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Recipes for Exclusion Limits

Abstract

We present recipes for computing exclusion limits based on profile likelihood ratio tests. The material is largely extracted from Ref. [**?**], where more details can be found.

The statistical test should be based on the profile likelihood ratio as described below:

For a model where $\mu \geq 0$, if one finds data such that $\hat{\mu} < 0$, then the best level of agreement between the data and any physical value of μ occurs for $\mu = 0$. We therefore define

$$\tilde{\lambda}(\mu) = \begin{cases} \frac{L(\mu,\hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(\hat{\mu},\hat{\boldsymbol{\theta}})} & \hat{\mu} \geq 0, \\ \frac{L(\mu,\hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(0,\hat{\hat{\boldsymbol{\theta}}}(0))} & \hat{\mu} < 0\ . \end{cases} \tag{1}$$

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.

The variable $\tilde{\lambda}(\mu)$ is used to obtain the test statistic, which we denote $\tilde{q}_\mu$. That is,

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

For the important case where one wants to find the median exclusion significance for the hypothesis μ assuming that there is no signal, then one has $\mu' = 0$ and therefore

$$\sigma_{\mathrm{A}}^2 = \frac{\mu^2}{q_{\mu,\mathrm{A}}}\ , \tag{3}$$

CHECK – IS THIS THE RIGHT SIGMA FOR P-VALUE FROM QMU-TILDE???

Using the alternative statistic $\tilde{q}_\mu$ defined by Eq. (2) and assuming the Wald approximation we find

$$\tilde{q}_\mu = \begin{cases} \frac{\mu^2}{\sigma^2} - \frac{2\mu\hat{\mu}}{\sigma^2} & \hat{\mu} < 0 \ , \\ \frac{(\mu-\hat{\mu})^2}{\sigma^2} & 0 \leq \hat{\mu} \leq \mu \ , \\ 0 & \hat{\mu} > \mu \ . \end{cases} \tag{4}$$

The pdf $f(\tilde{q}_\mu|\mu')$ is found to be

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

The special case $\mu = \mu'$ is therefore

$$f(\tilde{q}_\mu|\mu) = \frac{1}{2}\delta(\tilde{q}_\mu) + \begin{cases} \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\tilde{q}_\mu}} e^{-\tilde{q}_\mu/2} & 0 < \tilde{q}_\mu \leq \mu^2/\sigma^2 \ , \\ \frac{1}{\sqrt{2\pi}(2\mu/\sigma)} \exp\left[-\frac{1}{2}\frac{(\tilde{q}_\mu+\mu^2/\sigma^2)^2}{(2\mu/\sigma)^2}\right] & \tilde{q}_\mu > \mu^2/\sigma^2 \ . \end{cases} \tag{6}$$

The corresponding cumulative distribution is

$$F(\tilde{q}_\mu|\mu') = \begin{cases} \Phi\left(\sqrt{\tilde{q}_\mu} - \frac{\mu-\mu'}{\sigma}\right) & 0 < \tilde{q}_\mu \leq \mu^2/\sigma^2 \ , \\ \Phi\left(\frac{\tilde{q}_\mu-(\mu^2-2\mu\mu')/\sigma^2}{2\mu/\sigma}\right) & \tilde{q}_\mu > \mu^2/\sigma^2 \ . \end{cases} \tag{7}$$

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

$$p_\mu = 1 - F(\tilde{q}_\mu|\mu) \ , \tag{9}$$

and therefore the corresponding significance is

$$Z_\mu = \begin{cases} \sqrt{\tilde{q}_\mu} & 0 < \tilde{q}_\mu \leq \mu^2/\sigma^2 \ , \\ \frac{\tilde{q}_\mu+\mu^2/\sigma^2}{2\mu/\sigma} & \tilde{q}_\mu > \mu^2/\sigma^2 \ . \end{cases} \tag{10}$$

As when using q_μ, the upper limit on μ at confidence level $1-\alpha$ is found by setting $p_\mu = \alpha$ and solving for μ, which reduces to the same result as found when using q_μ, namely,

$$\mu_{\rm up} = \hat{\mu} + \sigma \Phi^{-1}(1-\alpha) \; . \tag{11}$$

That is, to the extent that the Wald approximation holds, the two statistics q_μ and $\tilde{q}_\mu$ lead to identical upper limits.

References

[1] S.S. Wilks, *The large-sample distribution of the likelihood ratio for testing composite hypotheses*, Ann. Math. Statist. **9** (1938) 60-2.