

A method for comparing non-nested models with application to astrophysical searches for new physics

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ABSTRACT

Searches for unknown physics and decisions between competing astrophysical models to explain data both rely on statistical hypothesis testing. The usual approach in searches for new physical phenomena is based on the statistical Likelihood Ratio Test (LRT) and its asymptotic properties. In the common situation, when neither of the two models under comparison is a special case of the other i.e., when the hypotheses are non-nested, this test is not applicable. In astrophysics, this problem occurs when two models that reside in different parameter spaces are to be compared. An important example is the recently reported excess emission in astrophysical γ -rays and the question whether its origin is known astrophysics or dark matter. We develop and study a new, simple, generally applicable, frequentist method and validate its statistical properties using a suite of simulations studies. We exemplify it on realistic simulated data of the Fermi-LAT γ -ray satellite, where non-nested hypotheses testing appears in the search for particle dark matter.

Key words: statistical – data analysis – astroparticle physics – dark matter.

1 MODEL COMPARISON IN ASTROPARTICLE PHYSICS

In astrophysics, hypothesis testing is ubiquitous, because progress is made by comparing competing models to experimental data. In the special case, where new physical phenomena are searched for, the most common choice of hypothesis test is the Likelihood Ratio Test (LRT), whose popularity is partly motivated by the fact that, assuming H_0 is true, the asymptotic distribution of the LRT statistic is a χ^2 . Such result holds if the regularity conditions specified in Wilks’s theorem hold (Wilks 1938). A key necessary condition is “nested-ness”, meaning that there is a full model of which both the models under H_0 and the alternative hypothesis, H_1 , are special cases. This is obviously the case for the search for new particles where the null hypothesis (or baseline model), H_0 , is given by “background” and H_1 is given by “background+signal of new particle”. However, cases where model comparison is non-nested are common: for instance, when a known astrophysical signal can be confused with new physics, see Ackermann et al. (2012) for an example from astroparticle physics, or if the models to be compared reside in different parameter spaces (Profumo & Linden 2012); as

in gamma-ray bursts (Guiriec et al. 2015). In these situations, Monte Carlo simulations of the measurement process are often the only possibility, but are challenged by stringent significance requirements, e.g., at the 5σ level. We present a solution that allows evaluation of accurate statistical significances for non-nested model comparison while avoiding extensive Monte Carlo simulations. As a concrete example, we apply the proposed procedure to the search for particle dark matter, where the method has particular importance.

One way to search for dark matter is to consider its hypothesized annihilation products, i.e., γ -rays, that can be detected by space borne or ground based γ -rays telescopes (Conrad, Cohen-Tanugi & Stigari 2015). Here, the issue of source confusion is one of the most challenging aspects of claiming discovery of a dark matter induced signal. A detected excess of γ -rays may either originate from dark matter annihilation or be caused by conventional, known astrophysical sources. Discrimination can be performed using their spectral distributions, however these are not necessarily part of the same parameter space (see below). This situation arises for example in the search for dark matter sources among the unidentified sources found by Fermi-LAT (Ackermann et al. 2012), the claimed detection of a signal consistent with dark matter in our own galaxy, which has gained much attention recently (Daylan et al. 2014), or (once a

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detection has been made) in the search for dark matter in dwarf galaxies (Ackermann et al. 2011, 2014, 2015; Geringer-Sameth & Koushiappas 2011; Geringer-Sameth et al. 2015). In the recent claims, the existence of a source of γ -rays (over some background) is established by a LRT, but the crucial and unsolved question is not whether a γ -ray source exists, but whether it can be explained by conventional sources of γ -rays as opposed to dark matter annihilation. This is a prime example of a non-nested model comparison. For definiteness, we can assume $f(y, E_0, \phi) \propto \phi E_0^\phi y^{-(\phi+1)}$ is the probability density function (pdf) of the γ -rays energies, denoted by y , originating from known cosmic sources and $g(y, M_\chi) \propto 0.73 \left(\frac{y}{M_\chi}\right)^{-1.5} \exp\{-7.8 \frac{y}{M_\chi}\}$ is the pdf of the γ -ray energies of dark matter (Bergström, Ullio & Buckley 1998). The goal is to decide if $f(y, E_0, \phi)$ is sufficient to explain the data (H_0) or if $g(y, M_\chi)$ (H_1) provides a better fit.

Although the issue of comparing non-nested models has been addressed since the early days of modern statistics (Cox 1961, 1962, 2013; Atkinson 1970; Quandt 1974), as well as in the more recent physical literature (Pilla, Loader & Taylor 2005; Pilla & Loader 2006), a method with the desired statistical properties, easy implementation and computational efficiency in astrophysics is still lacking.

This article is arranged as follows. Section 2 reviews the LRT, Wilks's theorem and their extensions to non-regular situations. Our proposal for testing non-tested models is introduced in Section 3, validated via simulation studies in Section 4, and applied to a realistic simulation of the Fermi-LAT γ -ray satellite in Section 5. General discussion appears in Section 6.

2 WILKS, CHERNOFF AND TRIAL FACTORS

Let $f(y; \alpha)$ and $g(y, \beta)$ be pdfs of the background and signal, where y is the detected energy, α and β are parameters. Suppose observed particles are a mixture of background and source, i.e.,

$$(1 - \eta)f(y, \alpha) + \eta g(y, \beta) \quad (1)$$

where $0 \leq \eta \leq 1$ is the proportion of signal counts. A hypothesis test can be specified as $H_0 : \eta = \eta_0$ versus $H_1 : \eta > \eta_0$, and if β is known the LRT statistic by

$$T(\beta) = -2 \log \frac{L(\eta_0, \hat{\alpha}_0, -)}{L(\hat{\eta}_1, \hat{\alpha}_1, \beta)}, \quad (2)$$

where $L(\eta, \alpha, \beta)$ is the likelihood function under (1). The numerator and denominator of (2) are the maximum likelihood achievable under H_0 and H_1 , respectively with $\hat{\alpha}_0$ being the MLE of α under H_0 and $\hat{\alpha}_1$ and $\hat{\eta}_1$ the MLEs under H_1 . (Wilks 1938) states that when H_0 is true and when testing for a one-dimensional parameter (in this case η), $T(\beta)$ is asymptotically distributed as a χ_1^2 (the subscript being the degrees of freedom). Among the regularity conditions which guarantee this result are:

RC1. The models are nested, meaning that there is a full model of which both H_0 and H_1 are special cases.

RC2. The set of possible parameters of H_0 is on the interior of that for the full model.

RC3. The full model is identifiable under H_0 .

Unfortunately in practice, it is common to encounter non-regular problems. Notice for example, if β is known but $\eta_0 = 0$, RC2 does not hold. In this case, Chernoff (1954) applies; it generalizes Wilks and states that if H_0 is on the boundary of the parameter space, the asymptotic distribution of $T(\beta)$ is an equal mixture of a χ_1^2 and a Dirac delta function at 0, namely $\frac{1}{2}\chi_1^2 + \frac{1}{2}\delta(0)$.

Further, if $\eta_0 = 0$ (on the boundary) and β is unknown, the model in (1) is not identifiable under H_0 and RC3 fails. This is known in statistics as a test of hypothesis where a nuisance parameter is defined only under H_1 , or ‘‘trial correction’’ in astrophysical literature. A solution based on theoretical result of Davies (1987) is proposed by Gross & Vitells (2010). In particular, under H_0 , $T(\beta)$ is a random process indexed by β , specifically if RC2 (but not RC3) holds $\{T(\beta), \beta \in \mathbf{B}\}$ is asymptotically a χ_1^2 -process. A natural choice of test statistic is $\sup_\beta T(\beta)$ and Gross & Vitells (2010) provides an approximation in the limit as $c \rightarrow \infty$ for the tail probability $P(\sup_\beta T(\beta) > c)$. Finally, if both RC2 and RC3 fail to hold (e.g., the important case of $\eta_0 = 0$ with β unknown), we show in our Supplementary Material that because $\{T(\beta), \beta \in \mathbf{B}\}$ is a $\frac{1}{2}\chi_1^2 + \frac{1}{2}\delta(0)$ random process,

$$P(\sup_\beta T(\beta) > c) \approx \frac{P(\chi_1^2 > c)}{2} + E[N(c_0)|H_0]e^{-\frac{c-c_0}{2}} \quad (3)$$

where $E[N(c_0)|H_0]$ is the expected number of upcrossings of the $T(\beta)$ process over the threshold c_0 under H_0 and c_0 is chosen $c_0 \ll c$. (Details of how to choose c_0 are given in Gross & Vitells (2010), where (3) is also asserted, but without proof.) Although this approximation holds as $c \rightarrow \infty$, when c is small, the right hand side of (3) is an upper bound for $P(\sup_\beta T(\beta) > c)$. Thus, basing inference on (3) is valid, though perhaps conservative.

3 STATISTICAL COMPARISON OF NON-NESTED MODELS

Suppose we wish to compare two pdfs, $f(y, \alpha)$ and $g(y, \beta)$, for which RC1 does not apply, that is the two pdfs are not special cases of a full model and do not share a parameter space. Notice that in both f and g free parameters (i.e., α and β respectively) are present and thus, the problem cannot be reduced to a test for simple hypotheses as in Cousins (2005), see Cox (1961) for more details. We require β to be one dimensional and α to lie in the interior of its parameter space. The goal is to develop a test of the hypothesis:

$$H_0 : f(y, \alpha) \text{ versus } H_1 : g(y, \beta) \quad (4)$$

Although $f(y, \alpha)$ and $g(y, \beta)$ are non-nested, we can construct a comprehensive model which includes both as special cases. There are two reasonable formulations. We encountered the first in (1); the second is proportional to $\{f(y, \alpha)\}^{1-\eta} \{g(y, \beta)\}^\eta$, with $0 \leq \eta \leq 1$ in both formulations. As discussed in Cox (1962, 2013); Atkinson (1970) and Quandt (1974), there are advantages and disadvantages to both. From our perspective, the additive form in (1) has the advantage of more appealing mathematical properties. Since no normalizing constant is involved, the maximization of the log-likelihood reduces to numerical optimization. In contrast to the test discussed in Section 2, the model in (1)

is not viewed as a mixture of astrophysical models in which a certain proportion of events, η , originates a process represented by one model, and the the remaining proportion, $1 - \eta$, originates from the completing process represented by the other model. Instead, (1) is a mathematical formalization used to embed the pdfs $f(y, \alpha)$ and $g(y, \beta)$ and their corresponding parameters spaces into an overarching model via the auxiliary parameter η (Quandt 1974). The overarching model has not astrophysical interpretation, but helps us reformulate the test in (4) into a suitable form, i.e.,

$$H_0 : \eta = 0 \quad \text{versus} \quad H_1 : \eta > 0. \quad (5)$$

Perhaps a more natural formulation of (4) would be $H_0 : \eta = 0$ versus $H_1 : \eta = 1$. Unfortunately, neither Wilks's or Chernoff's theorems apply to this formulation since they rely on the asymptotic normality of the MLE under H_0 , which can only hold if there is a continuum of possible values of η under H_1 , with $\eta = 0$ in its interior. With indirect dark matter detection, the formulation in (5) allows the alternative model to include both the case where dark matter and known cosmic sources are present simultaneously ($0 < \eta < 1$) and the case where only dark matter is present ($\eta = 1$). In situations where intermediate values of η are not physical we might, in addition to (5), test $H_0 : \eta = 1$ versus $H_1 : \eta < 1$, i.e., interchange the roles of the hypotheses as discussed in Cox (1962, 2013). In this case, the nuisance parameter α is required to be one dimensional i.e., $\alpha = \alpha$.

Under model (1), testing (5) is equivalent to testing η on the boundary with β only being defined under the alternative. We can apply the methods discussed in Section 2 to solve this problem. Notice that such methods can still be applied if the two models share additional parameters, γ , i.e., $f(y, \gamma, \alpha)$ and $g(y, \gamma, \beta)$. However, the maximized likelihoods in (2) must be replaced by their profile counterparts $L(0, \hat{\gamma}_0, \hat{\alpha}_0)$ and $L(\eta_1, \hat{\gamma}_1, \hat{\alpha}_1, \beta)$ (Davison 2003).

4 VALIDATION ON DARK MATTER MODELS

We illustrate the reliability of the method proposed for testing non-nested models using two sets of Monte Carlo simulations. In Test 1, we compare the two models introduced in Section 1 with the aim of distinguishing between a dark matter signal and a power law distributed cosmic source. In Test 2, we make the same comparison but in the presence of power law distributed background. In this case, H_0 specifies as

$$f(y, \delta, \lambda, E_0, \phi) = (1 - \lambda) \frac{\delta E_0^\delta}{k_\delta y^{\delta+1}} + \lambda \frac{\phi}{k_\phi y^{\phi+1}} E_0^\phi \quad (6)$$

and H_1 specifies

$$g(y, \delta, \lambda, E_0, M_\chi) = (1 - \lambda) \frac{\delta E_0^\delta}{k_\delta y^{\delta+1}} + \lambda \frac{e^{-7.8 \frac{y}{M_\chi}}}{y^{1.5} k_{M_\chi}}; \quad (7)$$

where k_ϕ , k_δ and k_{M_χ} are the normalizing constants for each pdf, $0 < \lambda < 1$, $\delta > 0$, $\phi > 0$, $E_0 = 1$, $y \in [E_0, 100]$ and $M_\chi \in [E_0, 100]$. Note that in this case, the formulation in (1), with mixture parameter λ , is first used to specify the signal existence over a (relatively well known) background, whilst in the next step, equation (1) is adopted as a merely mathematical tool to treat the non-nested case (as described previously).

For simplicity, in Test 2, λ , the proportion of events

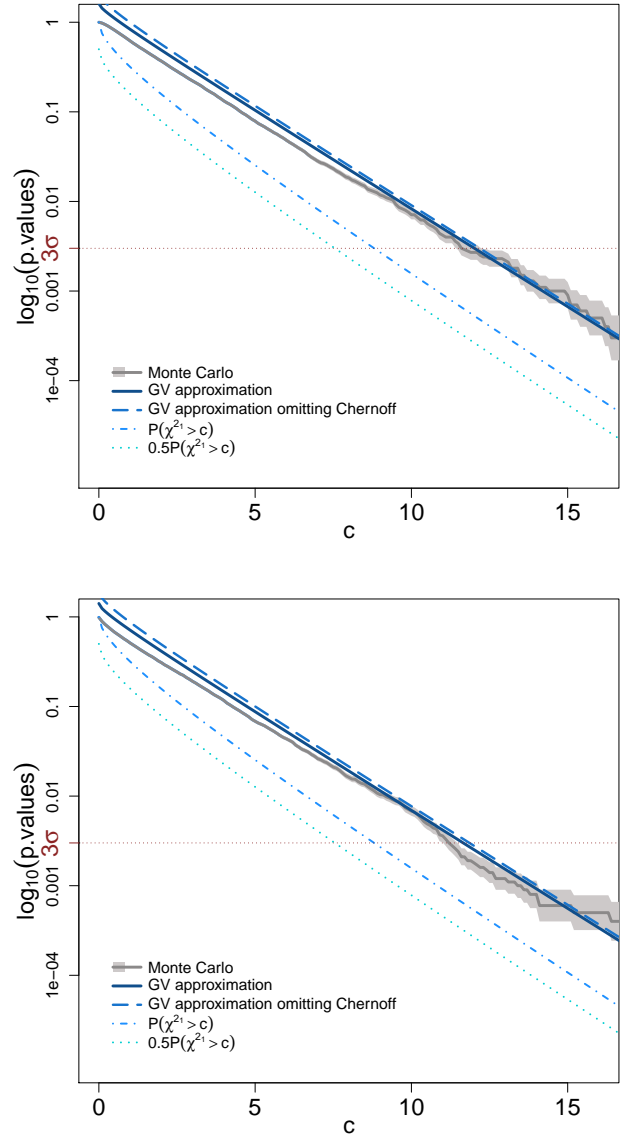


Figure 1. Comparing the approximation in (3) (solid blue lines) with Monte Carlo estimation of $P(\sup T(M_\chi) > c)$ (gray dashed lines), for Test 1 (upper panel) and Test 2 (lower panel). Approximations corresponding to (3) without the Chernoff correction (blue dashed lines), a χ^2 approximation (light blue dash-dotted lines) and a Chernoff-adjusted χ^2 approximation (light blue dotted lines) are also reported. Monte Carlo p-values were obtained by simulating 10,000 datasets under H_0 , each of size 10,000 for both simulations. For each simulated dataset $\sup_{M_\chi} T(M_\chi)$ was computed over an M_χ grid of size 100 for Test 1 and size 400 for Test 2. Monte Carlo errors (gray areas) were attained via error propagation (Cowan 1998).

coming from dark matter, was fixed to 0.2. In both tests, we estimated the average number of upcrossings $E[N(c_0)|H_0]$ using 1,000 Monte Carlo simulations. Finally, the approximation to $P(\sup_\beta T(\beta) > c)$ is calculated using (3) on a grid of values of c . The results are compared with the respective Monte Carlo p-values in Figure 1 along with the χ^2 and Chernoff corrections one might compute ignoring the regularity conditions in Section 2.

For small c , the approximation in (3) is greater than its Monte Carlo counterpart. As c increases, however, the

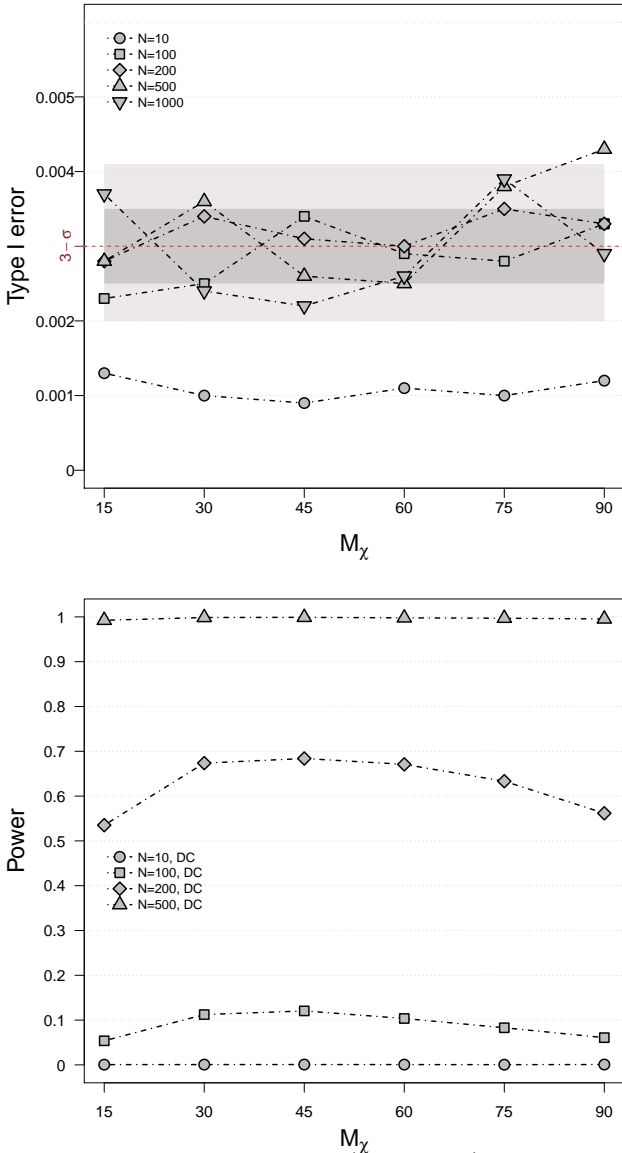


Figure 2. Simulated type I errors (upper panel) and power functions (lower panel) for Test 1 with at 3σ significance. Shaded areas indicate regions expected to contain 68% (dark gray) and 95% (light gray) of the symbols if the nominal type I error of 0.003 holds. For both the type I error and power curves 10000 Monte Carlo simulations were used.

approximation converges to the Monte Carlo estimates for a good approximation to the p-value, $P(\sup_\beta T(\beta) > c)$. The χ^2 and respective Chernoff-adjusted approximation lead to over optimistic p-values, whereas similar results to those attained with (3) are achieved when the factor of 2 that accounts for RC1 is omitted. This is not surprising since the right hand side of (3), is dominated by $E[N(c_0)|H_0]$ (which also explains the wide discrepancy between (3) and the χ^2 approximations in Figure 1) and in practice, when testing on the boundary of the parameter space, $E[N(c_0)|H_0]$ is typically calculated simulating a $\frac{1}{2}\chi_1^2 + \frac{1}{2}\delta(0)$ random process directly. Thus, the Chernoff correction is automatically implemented in the leading term of (3).

It is not uncommon in practice, e.g. in astronomy, for the number of counts to be considerably smaller than the 10,000 used in Figure 1. Thus, we conduct a simulation study

to verify the type I error (i.e., the rate of false rejections of H_0) of the method with smaller samples and verify that the approximate p-value in (3) holds. The upper panel of Figure 2 reports the simulated type I errors with a detection threshold on the p-value of 0.003 (3σ) for different sample sizes when conducting Test 1. For sample sizes of at least 100, the Monte Carlo results are consistent with the numerical 3σ error rate. The lower panel of Figure 2 shows the power (probability of detection) curves at 3σ of the same test for different sample sizes. For all the values of M_χ considered, a sample size of 500 is sufficient to achieve a power of nearly 1.

5 APPLICATION TO SIMULATED DATA FROM THE FERMI-LAT

The Fermi Large Area Telescope (LAT) (Atwood 2009) is a pair-conversion γ -ray telescope on board the earth-orbiting Fermi satellite. It measures energies and images γ -rays between about a 100 MeV and several TeV. One particular aspect is the γ -ray signal induced by dark matter annihilations, which gives rise to measurable signal from celestial objects, like the Milky Way center or dwarf galaxies. Here we apply the method proposed in this letter to a dataset simulated with realistic representations of the effects of the detector and present backgrounds. We considered a 5 years observation of putative dark matter source (dwarf galaxy-like) with dark matter annihilating into b-quark pairs and a mass of the dark matter particle of 35 GeV. This assumption is consistent with the most generic and popular models for dark matter, namely that it is in large part made of a Weakly Interacting Massive Particles (WIMP). It is also consistent with recent claims of evidence for dark matter. The signal normalization corresponds to about 200 events detected in the LAT. Roughly, this corresponds to a dark matter source at the distance of the dwarf galaxy Segue1 (and with comparable dark matter density) and an annihilation cross-section of $\sim 2 \cdot 10^{-25} \text{cm}^3 \text{s}^{-1}$). We find a 4.198σ significance in favor of the dark matter model. Scaling the event rate down to 50 (i.e. considering a lower cross-section by a factor of 4 or lower density by a factor of 16) we obtain 2.984σ significance (result not shown). Adding complexity, we introduce a background, for example γ -rays introduced by our own Galaxy. We then considered 2176 counts from a power-law distributed background source as in (6)-(7) and about 550 dark matter events. For simplicity, the mixture parameter λ is fixed at 0.2. In this case, we find 2.9σ significance in favor of the model in (7). As expected, introducing background significantly reduces the power for distinguishing a dark matter source from a conventional source. It should be noted however that (unlike in a full analysis) we do not attempt to reduce background by taking γ -ray directions into account.

6 SUMMARY & DISCUSSION

We have presented a two-step solution to a common problem in experimental astrophysics: comparing competing non-nested models. On the basis of the seminal work of Cox

| | H_0 | N | $\hat{\eta}$ | \tilde{M}_χ | sup LRT | Sig. |
|--------|------------|------|-----------------|------------------|-----------|---------------|
| Test 1 | $\eta = 0$ | 200 | 0.971 | 27 | 21.018 | 4.038σ |
| | $\eta = 1$ | 200 | p-value = 0.528 | | | |
| Test 2 | $\eta = 0$ | 2726 | 0.999 | 30 | 12.096 | 2.673σ |
| | $\eta = 1$ | 2726 | p-value = 1 | | | |

Table 1. Summary of the analysis on the Fermi LAT simulation comparing the models in Tests 1 and 2. Estimates and Significances refer to the tests $H_0 : \eta = 0$ versus $H_1 : \eta > 0$. P-values refer to the tests $H_0 : \eta = 1$ versus $H_1 : \eta < 1$.

(1962, 2013) and Atkinson (1970) the first step of our strategy requires the specification of a comprehensive model which extends the parameter space of the models to be compared. The problem of testing non-nested model is then reduced to the look-elsewhere effect, and thus the second step naturally recalls Gross & Vitells (2010) as an efficient solution to accurately approximate the significance of new signals. The resulting procedure is easy to implement, does not require extensive calculations on a case-by-case basis and is computationally more efficient than Monte Carlo simulations. Recent developments (Algeri et al. 2016) in the nested case illustrate additional desirable statistical properties of Gross & Vitells (2010) with respect to Pilla, Loader & Taylor (2005) and Pilla & Loader (2006). Given the nature of the methodology proposed in this letter, we expect these finding to carry over to the non-nested case.

An example of testing non-nested models arises in the search for particle dark matter. We use this example to validate and illustrate the procedure. We also demonstrate good performance in a realistic simulation of data that is collected with the Fermi-LAT γ -ray detector and used in the search for signal from dark matter annihilation.

Although any pair of hypothesized models can be expressed as a special case of (1), this formulation alone does not always provide a mechanism for a statistical hypothesis test. In the non-nested scenario analysed in this letter, valid inference for the test in (5) can be achieved by applying the methodology in Gross & Vitells (2010). This method, however, cannot handle multi-dimensional parameters that are defined only under H_1 , nor can it deal with nuisance parameters under H_0 which lie on the boundary of their parameter space. A possible approach to tackle the first limitation is to apply the theory in Vitells & Gross (2011) to the comprehensive model in (1). Whereas an extension of the method to overcome the second limitation could rely on the theory in Self & Liang (1987). In light of this, the methodology proposed is particularly suited to comparisons of non-nested models where these limitations often do not arise.

Software for the methodology illustrated in this letter is available at: <http://www.imperial.ac.uk/~sa2514/Research.html>.

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