$ ... p.d.f.'s
$\vec{X}_0 = \{x_0^{(1)}, x_0^{(2)}, \ldots, x_0^{(n)}\}$ ... measured values of $\vec{X}$

Def:

$$\boxed{\vec{X} \text{ is } \textit{worse} \text{ than } \vec{X}_0 \quad \Leftrightarrow \quad \underbrace{\prod_{k=1}^{n} f^{(k)}(x^{(k)})}_{F(\vec{X})} < \underbrace{\prod_{k=1}^{n} f^{(k)}(x_0^{(k)})}_{F(\vec{X}_0)}}$$

Backing of $\vec{X}_0$ for the hypothesis $\vec{f}$:

$$\boxed{\text{support of } \vec{X}_0 \text{ for } \vec{f} \quad = \quad \text{probability of obtaining } \vec{X} \text{ worse than } \vec{X}_0}$$

$$B(\vec{X}_0;\vec{f}) = \overbrace{\int \ldots \int}^{n-times}_{F(\vec{X})<F(\vec{X}_0)} F(\vec{X})\ \underbrace{dx^{(1)} \ldots x^{(n)}}_{d\vec{X}} \tag{6}$$

Gaussian distributed random observables $x^{(1)} \ldots x^{(n)}$:

$$f^{(k)}(x) = \frac{1}{(2\pi)^{1/2}\sigma_k} \exp\left[-\frac{(x-\mu_k)^2}{2\sigma_k^2}\right], \qquad k = 1, \ldots, n \tag{7}$$

then

$$F(\vec{X}) = \frac{1}{(2\pi)^{n/2}\prod_{k=1}^{n}\sigma_k} \exp\left[-\frac{\chi^2(\vec{X})}{2}\right] \tag{8}$$

where

$$\chi(\vec{X}) \equiv \sqrt{\sum_{k=1}^{n} \frac{(x^{(k)}-\mu_k)^2}{\sigma_k^2}} \tag{9}$$

the backing of $\vec{X}_0$ for $\vec{f}$ (which is essentially the backing for the given set of μ_k's and σ_k's):

$$B(\vec{X}_0;\vec{f}) = \overbrace{\int\ldots\int}^{n-times}_{\chi^2>\chi_0^2} F(\vec{X})\, d\vec{X} = \frac{1}{(2\pi)^{n/2}} \overbrace{\int\ldots\int}^{n-times}_{\chi^2>\chi_0^2} \exp(-\chi^2(\vec{\kappa})/2)\, d\vec{\kappa},$$

where $\chi_0 = \chi(\vec{X}_0)$, $\kappa^{(k)} = (x^{(k)}-\mu_k)/\sigma_k$, and $\chi^2 = (\kappa^{(1)})^2 + \ldots + (\kappa^{(n)})^2$. Since the integrand depends on χ^2 only it is useful to switch to the n-dim spherical coordinates. All integration but the one with respect to χ is trivial. Thus using

$$d\vec{\kappa} = \frac{n\pi^{n/2}}{\Gamma(\frac{n}{2}+1)}\chi^{n-1}\, d\chi \tag{10}$$

and considering $\Gamma(\frac{n}{2}+1) = \frac{n}{2}\Gamma(\frac{n}{2})$ we get

$$B(\vec{X}_0;\vec{f}) = \frac{1}{2^{n/2-1}\Gamma(\frac{n}{2})}\int_{\chi_0}^{\infty} \exp(-\chi^2/2)\, \chi^{n-1}\, d\chi \tag{11}$$

let $\chi = \sqrt{z}$:

$$B(\vec{X}_0;\vec{f}) = \frac{1}{2^{n/2}\Gamma(\frac{n}{2})}\int_{\chi_0^2}^{\infty} e^{-z/2}\, z^{n/2-1}\, dz = \int_{\chi_0^2}^{\infty} p_{\chi^2}^{(n)}(z)\, dz. \tag{12}$$

$$\boxed{\text{the backing of } \vec{X}_0 \text{ is equal to the probability that } z > \chi_0^2 \text{ for } z \text{ distributed as } p_{\chi^2}^{(n)}(z)}$$

Def of χ^2-distribution function (an n observables case):

$$p_{\chi^2}^{(n)}(z) = \frac{e^{-z/2}\, z^{n/2-1}}{2^{n/2}\Gamma(\frac{n}{2})} \tag{13}$$

3 The Best Fit

$\vec{X} = \{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$ ... independent Gaussian distributed random observables
$f(x; \mu_k, \sigma_k),\ k = 1, \ldots, n$ ... Gaussian p.d.f.'s
$\vec{X}_0 = \{x_0^{(1)}, x_0^{(2)}, \ldots, x_0^{(n)}\}$ ... measured values of $\vec{X}$

$\{\sigma_1, \ldots, \sigma_n\}$ ... the errors of measurements
they should better be the errors on theoretical predictions but the common practice is to use the errors of measurements
see [L.Lyons: Statistics for Nuclear and Particle Physicists, p.102 on]

let the observables $\vec{X}$ be functions of some parameters $\vec{p} = \{p_1, \ldots, p_m\},\ m < n$
then

$$\mu_1 = \mu_1(\vec{p}),\ \ldots\ , \mu_n = \mu_n(\vec{p})$$

Which $\vec{p}$ is the best supported one by the measurement $\vec{X}_0$?
Obviously, the one that minimizes

$$\chi^2(\vec{p}) = \sum_{k=1}^{n} \frac{[x_0^{(k)} - \mu_k(\vec{p})]^2}{\sigma_k^2} \tag{14}$$

because it has the greatest backing!
Note, that in this situation there is only $n - m$ d.o.f.!
Thus the backing is given by $(n - m)$-dim χ^2-distribution $p_{\chi^2}^{(n-m)}(z)$.

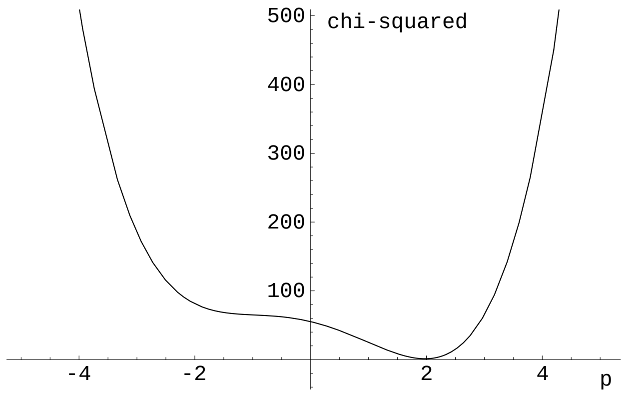
EXAMPLE:

measurements and errors:
$x_0^{(1)} = 6 \pm 1$
$x_0^{(2)} = 11 \pm 2$

dependency on parameters:
$\mu_1(p) = 1 + 2p$
$\mu_2(p) = 3p^2$

the value of χ^2 parameterized by p:

$$\chi^2(p) = \frac{[x_0^{(1)} - \mu_1(p)]^2}{\sigma_1^2} + \frac{[x_0^{(2)} - \mu_2(p)]^2}{\sigma_2^2} = (5 - 2p)^2 + \frac{1}{4}(11 - 3p^2)^2$$



searching for the minimum of $\chi^2(p)$:

$$\frac{d\chi^2(p)}{dp} = 9p^3 - 25p - 20 = 0$$

the numerical solution:

$$p_0 = 1.97552$$

this is the value of p for which the theoretical predictions for observables,

$$\mu_1(p_0) = 4.95104, \quad \mu_2(p_0) = 11.708,$$

have the greatest support from measured data $\vec{X}_0 = \{6, 11\}$

the backing:

$$\text{d.o.f.} = 2 - 1 = 1$$

$$\chi_0^2 = \chi^2(p_0) = 1.22565$$

the Chi Square Calculator (`http://www.stat.sc.edu/~west/applets/chisqdemo.html`):

$$B(\underbrace{\{6, 11\}}_{\vec{X}_0}; \underbrace{4.95104 \pm 1}_{\mu_1 \pm \sigma_1}, \underbrace{11.708 \pm 2}_{\mu_2 \pm \sigma_2}) = 15.98\%$$

summary table:

observable	measured	fitted	$\lvert\text{measured} - \text{fitted}\rvert/\sigma$
$x^{(1)}$	6 ± 1	4.95104	1.04896
$x^{(2)}$	11 ± 2	11.708	0.354019

(15)