A fast and stable approximation to the Barlow-Beeston template fit

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Abstract

In their paper from 1993, Barlow and Beeston presented an exact likelihood for the problem of fitting a composite model consisting of binned templates obtained from Monte-Carlo simulation which are fitted to equally binned data. Solving the exact likelihood is a technical challenge, and so Conway in 2011 proposed an approximated likelihood that overcomes them. Conway’s approximate likelihood and a new approximate likelihood are derived from the exact one in this paper. The new approximation is expected perform better than Conway’s. The likelihoods are extended to the problem of fitting weighted data and weighted templates. The performance of estimates obtained with all three likelihoods are studied on a toy example. The exact likelihood performs best, closely followed by the new approximate likelihood, putting Conway’s likelihood in third place.

1. Introduction

A common scenario in (astro)particle physics is the following. A data sample is described by a point density (in one or more dimensions) which is composed of two or more components. The analyst wants to know how many points originate from each component; this number is called the yield. If the component \( p.d.f.s \) are known and linearly independent, one can obtain estimates for the yields from an extended maximum-likelihood fit \([1]\), which is based on maximizing the exact likelihood for this problem.

In their paper from 1993 \([2]\), Barlow and Beeston describe a similar likelihood for the problem of fitting a composite model consisting of binned templates obtained from Monte-Carlo simulation which are fitted to equally binned data. In this scenario, the component \( p.d.f.s \) are not available in parametrized form, but are obtained implicitly from simulation. Barlow and Beeston give the exact likelihood for this problem, in which the shapes of the templates are not exactly known since the simulated sample is finite. Therefore, the value of each template in each bin is a nuisance parameter, constrained through Poisson statistics by
the simulated sample. Since the likelihood is exact for this case, all proven properties for maximum-likelihood estimates carry over, in particular, one obtains asymptotically correct uncertainty estimates for the yields.

The exact likelihood has many nuisance parameters, one per bin and component. Since the number of bins can be large (especially when the data are multidimensional), Barlow and Beeston describe an algorithm to estimate the nuisance parameters by solving a non-linear equation per bin for a given set of yields, which are thus internally solved. The only remaining external parameters are the yields, which are optimized numerically in the unusual way, for example, with the MIGRAD algorithm in MINUIT [3].

Unfortunately, this approach has some drawbacks. It was observed by Conway [4] that the finite accuracy of the non-linear solver introduces discontinuities in the log-likelihood that confuses the algorithms employed by MIGRAD. This can lead to fits that fail to converge or incorrect uncertainty estimates. In addition to this issue, solving a non-linear equation per bin is somewhat computationally expensive.

Conway proposes a simplified treatment [4] to address these issues, and replaces the exact likelihood by a simplified one where the uncertainty in the template is captured by a multiplicative factor, which in turn is constrained by a Gaussian penalty term. This introduces only one nuisance parameter per bin instead of one per component per bin. This simplification allows one to estimate the nuisance parameter by bin-by-bin by solving a quadratic equation, which has an analytical solution. The numerical computation of the simplified likelihood does not suffer from aforementioned instabilities and is also faster.

Conway did not derive the simplified likelihood rigorously from the exact likelihood of Barlow and Beeston; it is introduced ad hoc. This is unsatisfactory, because a rigorous derivation allows one to judge in which limit the approximate likelihood is an adequate replacement of the exact likelihood. A derivation of Conway’s likelihood is provided here. This exercise lead to the discovery of another approximate likelihood that offers the same technical benefits while requiring fewer approximations and treats simulation and data symmetrically. The new approximate likelihood is expected to perform better than Conway’s method on average, which is confirmed in the study of a toy example.

All likelihoods derived in this paper are further transformed so that the minimum value is asymptotically chi-square distributed, following the approach of Baker and Cousins [5]. This allows one to use the minimum value as a goodness-of-fit test statistic, and it stabilizes the numerical minimization of this function.

2. Derivation of the approximate likelihood

Baker and Cousins [5] note that likelihoods for binned data can be transformed so that the estimate value doubles as an asymptotically chi-square-distributed test statistic $Q$. The following monotonic transformation is applied
to the likelihood \( L \), here without loss of generality given for a single bin,

\[
Q(\vec{p}) = -2 \ln \left( \frac{L(n; \mu(\vec{p}))}{L(n; n)} \right),
\]

(1)

where \( n \) is the count of samples in the bin, \( \mu \) is the model expectation, which is a function of model parameters \( \vec{p} \). In the constant denominator, \( \mu \) is replaced by \( n \). If the model is correct, \( Q \) follows a chi-square distribution with \( n_{dof} \) degrees of freedom in the asymptotic limit of infinite sample size, where \( n_{dof} \) is the difference between the number of bins and the number of fitted parameters.

In the approximations that are considered here, the simulation adds zero additional degrees of freedom, since each additional bin in the simulation part has one corresponding nuisance parameter. Therefore, the simulated part can be ignored when calculating \( n_{dof} \) of the total likelihood, which is still given by the difference of the number of bins and the number of yields.

Eq. 1 applied to the exact likelihood described by Barlow and Beeston gives

\[
Q = 2(\mu - n - n(\ln \mu - \ln n)) + 2 \sum_k \xi_k - a_k - a_k(\ln \xi_k - \ln a_k),
\]

(2)

where \( \mu = \sum_k y_k \xi_k / M_k \) is the bin expectation, \( \xi_k \) is the unknown amplitude of the \( k \)-th component, \( a_k \) is the observed simulated count, \( y_k \) is the yield of the \( k \)-th component, and \( M_k \) is a normalization computed by adding all \( a_k \) from different bins.

Without loss of generality, the template amplitudes can be parametrized as \( \xi_k = a_k \beta_k \), since the extremum of the likelihood is also invariant to monotonic transformations of the parameters. The factors \( \beta_k \) tend to 1 in the asymptotic limit of an infinite simulated sample. The central approximation of Conway is to set \( \beta_k \approx \beta \); the component factors are replaced by a single factor,

\[
\mu = \sum_k \frac{y_k \xi_k}{M_k} = \sum_k \frac{y_k \beta_k a_k}{M_k} \approx \beta \sum_k \frac{y_k a_k}{M_k}. \tag{3}
\]

This approximation is valid in the limit where the bin expectation is dominated by a single component. Applied to Eq. 2, one gets

\[
Q \approx 2(\beta \mu_0 - n - n(\ln(\beta \mu_0) - \ln n)) + 2 \sum_k \beta a_k - a_k(\ln(\beta a_k) - \ln a_k)
\]

(4)

\[
= Q_p(n; \beta \mu_0) + 2 \sum_k (\beta - 1)a_k - a_k \ln \beta
\]

\[
= Q_p(n; \beta \mu_0) + 2 \left[ (\beta - 1) \left( \sum_k a_k \right) - \left( \sum_k a_k \right) \ln \beta \right]
\]

\[
= Q_p(n; \beta \mu_0) + 2a((\beta - 1) - \ln \beta),
\]

with \( a = \sum_k a_k \). At this point, the derivation branches into one in which the equivalent of Conway’s likelihood is derived by applying further approximations.
The other branch uses only equivalent transformations to bring Eq. 4 into a symmetric form.

2.1. Conway’s approximation

The first part \( Q_p(n; \beta \mu_0) \) of Eq. 4 already corresponds to Conway’s likelihood, one only needs to modify the second part. The logarithm \( \ln \beta \) is approximated by a Taylor series around \( \beta = 1 \) to second order. One obtains

\[
Q = Q_p(n; \beta \mu_0) + 2a((\beta - 1) - \ln \beta)
\approx Q_p(n; \beta \mu_0) + 2a((\beta - 1) - (\beta - 1) + \frac{1}{2}(\beta - 1)^2)
= Q_p(n; \beta \mu_0) + a(\beta - 1)^2.
\]

This approximation is valid in the asymptotic limit \( a \to \infty \), but in practice that is at odds with the fact that the simulation sample is frequently smaller than the data sample, so that \( a \) may be small in some bins with nonzero \( n \).

In Conway’s likelihood, the second term is divided by the variance \( V(\beta) \) of \( \beta \), not multiplied by \( a \). In the following, it is demonstrated that \( V(\beta) \approx 1/a \).

Recall the definition \( \beta = \mu/\mu_0 \), where \( \mu_0 \) is considered constant. One finds via error propagation,

\[
V(\beta) = \frac{V(\mu)}{\mu_0^2}.
\]

With

\[
V(\mu) = \sum_k \frac{y_k^2 V(\xi_k)}{M_k^2}
\]

and estimates \( V(\xi_k) = \xi_k \approx a_k \) (the \( \xi_k \) are Poisson distributed), one obtains

\[
V(\beta) = \frac{\sum_k \frac{y_k^2 a_k}{M_k^2}}{\left(\sum_k \frac{y_k a_k}{M_k^2}\right)^2}.
\]

In the limit where one of the components is dominant \( a_k \approx a \) (which is valid in the same limit as the central approximation \( \beta_k \approx \beta \)), one gets

\[
V(\beta) \approx \frac{\sum_k \frac{y_k^2}{M_k^2} a}{\left(\sum_k \frac{y_k}{M_k} a\right)^2} = \frac{1}{a}.
\]

So, finally the equivalent of Conway’s likelihood is obtained,

\[
Q = Q_p(n; \beta \mu_0) + \frac{(\beta - 1)^2}{V(\beta)}.
\]

In practical applications, \( V(\beta) \) is computed with Eq. 8.

As shown by Conway [4], an estimate for \( \beta \) can be obtained by solving the score function \( \partial Q/\partial \beta = 0 \) based on Eq. 10 which leads to a quadratic equation for \( \beta \), which has only one valid solution.
2.2. Alternative approximation

Starting again from Eq. 4, the score function $\frac{\partial Q}{\partial \beta} = 0$ are directly solved. One obtains

$$\mu_0 - \frac{n}{\beta} + a\left(1 - \frac{1}{\beta}\right) = 0 \quad \Rightarrow \quad \beta = \frac{n + a}{\mu_0 + a},$$

(11)

without any further approximation. This formula for $\beta$ is even simpler than the one derived by Conway, and can be easily interpreted. If $a \ll n$, $\beta$ adjusts $\mu_0$ to $n$, irrespective of the actual value of $\mu_0$. The bin provides no information on the component yields, which enter only through the potential tension between $\mu_0$ and $n$. For $a \to \infty$, $\beta$ goes to 1 and $Q \to Q_p(n; \mu_0)$, which is identical to the exact likelihood for the case when the templates are exactly known.

The alternative likelihood in Eq. 4 treats data and simulation symmetrically, which becomes more clear with a few transformations,

$$Q = Q_p(n; \beta \mu_0) + 2a((\beta - 1) - \ln \beta)$$

$$= Q_p(n; \beta \mu_0) + 2((\beta a - a) - a(\ln(\beta) + \ln a - \ln a))$$

$$= Q_p(n; \beta \mu_0) + 2((\beta a - a) - a(\ln(\beta a) - \ln a))$$

$$= Q_p(n; \beta \mu_0) + Q_p(a; \beta a).$$

(12)

To summarize, this alternative approximate likelihood is derived from the exact likelihood by using fewer approximations than Conway’s likelihood, and it describes both the simulated and the data sample with Poisson statistics. As shown by Barlow and Beeston [2], maximum-likelihood estimation based on Poisson statistics performs better than a likelihood based on a Gaussian approximation. The alternative likelihood should therefore perform better in fits where the simulated sample used to produce the templates is small.

Bins in which $a$ is zero should be ignored in the calculation, since they do not contribute anything to the yields. In practice, one can replace $a$ with a tiny number in this case, so that Eq. 11 and Eq. 12 always produces a valid number instead of dividing by zero or taking the logarithm of zero.

3. Weighted templates and weighted data

In practice, the data and the simulation samples may be weighted. Simulations are often weighted to reduce discrepancies between the simulated and the real experiment, or as a form of importance sampling. Data may be weighted to correct losses from finite detection efficiency. In both cases, a count $n$ is replaced by a sum of weights $\sum_i w_i$. Barlow and Beeston discuss this case in their paper and show how the exact likelihood can be adapted to this case, but their solution is not complete since it does not handle the additional variance introduced by weights of varying size. A full solution is given here which is asymptotically valid.

Eq. 10 and Eq. 12 are adapted to describe sum of weights asymptotically correct by replacing $Q_p$ with the approximate likelihood for sums of independent
weights, described by Bohm and Zech [6]. In this approach, the sum of weights \( \sum_i w_i \) and the prediction \( \mu \) are scaled with a factor \( s = \sum_i w_i / \sum_i w_i^2 \). With the so-called effective count \( n_{\text{eff}} = (\sum_i w_i)^2 / \sum_i w_i^2 \), the full replacement is

\[ Q_P(n; \mu) \to Q_P(n_{\text{eff}}; s\mu). \] (13)

This replacement can be applied to both parts of Eq. 12,

\[ Q = Q_P(n_{\text{eff}}; \beta s \mu_0) + Q_P(a_{\text{eff}}; \beta a_{\text{eff}}), \] (14)

where \( a_{\text{eff}} \) is the equivalent of \( n_{\text{eff}} \) computed from the weights in the simulation.

These replacements also modify the solution for \( \beta \). By identifying the corresponding variables in Eq. 12 and Eq. 14 one finds

\[ \beta = \frac{n_{\text{eff}} + a_{\text{eff}}}{s \mu_0 + a_{\text{eff}}}. \] (15)

4. Toy study

The properties of estimated yields are studied, which are obtained by minimizing Eq. 2 corresponding to the exact likelihood derived by Barlow and Beeston, as well as its approximations Eq. 10 and Eq. 12. Of interest is the bias of the estimates and the bias of the estimated uncertainty of the yields. Either bias should be small.

The minimization is performed with the MINUIT [3] algorithm MIGRAD as implemented in iminuit [7]. In case of Eq. 2 the nuisance parameters are found by MIGRAD in the usual way, the alternative solution for estimating the nuisance parameters described by Barlow and Beeston is not used, due to the instabilities which this causes.
The toy example consists of two components, a normally distributed signal and a truncated exponentially distributed background. The normal distribution has parameters $\mu = 1$, $\sigma = 0.1$, and the true yield is 250. The exponential is truncated to the interval $[0, 2]$, the slope is 1 and true yield is 750. For the templates, $N_{mc}$ samples are generated per component, where $N_{mc}$ varies from 100 to 10000. In repeated toy experiments, the shape parameters are fixed, but the component yields in the data sample and in the templates are drawn from a Poisson distribution. All samples are sorted into histograms with 15 equidistant bins over the interval $[0, 2]$. An example is shown in Fig. 1.

The fit is repeated 1000 times with randomly generated data and templates per value of $N_{mc}$ to measure the bias of the estimate itself and the bias of its variance estimate. Such sets of experiments are run for $N_{mc} = 50, 100, 200, 500, 1000, 10000$. It is expected that the results converge as the sample used to compute the templates grows. To judge the performance, the pull distribution of the estimated signal yield is computed, where the pull is defined as

$$z = (\hat{s} - s) / \hat{V}_{s}^{1/2},$$

(16)

with true signal yield $s$, estimate $\hat{s}$, and $\hat{V}_{s}$ is the variance estimated by MINUIT’s HESSE algorithm for $\hat{s}$. The performance is judged by the method is indicated by the degree of agreement of the mean of $z$ with 0 and the standard deviation with 1.

The results are shown in Fig. 2. The performance of all likelihood functions is roughly comparable, unless the sample size to generate the templates is very small ($N_{mc} < 100$). For $N_{mc} = 50$, only the approximation derived in this work produces passable results, while the fits with the functions from Conway and Barlow-Beeston become unstable and produce outliers that distort the mean and standard deviation of $z$. For all other values of $N_{mc}$, the fit based on the full Barlow-Beeston performs best, closely followed by the approximation derived in this work. Conway’s likelihood performs a bit worse, with a slightly larger absolute bias and a standard deviation further away from 1. At $N_{mc} = 10000$, the uncertainty in the templates becomes negligible compared to the uncertainty in the data, and the $z$ distributions of all three fits converge.

The fits have been timed on the example shown in Fig. 1. While the details depend on the problem, the implementation of the likelihood functions (here in Python) and the machine on which the fits are run (here a 2.8 GHz Quad-Core CPU), a coarse comparison of the time it took for the fits to converge is enlightening. The approximate likelihood derived in this work is the fastest, followed by Conway’s likelihood which is 25% slower, and tailed by the exact likelihood which takes 16 times as long. This large gap is caused by the large number of nuisance parameters in the exact likelihood. The runtime of MINUIT’s algorithms roughly scales quadratically with the number of fitted parameters, and thus in case of the exact likelihood, it scales with the number of bins. Repeating the fits with 100 bins kept the ratio between the two approximate likelihoods roughly the same, while the gap to the exact likelihood became a factor of 800.

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Figure 2: Pull distributions for estimates obtained from maximizing the exact likelihood (Barlow-Beeston), and the approximate likelihoods of Conway and the one derived in this work.
5. Conclusions

Conway’s approximate likelihood was rigorously derived from the exact likelihood described by Barlow and Beeston, to shed some light on the limit in which the approximation is valid. An alternative approximate likelihood was derived as well, which requires fewer approximations and treats data and simulation symmetrically as Poisson distributed, while Conway uses a different treatment for the simulation. It was further shown how the likelihoods need to be modified to approximately describe weighted data or weighted templates. All likelihood functions were transformed so that the minimum value is asymptotically chi-square distributed, to double as a goodness-of-fit test statistic. A toy study on particular example showed that yields obtained with the alternative approximate likelihood have good small sample properties, which are only slightly worse than those obtained with the exact likelihood and better than those obtained with Conway’s likelihood. The approximate likelihoods have been implemented in Python and are available in the iminuit library \cite{7} as the class iminuit.cost.BarlowBeestonLite.

References

[1] Roger J. Barlow. Extended maximum likelihood. *Nucl. Instrum. Meth. A*, 297:496–506, 1990.

[2] Roger J. Barlow and Christine Beeston. Fitting using finite Monte Carlo samples. *Comput. Phys. Commun.*, 77:219–228, 1993.

[3] F. James and M. Roos. Minuit: A System for Function Minimization and Analysis of the Parameter Errors and Correlations. *Comput. Phys. Commun.*, 10:343–367, 1975.

[4] J. S. Conway. Incorporating Nuisance Parameters in Likelihoods for Multisource Spectra. In *PHYSTAT 2011*, pages 115–120, 2011.

[5] Steve Baker and Robert D. Cousins. Clarification of the Use of Chi Square and Likelihood Functions in Fits to Histograms. *Nucl. Instrum. Meth.*, 221:437–442, 1984.

[6] G. Bohm and G. Zech. Statistics of weighted Poisson events and its applications. *Nucl. Instrum. Meth. A*, 748:1–6, 2014.

[7] Hans Dembinski, Piti Ongmongkolkul, Christoph Deil, Henry Schreiner, Matthew Feickert, Andrew, Chris Burr, Jason Watson, Fabian Rost, Alex Pearce, Lukas Geiger, Bernhard M. Wiedemann, Christoph Gohlke, Gonzalo, Jonas Drotleff, Jonas Eschle, Ludwig Neste, Marco Edward Gorelli, Max Baak, Omar Zapata, and odidev. scikit-hep/iminuit: v2.11.2, March 2022.