Confidence intervals for efficiencies in particle physics experiments

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Abstract

We compute bias and variance of an efficiency estimator for a random processes, in which the success probability is constant but the number of trials is drawn from a Poisson distribution. The standard estimator, although being a non-linear function in this case, is unbiased. Compared to the case where the number of trials is fixed, the variance is increased or decreased depending on the expected number of trials. We further compute the variance for the case where the numbers of successes and failures have a variance which exceeds that of a Poisson process. This is the case, for example, when these numbers are obtained from a mixture of signal and background events in which the background is subtracted imperfectly. We compute generalised Wilson intervals based on these variances and study their coverage probability. We conclude that the standard Wilson interval is also suitable when the number of trials is Poisson distributed.

1. Introduction

In (astro)particle physics experiments, a cross-section or a flux is computed from the number of times a particular type of event occurs in a given integrated luminosity interval or occurs for a given integrated exposure. This is essentially a rate measurement, where the integrated luminosity or exposure plays the role of time. The rate of interest is usually observed imperfectly with an efficiency smaller than one. The efficiency $p$ of a detector device or a selection is

$$p = \frac{n_1}{n_1 + n_2} = \frac{n_1}{n},$$

(1)

where $n_1$ is the expected number of events which are selected, $n_2$ is the expected number of events that are rejected, and $n$ is the total expected number of trials. The value of $p$ is usually estimated either from Monte-Carlo simulations or from calibration samples, using the estimator $\hat{p}$, obtained by replacing the expectation values $n_k$ with their sample values $\hat{n}_k$,

$$\hat{p} = \frac{\hat{n}_1}{\hat{n}_1 + \hat{n}_2}. $$

(2)

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If the true efficiency $p$ is constant and $\hat{n}_1 + \hat{n}_2 = n$ is fixed, then $\hat{n}_1$ is binomially distributed. Since $\hat{p}$ is a linear function of $\hat{n}_1$, $\hat{p}$ is an unbiased estimate of $p$,

$$E[\hat{p}] = \frac{E[\hat{n}_1]}{n} = \frac{n_1}{n} = p,$$

and the variance of $\hat{p}$ can be calculated exactly to

$$\text{var}(\hat{p}) = E[(\hat{p} - p)^2]
= \sum_{\hat{n}_1=0}^{\infty} \left( \frac{\hat{n}_1}{n} - p \right)^2 B(\hat{n}_1; n, p)
= \frac{1}{n^2} \sum_{\hat{n}_1=0}^{\infty} (\hat{n}_1 - pn)^2 B(\hat{n}_1; n, p)
= \frac{E[(\hat{n}_1 - n_1)^2]}{n^2} = \frac{p(1-p)}{n} = \frac{n_1n_2}{(n_1 + n_2)^2},$$

where we used the known second central moment of the binomial distribution.

This binomial model is the standard starting point on which confidence intervals for the efficiency estimator are derived. Confidence intervals are constructed so that they contain the true value with a fixed probability in repeated identical experiments, the coverage probability.

Coverage probability is a useful concept, even if an experiment is not actually identically repeated. We illustrate this with the common case where the efficiency $p$ depends on some variable $x$. In that case, efficiency estimates are usually computed in bins of $x$. In general, the true values of $p$ and $n$ in each bin differ, and thus the bins are not repetitions of identical experiments, but the result in each bin is one realisation from the potential set of identical experiments with fixed $p$ and Poisson-distributed $n$. If we use confidence intervals for each bin that have the same known coverage probability, then the whole set of intervals over all bins also has that coverage probability for the true values $p(x)$. This allows one to judge whether a model curve $p(x)$ agrees with the measurements. If it does, the fraction of the intervals that intersect with the curve approaches the coverage probability (for standard 68% intervals this is the well-known rule of $2/3$).

A universally accepted formula for the confidence interval of an efficiency is not at hand. Because of the discreteness of the counts, it is not possible to construct intervals which contain the true value with a fixed probability for all true values. The Clopper-Pearson intervals always contain the true value with at least the given probability, but severely overcover on average. This is not always desired. In the example from the previous paragraph, the fraction of Clopper-Pearson intervals that overlap with the model curve $p(x)$ would be considerably larger than 68%. Therefore other intervals have been proposed. The Wilson interval has an average coverage probability closer to the nominal value for randomly chosen values of $p$ and $n$, at the cost of undercovering for some values. In this note, we will focus on the Wilson interval, because it has attractive properties and is easy to generalise.

A major point of this note is to correct the assumption that a fixed $n$ is a good model of reality in particle physics experiments. The number of trials $n$ in a typical experiment is Poisson distributed, since experiments are run for a fixed time rather than until a fixed number of trials has been accumulated. This modifies the variance of $\hat{p}$ compared to what is expected from the binomial model. Since the Wilson interval is based on this variance, we investigate the
impact of the modified variance on the Wilson interval. We further consider that the counts \( \hat{n}_k \) in practice are often not directly known and have to be estimated, which increases their variance compared to Poisson fluctuations. We also compute the variance of \( \hat{p} \) under these conditions and obtain a generalised Wilson interval for this case.

2. Poisson-distributed counts

We are considering the case where \( p \) is a fixed number and the actual number of trials \( \hat{n} \) is Poisson-distributed around an expectation \( n \). There are two equivalent ways to calculate the probability for observing a particular value of \( \hat{p} \) in this case. The first is based on the straightforward product of the probabilities of the binomial distribution \( B \) and the Poisson distribution \( \text{Pois} \), while the second uses the probabilities from two Poisson distributions. The probability to observe the sample pair \( \hat{n}_1, \hat{n} \) is

\[
P(\hat{n}_1, \hat{n}; p, n) = B(\hat{n}_1; \hat{n}, p) \text{Pois}(\hat{n}; n) \\
= \frac{\hat{n}!}{\hat{n}_1!(\hat{n} - \hat{n}_1)!} p^{\hat{n}_1}(1 - p)^{\hat{n} - \hat{n}_1} e^{-n} \frac{n^{\hat{n}}}{\hat{n}!} \\
= \frac{1}{\hat{n}_1! \hat{n}_2!} n^{\hat{n}_1} (1 - p)^{\hat{n} - \hat{n}_1} e^{-n} \frac{n^{\hat{n}_1}}{\hat{n}_1!} \frac{n^{\hat{n}_2}}{\hat{n}_2!} \\
= \frac{e^{-n_1} n_1^{\hat{n}_1}}{\hat{n}_1!} \frac{e^{-n_2} n_2^{\hat{n}_2}}{\hat{n}_2!} \text{Pois}(\hat{n}_1; n_1) \text{Pois}(\hat{n}_2; n_2),
\]

with \( n_1 = pn \) and \( n_2 = n - n_1 = (1 - p)n \). Both forms are equivalent, so one can use the most convenient form for each calculation.

We calculate the bias and variance of the efficiency estimator \( \hat{p} \) again under these new conditions. The estimator is undefined for \( \hat{n} = 0 \), so one has to decide how this case should be handled. We could, for example, assign the value 1/2 to \( \hat{p} \), but that would not be correspond to actual practice. Instead, we skip this outcomes with \( \hat{n} = 0 \) and compute the expectation of the remaining cases. This leads to some surprising properties, as we will see.

Calculating the bias again is important since the estimator \( \hat{p} \) is now a nonlinear function of the arguments \( \hat{n}_1 \) and \( \hat{n} \). Non-linear functions in general lead to biased estimators, but \( \hat{p} \) is still unbiased. To show this, we compute the expectation of \( \hat{p} \),

\[
E[\hat{p}] = \frac{1}{1 - \text{Pois}(0; n)} \sum_{\hat{n}_1=1}^{\infty} \sum_{\hat{n}_1=0}^{\infty} \frac{\hat{n}_1}{\hat{n}} B(\hat{n}_1; \hat{n}, p) \text{Pois}(\hat{n}; n) \\
= \frac{1}{1 - \text{Pois}(0; n)} \sum_{\hat{n}_1=1}^{\infty} \frac{\hat{n}p}{\hat{n}} \text{Pois}(\hat{n}; n) = p.
\]
Next, we compute the variance of $\hat{p}$ and get
\[
\text{var}(\hat{p}) = E[(\hat{p} - p)^2]
\]
\[
= \frac{1}{1 - \text{Pois}(0; n)} \sum_{\hat{n}_1 = 1}^{\infty} \sum_{\hat{n}_2 = 0}^{\hat{n}_1} \left( \frac{\hat{n}_1}{\hat{n}_2} - p \right)^2 \text{B}(\hat{n}_1; \hat{n}, p) \text{Pois}(\hat{n}; n)
\]
\[
= \frac{1}{1 - \text{Pois}(0; n)} \sum_{\hat{n} = 1}^{\infty} \frac{p(1 - p)}{\hat{n}} \text{Pois}(\hat{n}; n).
\]

We used Eq. 4 to replace the inner sum. The remaining calculation can be carried out numerically. Terms with large deviations $|\hat{n} - n|$ quickly approach zero and thus only a few terms of the sum around the expectation value $n$ need to be evaluated. Alternatively, one can compute the variance based on Monte-Carlo simulation, by computing the average $\langle (\hat{p} - p)^2 \rangle$ over many randomly drawn samples. Due to law of large numbers, this approaches $E[(\hat{p} - p)^2]$.

Results of solving Eq. 7 numerically are shown in Fig. 1 and compared to results from Eq. 4. The results agree in the limit $n \to \infty$, but differ for $n \lesssim 10$.

We can express the variance of $\hat{p}$ as the product of Eq. 4 with a correction $f(n)$,
\[
\text{var}(\hat{p}) = \frac{p(1 - p)}{n} f(n).
\]

The correction $f(n)$ is shown in Fig. 2 for a numerical and a Monte-Carlo calculation of Eq. 7. It starts off smaller than one, due to the exclusion of samples with $\hat{n} = 0$, and then rises above one with a maximum in the range $n = 3 \ldots 4$ and then approaches one as $n$ increases further.

Since Eq. 7 is still comparably expensive to compute, we offer a fast approximation. We start by expanding the estimator $\hat{p} = \hat{n}_1 / (\hat{n}_1 + \hat{n}_2)$ at $\hat{n}_k = n_k$ in
a Taylor series,

\[ \hat{p} = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \frac{\hat{n}_1 - n_1}{i!} \frac{\hat{n}_2 - n_2}{j!} \frac{\partial^{i+j} \hat{p}}{\partial \hat{n}_1^i \partial \hat{n}_2^j}(n_1, n_2), \] \hspace{1cm} (9)

treating the integer values \( \hat{n}_k \) like real numbers. This expansion approximates the asymptotic limit \( n_k \to \infty \). We can rewrite this as

\[ \hat{p} - p = \sum_{j=1}^{\infty} \frac{\hat{n}_2 - n_2}{j!} \frac{\partial^{j} \hat{p}}{\partial \hat{n}_2^j}(n_1, n_2) + \sum_{i=1}^{\infty} \frac{\hat{n}_1 - n_1}{i!} \frac{\partial^{i} \hat{p}}{\partial \hat{n}_1^i}(n_1, n_2) + \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{\hat{n}_1 - n_1}{i!} \frac{\hat{n}_2 - n_2}{j!} \frac{\partial^{i+j} \hat{p}}{\partial \hat{n}_1^i \hat{n}_2^j}(n_1, n_2). \] \hspace{1cm} (10)

The variance of \( \hat{p} \) can then be computed by squaring both sides and computing the expectation on both sides. The expectation is a linear operator and therefore distributive to each term of the sum on the right-hand side. These terms consists of constants multiplied with

\[ \mathbb{E}[(\hat{n}_1 - n_1)^i(\hat{n}_2 - n_2)^j] = \mathbb{E}[(\hat{n}_1 - n_1)^i] \mathbb{E}[(\hat{n}_2 - n_2)^j]. \] \hspace{1cm} (11)

The expectations of \( \hat{n}_1 \) and \( \hat{n}_2 \) factor, because they are independently distributed. The expectation \( \mathbb{E}[(\hat{n}_k - n_k)^j] \) is the \( j \)-th central moment of the Poisson distribution, which can be computed to any order from the moment generating function. Putting all this together, the correction to first order in \( n^{-1} \) is

\[ f_{n \to \infty}(n) = \frac{n + 1}{n} + O(n^{-2}). \] \hspace{1cm} (12)
Although the simplicity of this formula is attractive, it improves the accuracy of Eq. 8 only marginally. A correction to third order performs better,

\[ f_{n \to \infty}(n) = \frac{2n + n^2 + n^3 + 6}{n^3} + O(n^{-4}), \]  

(13)

and produces accurate results for \( n \gtrsim 5 \). It fails to describe the true variance as \( n \) approaches zero, however. Another expansion of Eq. 7 around \( n_1 = n_2 = 0 \) to second order yields

\[ f_{n \to 0}(n) = n + n^2/4 + O(n^3), \]  

(14)

We combined the two limits empirically with a transition function to obtain an approximation with an accuracy better than 1.7% over the whole range,

\[ f_{\text{approx}}(n) = (1 - z(n)) \left( n - \frac{n^2}{4} \right) + z(n) \left( \frac{2n + n^2 + n^3 + 6}{n^3} \right), \]  

(15)

\[ z(n) = \left( 1 + e^{-(\ln_{q=0.82}(n) - \ln_{q=0.82}(2.92))/0.18} \right)^{-1}, \]  

(16)

in which we use the \( q \)-logarithm \( \ln_q(x) = (x^{1-q} - 1)/(1-q) \) for \( q \neq 1 \). The approximation and the two limiting functions are shown in Fig. 2.

3. Poisson-distributed counts with additional fluctuations

We now consider the common case where the estimates \( \hat{n}_k \) cannot be obtained by direct counting, but need to be estimated in some other way that inflates their variance. A typical case in high-energy physics is that the estimates \( \hat{n}_k \) are obtained from a fit to the invariant mass distribution of decay candidates. Such a fit removes a background contribution on average, but it adds additional variance to the estimate, since the background fluctuates.

This case and any other, where an additional random contribution is added to a sample from a Poisson process, can be modeled in the following way,

\[ \hat{n}_1 = n_1 + z_1 \sqrt{n_1} + z_2 \sigma_{1,b}, \]  

(17)

and likewise for \( \hat{n}_2 \). Here, the \( z \) are random numbers with \( \text{E}[z] = 0 \) and \( \text{E}[z^2] = 1 \) and \( \sigma_{1,b}^2 \) is the additional variance that does not originate from the Poisson process. We assume that the random process which generates the extra variance is uncorrelated to the Poisson process. The variance of \( \hat{n}_k \) then is

\[ \text{var}(\hat{n}_k) = n_k + \sigma_{k,b}^2. \]  

(18)

In general, \( \sigma_{k,b}^2 \) is difficult to estimate, but an estimate for \( \text{var}(\hat{n}_k) \) is usually available. In the fit that was just described, \( \text{var}(\hat{n}_k) \) is estimated by inverting the Hessian matrix of the log-likelihood at the best fit values and taking the diagonal component that corresponds to the parameter \( \hat{n}_k \) (the so-called HESSE method in MINUIT [3]). We thus use the substitution

\[ \sigma_{k,b} = \sqrt{\text{var}(\hat{n}_k) - n_k}. \]  

(19)

We compute the variance of the efficiency estimate \( \hat{p} \) under these conditions. The estimate is

\[ \hat{p} = \frac{\hat{n}_1}{\hat{n}_1 + \hat{n}_2} = \frac{n_1 + z_1 \sqrt{n_1} + z_3 \sigma_{1,b}}{n_1 + z_1 \sqrt{n_1} + z_3 \sigma_{1,b} + n_2 + z_2 \sqrt{n_2} + z_4 \sigma_{2,b}}, \]  

(20)
and its variance is to second order
\[ \text{var}(\hat{p}) \approx JC_zJ^T, \]  
with the covariance matrix
\[
C_z = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & \rho \\
0 & 0 & \rho & 1
\end{pmatrix},
\]  
for the \( z_k \), where \( \rho \) is the correlation coefficient between the two background contributions. Estimating \( \rho \) from data is not straightforward, but fortunately \( \rho \) is often zero. If \( n_1 \) and \( n_2 \) are estimated from independent samples, the backgrounds are usually independently sampled as well. The row-matrix \( J \) is given by the derivatives \( J_i = \partial \hat{p}/\partial z_k \) evaluated at \( z_k = 0 \). We obtain
\[
\text{var}(\hat{p}) \approx p(1-p)\frac{n}{n_1 + n_2} + \frac{n_1^2 \text{var}(\hat{n}_2) + n_2^2 \text{var}(\hat{n}_1)}{(n_1 + n_2)^4} - 2\rho \frac{p(1-p)\sigma_{1,b}\sigma_{2,b}}{n^2}.
\]  
which reduces to Eq. 4 for \( \sigma_{k,b} = 0 \). Substitution of \( \sigma_{k,b} \) gives
\[
\text{var}(\hat{p}) \approx n_1^2 \text{var}(\hat{n}_2) + n_2^2 \text{var}(\hat{n}_1) - 2p \frac{n_1 n_2 \sqrt{\text{var}(\hat{n}_1) - n_1 \sqrt{\text{var}(\hat{n}_2) - n_2}}}{(n_1 + n_2)^4}.
\]  
For \( \rho = 0 \) we get the simple formula
\[
\text{var}(\hat{p}) \approx \frac{n_1^2 \text{var}(\hat{n}_2) + n_2^2 \text{var}(\hat{n}_1)}{(n_1 + n_2)^4}.
\]  
Eq. 24 is a good approximation for \( n \gg 1 \) and \( \sigma_{k,b} \ll n \). In contrast to the previous section, we will not attempt to compute \( \text{var}(\hat{p}) \) more accurately, since that would require additional information about the process which introduces the extra fluctuations. One needs the higher moments of \( z_3 \) and \( z_4 \), which are usually not readily available. It is possible to improve the result in the limit \( \sigma_{k,b}/n \to 0 \) by replacing the first term in Eq. 23 with Eq. 8 and using Eq. 16 for \( f(n) \).

To demonstrate the validity of Eq. 25 we simulate an analysis in which the estimates \( \hat{n}_k \) are obtained from a fit to data which consists of a gaussian signal and uniformly distributed background. The peak is modelled with a normal distribution whose amplitude, location, and width are free parameters. The background is modelled with a second degree Bernstein polynomial. The simulation is run 1000 times. In each run, the number of successes and failures are sampled independently from Poisson-distributions with expectations \( pn \) and \( (1-p)n \), respectively. The expected number of background events for both successes and failures is taken to be \( 0.2n \), and also Poisson distributed. Since the background events are independently sampled from the successes and failures, we have \( \rho = 0 \).

The results of the simulation are shown in Fig. 3. The results of Eq. 25 show satisfactory agreement with the true variance of the estimate \( \hat{p} \), but we also point out deviations up to 18% (6%) in case of \( n = 50 \) (\( n = 1000 \)). Convergence is rather slow. The approximate formula underestimates the true
Figure 3: Standard deviation of the efficiency estimate $\hat{p}$ for the simulated analysis described in the text, in which the estimates $\hat{n}_k$ are obtained from a fit to a mixture of signal and background. Shown are the standard deviations over the repetitions (lines) and the square-root of the average variance estimates (dots) for different total expected number of events $n$. An alternative calculation in which the first term in Eq. 23 is corrected with Eq. 16 is also shown (crosses).

The ansatz of the standard Wilson interval is to regard the normalised residual of $\hat{p}$ as approximately standard-normal distributed, so that its square approximation for central values of $\rho$ and overestimates for values close to zero or one. This accuracy is usually good enough to draw an error bar in a plot, however.

For more accurate calculations, bootstrap methods could be used.

Sometimes, it is more convenient to estimate $\hat{n}_1$ and $\hat{n}$ instead of $\hat{n}_1$ and $\hat{n}_2$ to compute $\hat{p}$, so we also compute the variance for this case. The variance of $\hat{n}$ is $\text{var}(\hat{n}) = n + \sigma_{1,b}^2 + \sigma_{2,b}^2 + 2\rho \sigma_{1,b} \sigma_{2,b}$ and the substitution for $\sigma_{2,b}$ becomes

$$\sigma_{2,b} = \sqrt{\text{var}(\hat{n}) - \text{var}(\hat{n}_1)} - n + n_1(1 - \rho^2) + \rho^2 \text{var}(\hat{n}_1) - \rho \sqrt{\text{var}(\hat{n}_1) - n_1},$$

which yields

$$\text{var}(\hat{p}) \approx \frac{n^2 \text{var}(\hat{n}_1) + \text{var}(\hat{n})n_1^2 - 2nn_1 \text{var}(\hat{n}_1)}{n^4} + 2\rho \frac{n_1}{n^3} \left(\rho \left(\text{var}(\hat{n}_1) - n_1\right) - \sqrt{\text{var}(\hat{n}_1) - n_1} \sqrt{\rho^2 \left(\text{var}(\hat{n}_1) - n_1\right) + \text{var}(\hat{n}) - n + n_1 - \text{var}(\hat{n}_1)}\right).$$

This formula is very complicated, but when $\rho$ is zero, it reduces to

$$\text{var}(\hat{p}) \approx \frac{n^2 \text{var}(\hat{n}_1) + \text{var}(\hat{n})n_1^2 - 2nn_1 \text{var}(\hat{n}_1)}{n^4}.$$  

4. Generalised Wilson intervals

The ansatz of the standard Wilson interval is to regard the normalised residual of $\hat{p}$ as approximately standard-normal distributed, so that its square approximations for central values of $\rho$ and overestimates for values close to zero or one. This accuracy is usually good enough to draw an error bar in a plot, however.

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Sometimes, it is more convenient to estimate $\hat{n}_1$ and $\hat{n}$ instead of $\hat{n}_1$ and $\hat{n}_2$ to compute $\hat{p}$, so we also compute the variance for this case. The variance of $\hat{n}$ is $\text{var}(\hat{n}) = n + \sigma_{1,b}^2 + \sigma_{2,b}^2 + 2\rho \sigma_{1,b} \sigma_{2,b}$ and the substitution for $\sigma_{2,b}$ becomes

$$\sigma_{2,b} = \sqrt{\text{var}(\hat{n}) - \text{var}(\hat{n}_1)} - n + n_1(1 - \rho^2) + \rho^2 \text{var}(\hat{n}_1) - \rho \sqrt{\text{var}(\hat{n}_1) - n_1},$$

which yields

$$\text{var}(\hat{p}) \approx \frac{n^2 \text{var}(\hat{n}_1) + \text{var}(\hat{n})n_1^2 - 2nn_1 \text{var}(\hat{n}_1)}{n^4} + 2\rho \frac{n_1}{n^3} \left(\rho \left(\text{var}(\hat{n}_1) - n_1\right) - \sqrt{\text{var}(\hat{n}_1) - n_1} \sqrt{\rho^2 \left(\text{var}(\hat{n}_1) - n_1\right) + \text{var}(\hat{n}) - n + n_1 - \text{var}(\hat{n}_1)}\right).$$

This formula is very complicated, but when $\rho$ is zero, it reduces to

$$\text{var}(\hat{p}) \approx \frac{n^2 \text{var}(\hat{n}_1) + \text{var}(\hat{n})n_1^2 - 2nn_1 \text{var}(\hat{n}_1)}{n^4}.$$
proximately satisfies,
\[
z^2 \approx \frac{(\hat{p} - p)^2}{\text{var}(\hat{p})},
\]
where \(z\) is standard-normally distributed. For a given value of \(z^2\) and the observed value \(\hat{p}\), one finds the interval in \(p\) that satisfies the equation. The value \(z^2\) is computed from the inverse of the cumulative \(\chi^2\) distribution with one degree of freedom, evaluated at the desired coverage probability. The crucial improvement of the Wilson interval over the normal approximation interval is that \(\text{var}(\hat{p})\) is correctly considered as a function of \(p\) when solving the equation, while the latter uses a constant value for \(\text{var}(\hat{p})\), evaluated at the point \(p = \hat{p}\).

We follow this approach to compute a Wilson interval for the case of Poisson-distributed counts without extra fluctuations. We insert Eq. 8 in Eq. 29 and get a quadratic equation in \(p\),
\[
(\hat{p} - p)^2 = z^2 p(1 - p)\frac{n}{f(n)},
\]
which we solve for \(p\) to obtain a Wilson interval
\[
p_{1,2} = \frac{1}{1 + \frac{z^2}{n} f(n)} \left( \hat{p} + \frac{z^2}{2n} f(n) \pm \frac{z}{n} \sqrt{-\hat{p}(1 - \hat{p})n f(n) + \frac{z^2}{4} f(n)^2} \right),
\]
To obtain the standard 68 % interval, one sets \(z = 1\). For \(f(n)\), and can insert Eq. 16. We note that this is interval is not a full implementation of Wilson’s approach, since deviations of \(n\) from \(\hat{n}\) are not taken into account. For small \(n\), this interval may be too narrow, as we will see in the next section. Therefore, we do not recommend this Wilson interval over the standard one, even though it is computed with an improved estimate of the variance.

More useful is the generalisation of the Wilson interval for the case of Poisson-distributed counts with independent extra fluctuations (\(\rho = 0\)). We insert Eq. 23 into Eq. 29 and again get a quadratic equation in \(p\),
\[
(\hat{p} - p)^2 = \frac{z^2}{n^2} \left( (\sigma_{1,b}^2 + \sigma_{2,b}^2 - n)p^2 + (n - 2\sigma_{1,b}^2)p + \sigma_{1,b}^2 \right).
\]
Solving for \(p\) yields
\[
p_{1,2} = \frac{1}{1 + \frac{z^2}{n} (1 - \frac{\sigma_{1,b}^2 + \sigma_{2,b}^2}{n})} \left( \hat{p} + \frac{z^2}{2n} \left( 1 - \frac{2\sigma_{1,b}^2}{n} \right) \pm \frac{z}{n} \sqrt{\hat{p}^2 (\sigma_{1,b}^2 + \sigma_{2,b}^2 - n) + \hat{p}(n - 2\sigma_{1,b}^2) + \sigma_{1,b}^2 + \frac{z^2}{4} \left( 1 - 4\frac{\sigma_{1,b}^2 \sigma_{2,b}^2}{n^2} \right)} \right).
\]
The \(\sigma_{k,b}\) are then substituted according to Eq. 19. The generalised Wilson interval reduces to the original for \(\sigma_{k,b} \to 0\). Results for non-zero values of \(\sigma_{k,b}\) are shown in Fig. 4. When the extra fluctuations are large, the interval becomes similar to the normal approximation interval \(\hat{p} \pm \sqrt{\text{var}(\hat{p})}\), but it has a better limit for \(\sigma_{k,b} \to 0\). The original Wilson interval has the nice property that the interval boundaries are automatically restricted to the range \(p \in [0,1]\), but this is not the case for the generalised interval.
Figure 4: Wilson intervals computed with Eq. 33 when extra fluctuations are present. Shown are intervals as a function of the estimate $\hat{p}$ for $n = 10$ and different amounts of additional fluctuations. Also shown for comparison is the normal approximation interval $\hat{p} \pm \sqrt{\text{var}(\hat{p})}$ for one of the cases. All intervals have been clipped to the range $[0, 1]$.

5. Coverage probability of different intervals

The coverage probability is given by the fraction of intervals that cover the true value in repeated identical experiments. We compute the coverage probability of the Wilson interval and other popular intervals:

- Clopper-Pearson interval [1]. This is based on the exact Neyman construction of the interval. It is guaranteed to cover the true value with at least the requested coverage probability.

- Normal approximation interval. Like the Wilson interval, this interval assumes that sample deviations from the true value are normally distributed, but the variance of these deviations is considered to be constant, with $\text{var}(\hat{p})$ evaluated at $p = \hat{p}$.

- Bayesian intervals. We calculate Bayesian credible intervals for uniform and Jeffreys priors [5] in $p$, respectively. Bayesian intervals are not designed to have any particular coverage probability, but can have good coverage properties in practice. The Jeffreys prior used here is the one for the binomial distribution.

We compute the coverage probability of these intervals for binomially and Poisson distributed samples. The deviation of the actual coverage probability from the expected probability is shown as a function of the true efficiency $p$ and the expected total number of counts $n$ in Fig. 5 and Fig. 6. The coverage probability is not a smooth function of $p$ and $n$ due to the discreteness of the binomial and Poisson distributions. This is very apparent in case of binomially distributed samples, and to a lesser degree also in case of Poisson distributed samples.
Figure 5: Deviation of the coverage probability from the expected value as a function of $p$ and the expected total number of events $n$. Samples in the top left plot are drawn from the binomial distribution, for the other plots they are drawn from the Poisson distribution. The plot in the top right corner shows the standard Wilson interval based on Eq. 4. The plot in the bottom left corner shows the generalised Wilson interval based on Eq. 13 and the plot in the bottom right corner shows the interval based on Eq. 16.
Figure 6: Deviation of the coverage probability from the expected value as a function of $p$ and the expected total number of events $n$. Samples are drawn from the binomial (Poisson) distribution for the plot on the left-hand (right-hand) side.
Figure 7: Coverage probability averaged over $p$ as a function of the expected total number of events $n$. Samples are drawn from the binomial (Poisson) distribution on in the upper (lower) plot.
samples. The coverage probability averaged over values of $p$ is shown in Fig. 7 using a uniform prior for $p$. The choice of this prior is arbitrary, but the qualitative results that we draw do not depend strongly on the prior.

We evaluate these results according to the following criteria

- Intervals with a coverage probability closer to the expected value are preferred.
- Intervals are disqualified, if they do not cover the true value at all for some combinations of $p$ and $n$.

The Clopper-Pearson and normal approximation intervals severely over- and undercover, respectively. When it is essential to be conservative, the Clopper-Pearson interval is the correct choice, but not in most practical cases. The average coverage probability is closest to the expected probability for the Bayesian credible interval with the Jeffreys prior. However, the Bayesian intervals have zero coverage for some values of $n$ and $p$, which disqualifies them according to our criteria.

The Wilson intervals have a coverage probability close to the expected value and only slightly overcover on average. They never have zero coverage for some values of $n$ and $p$. The standard Wilson interval based on the variance for binomially distributed samples in Eq. 4 also performs well when the samples are Poisson distributed. It overcovers when $p$ is close to zero and one, and slightly undercovers when $p$ is near 1/2. When the Wilson interval is constructed with the correct variance for Poisson distributed samples, the latter is more pronounced. Undercoverage can be avoided completely by using the approximate variance based on Eq. 13, which makes the interval conservative for small $n$.

In conclusion, the standard Wilson interval is a good choice even when the samples are Poisson distributed. Its coverage probability is close to the expected value, it undercovers only mildly, and is readily available in statistical software or easily implemented by hand.

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The calculations in this paper use the following scientific software libraries: Numba [6], ROOT [7], Numpy [8], SciPy [9], iminuit [10], matplotlib [11], and SymPy [12]. HD acknowledges funding from the Deutsche Forschungsgemeinschaft (DFG – German Research Foundation) under award DE 3061/1-1.

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