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Recipes for Exclusion Limits

We summarize the mathematics needed for computing exclusion limits based on profile likelihood ratio tests. The material is largely extracted from Ref. [1], where more details can be found. We consider testing a hypothesized signal strength μ, defined such that $\mu = 0$ is the background-only model, and $\mu = 1$ corresponds to the nominal signal model. The result of the significance test is a p-value, p_μ. If one finds $p_\mu < 0.05$, then this value of μ is excluded at 95% confidence level. The upper limit on μ is the highest value of μ not excluded, in practice found by solving $p_\mu = 0.05$ for μ.

Here we assume the search is carried out using a histogram where signal could be present, represented as a set of numbers $\mathbf{n} = (n_1, \ldots, n_N)$, where the expectation value of n_i can be written

$$E[n_i] = \nu_i = \mu s_i + b_i \ . \tag{1}$$

Here s_i and b_i are the expected numbers of entries in bin i, and μ is the strength parameter. The values s_i and b_i will depend in general on a set of nuisance parameters $\boldsymbol{\theta}$.

The analysis may use one or more control histograms to constrain the nuisance parameters. A control histogram is represented by $\mathbf{m} = (m_1, \ldots, m_M)$ with expectation values

$$E[m_i] = u_i(\boldsymbol{\theta}) \ , \tag{2}$$

where the functions $u_i(\theta)$ are given functions of the nuisance parameters $\boldsymbol{\theta}$.

These ingredients are used in a statistical test of the strength parameter μ by using the profile likelihood ratio. Often one assumes that the presence of signal can only increase the expected number events, i.e., a physical model requires $\mu \geq 0$ Nevertheless, the estimator $\hat{\mu}$ is taken to be the value of μ that maximizes the likelihood, even if this value is negative. If a data set gives $\hat{\mu} < 0$, then the best level of agreement between the data and any physical value of μ occurs for $\mu = 0$. Therefore to measure the level of agreement between the data and a hypothesized value of the strength parameter μ we take the ratio of the profile likelihood at the hypothesized μ to the maximum likelihood for a physical model, i.e.,

$$\tilde{\lambda}(\mu) = \begin{cases} \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} & \hat{\mu} \geq 0, \\ \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(0, \hat{\hat{\boldsymbol{\theta}}}(0))} & \hat{\mu} < 0 \ . \end{cases} \tag{3}$$

Here $\hat{\hat{\boldsymbol{\theta}}}(0)$ and $\hat{\hat{\boldsymbol{\theta}}}(\mu)$ refer to the conditional ML estimators of $\boldsymbol{\theta}$ given a strength parameter of 0 or μ, respectively.

We then define the test statistic $\tilde{q}_\mu$ as

$$\tilde{q}_\mu = \begin{cases} -2\ln\tilde{\lambda}(\mu) & \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \end{cases} \quad = \quad \begin{cases} -2\ln\frac{L(\mu,\hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(0,\hat{\hat{\boldsymbol{\theta}}}(0))} & \hat{\mu} < 0\ , \\ -2\ln\frac{L(\mu,\hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(\hat{\mu},\hat{\boldsymbol{\theta}})} & 0 \le \hat{\mu} \le \mu\ , \\ 0 & \hat{\mu} > \mu\ . \end{cases} \tag{4}$$

Large values of $\tilde{q}_\mu$ corresponding to increasing disagreement between the data and the hypothesized μ. For a sufficiently large data sample, the pdf $f(\tilde{q}_\mu|\mu)$ is found to approach

$$f(\tilde{q}_\mu|\mu) = \frac{1}{2}\delta(\tilde{q}_\mu) + \begin{cases} \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\tilde{q}_\mu}}e^{-\tilde{q}_\mu/2} & 0 < \tilde{q}_\mu \le \mu^2/\sigma^2\ , \\ \frac{1}{\sqrt{2\pi}(2\mu/\sigma)}\exp\left[-\frac{1}{2}\frac{(\tilde{q}_\mu+\mu^2/\sigma^2)^2}{(2\mu/\sigma)^2}\right] & \tilde{q}_\mu > \mu^2/\sigma^2\ . \end{cases} \tag{5}$$

Equation (5) requires the standard deviation σ of $\hat{\mu}$, under assumption of a signal strength μ. This can be found by first estimating the covariance matrix from the matrix of second derivatives of the log-likelihood function, evaluated with the Asimov data set that corresponds to the strength parameter μ that is being tested. That is, the Asimov data values are

$$n_{\mathrm{A},i} = \mu s_i + b_i\ , \tag{6}$$

$$m_{\mathrm{A},i} = u_i\ . \tag{7}$$

We denote the likelihood evaluated with the Asimov data values as $L_{\mathrm{A}}(\mu)$. Note that this depends both on the strength parameter μ being tested as well as on the value of μ that defines the Asimov data in Eq. (6). When finding the p-value, these two values are the same.

For the inverse covariance matrix one finds (see [1] Eq. (28)),

$$V_{jk}^{-1} = -\frac{\partial^2 \ln L_{\mathrm{A}}}{\partial\theta_j\partial\theta_k} = \sum_{i=1}^{N}\frac{\partial\nu_i}{\partial\theta_j}\frac{\partial\nu_i}{\partial\theta_k}\frac{1}{\nu_i} + \sum_{i=1}^{M}\frac{\partial u_i}{\partial\theta_j}\frac{\partial u_i}{\partial\theta_k}\frac{1}{u_i}\ . \tag{8}$$

In Eq. (8) the parameter μ is regarded as one of the θ_i (say, θ_0). To find σ, evaluate the derivatives of $\ln L_{\mathrm{A}}$ numerically, use this to find the inverse covariance matrix, and then invert and extract the variance of $\hat{\mu}$. One can see directly from Eq. (8) that this variance depends on the parameter values assumed for the Asimov data set, in particular on the assumed strength parameter μ.

The cumulative distribution for $\tilde{q}_\mu$ corresponding to the pdf (5) is

$$F(\tilde{q}_\mu|\mu) = \begin{cases} \Phi\left(\sqrt{\tilde{q}_\mu}\right) & 0 < \tilde{q}_\mu \le \mu^2/\sigma^2\ , \\ \Phi\left(\frac{\tilde{q}_\mu+\mu^2/\sigma^2}{2\mu/\sigma}\right) & \tilde{q}_\mu > \mu^2/\sigma^2\ . \end{cases} \tag{9}$$

The p-value of the hypothesized μ is as before given by one minus the cumulative distribution,

$$p_\mu = 1 - F(\tilde{q}_\mu|\mu)\ , \tag{10}$$

and therefore the corresponding significance is

$$Z_\mu = \begin{cases} \sqrt{\tilde{q}_\mu} & 0 < \tilde{q}_\mu \leq \mu^2/\sigma^2 \ , \\ \frac{\tilde{q}_\mu + \mu^2/\sigma^2}{2\mu/\sigma} & \tilde{q}_\mu > \mu^2/\sigma^2 \ . \end{cases} \tag{11}$$

The upper limit on μ at confidence level $1 - \alpha$ is found by setting $p_\mu = \alpha$ and solving for μ, which gives

$$\mu_{\mathrm{up}} = \hat{\mu} + \sigma \Phi^{-1}(1 - \alpha) \ . \tag{12}$$

Note that because σ depends in general on μ, Eq. (12) must be solved numerically.

References

[1] G. Cowan, K. Cranmer, E. Gross and O. Vitells, *Asymptotic formulae for likelihood-based tests of new physics*, accepted by EPJC; arXiv:1007.1727.