Bayesian Blocks in High Energy Physics:  
Better Binning made easy!

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The Bayesian Block algorithm, originally developed for applications in astronomy, can be used to improve the binning of histograms in high energy physics. The visual improvement can be dramatic, as shown here with two simple examples. More importantly, this algorithm and the histogram is produces a non-parametric density estimate, providing a description of background distributions that does not suffer from the arbitrariness of ad hoc analytical functions. The statistical power of an hypothesis test based on Bayesian Blocks is nearly as good as that obtained by fitting analytical functions. Two examples are provided: a narrow peak on a smoothly-falling background, and an excess in the tail of a background that falls rapidly over several orders of magnitude. These examples show the usefulness of the binning provided by the Bayesian Blocks algorithm both for presentation of data and when searching for new physics.

I. INTRODUCTION

Histograms are ubiquitous in particle physics, yet histogram binning is usually settled in an ad hoc manner. Most of the time, a subjectively natural range and bin width is chosen, motivated mainly by obtaining a nice-looking plot. Objective methods have been proposed [1–6] that determine binning according to some optimization procedure. For example, Scott’s Rule [11] and the Freedman-Diaconis Rule [2] determine the number of fixed-width bins by the number of entries and a measure of the spread of the distribution (root-mean-square for Scott’s Rule and interquartile range for Freedman-Diaconis Rule). Knuth’s Rule [4] takes the structure of the distribution into account but uses bins of fixed width. The Bayesian Block algorithm, in contrast, allows the bin widths to vary.

The Bayesian Blocks algorithm was developed in an astronomy context by Scargle [7, 8]. His objective was to set bin edges, called “change points”, at times when the light flux from an astrophysical object suddenly changed. The flux is represented by the arrival times \( t_i \) of photons in a telescope; given a set of event data \( \{t_i\} \) for \( i = 1, \ldots, N \), the algorithm uniquely determines the number and placement of the change points.

In our analysis, the change points play the role of histogram bin boundaries for a set of event data \( \{x_i\} \). The resulting histogram is objective rather than subjective. Ranges in \( x \) in which the data are sparse result in larger bins, and ranges in which the data are concentrated result in smaller bins. Furthermore, if the (empirical) probability density function (pdf) changes slowly, then the bins are wide, and if it changes rapidly, the bins will be narrower. The prospect of a self-adjusting histogram is attractive especially in contexts in which the distributions falls over orders of magnitude: typical histograms plotted on a semi-logarithmic scale either lose the structure at the high values of the pdf or are plagued by statistical fluctuations in the tails. Sometimes researchers employ unequal binning but the bins are still chosen in an arbitrary manner, and the results are seldom completely satisfactory.

We apply the Bayesian Blocks algorithm to histogramming in collider physics. We provide illustrations of how this algorithm produces clear and pleasing histograms with no subjective input from the analyzer. Naturally, the Bayesian Block algorithm can be applied to any scientific field in which histograms are employed.

Beyond producing pleasing histograms, we have discovered that the binning provided by the Bayesian Blocks algorithm can be used in searches for new physics with important advantages. Since the binning is statistically optimal in a well-defined sense, hypothesis tests such as comparing a null distribution based on standard model expectations with an alternative that includes a well-defined signal are effective. Furthermore, since the binning is determined by an algorithm, the null or background model is not arbitrary and is, essentially, non-parametric. As a consequence, issues of which analytical functions to use to represent the background distribution are completely avoided with little loss of discriminating power. We give two very different examples to illustrate this point: the first example considers a narrow peak on a large and smooth background, and the other example considers a broad excess at the tail of a rapidly-falling distribution.

The remainder of this paper is structured as follows. A brief technical description of the Bayesian Blocks algorithm is given in Section II followed by illustrations from collider physics in Section III. Section IV explores the use of the algorithm in the search for a narrow peak such as \( h \to \gamma \gamma \), while Section V shows how the algorithm can be used in searching for black holes. We conclude in Section VI.

II. THE BAYESIAN BLOCK ALGORITHM

The Bayesian Blocks algorithm is a nonparametric modeling technique for determining the optimal segmentation of a given set of univariate random variables. Each
blocks (or bin, in the context of histograms) is consistent with a pdf with compact support; the entire dataset is represented by the collection of finite pdfs. For this analysis (and for most current implementations of Bayesian Blocks), each pdf is a uniform distribution, which thereby defines the ‘Piecewise Constant Model’ as discussed in Ref. [7]. The number of blocks and the edges of the blocks are determined through optimization of a ‘fitness function’, which is essentially a goodness-of-fit statistic dependent only on the input data and a regularization parameter (discussed below).

The set of blocks is gapless and non-overlapping, where the first block edge is defined by the first data point, and the last block edge is defined by the last data point. A block can contain between 1 to \(N\) data points, where the sum of the contents of all the blocks must equal \(N\). The fitness of a given set of blocks is equal to the sum of the fitnesses of the individual blocks, and therefore the total fitness, \(F_{\text{total}}\), for a given dataset is:

\[
F_{\text{total}} = \sum_{i=0}^{K} f(B_i),
\]

where \(f(B_i)\) is the fitness for an individual block, and \(K\) is the total number of blocks. The additivity of the block fitnesses is leveraged by the Bayesian Blocks algorithm in order to greatly improve the total execution time.

Given an ordered set of \(N\) data points, the algorithm determines the optimal set of \(K + 1\) change points (and therefore \(K\) blocks) by iterating through the data points, and caching the current maximum fitness values and corresponding indices. For example, during iteration \(n\) (where data point \(n\) is being evaluated), the potential total fitnesses are calculated from: Eq. [1] as:

\[
F_{\text{total}}(n, m) = F_m + f(B^m_n), \quad m = 1, 2, \ldots, n - 1
\]

where \(F_m\) is the optimal fitness as determined during iteration \(m\), and \(f(B^m_n)\) is the fitness of the block bound between data points \(n\) and \(m\). This potential total fitness is calculated \(n - 1\) times at each iteration, and the maximum of those fitnesses along with the relevant change points are stored and used during the subsequent iterations. After the final iteration, \(N\), the change-points associated with the maximum total fitness are returned. This method guarantees that the global maximum fitness is obtained with a runtime of \(O(N^2)\), which is much more efficient than an exhaustive search of all \(2^N\) potential configurations.

For a series of discrete, independent events, the fitness function for an individual block, \(f(B_i)\), can be defined as an unbinned log-likelihood (the Cash statistic [8]):

\[
f(B_i) = \ln L_i(\lambda) = N_i \ln \lambda - \lambda T_i.
\]

This modified Cash statistic is derived from the Poisson likelihood of \(N\) events sampled from a model with amplitude \(\lambda\) over a range \(T\). It follows that the total fitness \(F_{\text{total}}\) is:

\[
F_{\text{total}} = \sum_{i=1}^{K} \ln L_i^{\text{max}}(\lambda).
\]

The fitness described above must be modified by a penalty term for the number of blocks. Without explicitly adding this additional parameter, there is an implicit assumption of a uniform prior on the number of blocks between 0 and \(N\). This is unreasonable in most cases, as typically \(N_0 \ll N\), where \(N_0\) is the number of blocks. In Ref. [7], a geometric prior of the form was chosen:

\[
P(N_b) = P_0 \gamma^{N_b},
\]

where \(\gamma\) is the single free parameter, and \(P_0\) is a normalization constant. This prior must be tuned in order to achieve a reasonable binning for a given dataset. An overly conservative value will suppress the detection of true change-points, while too liberal a value will lead to spurious change points (eventually reaching the limit of \(N_b = N\)). The prior can be interpreted as a control on the false-positive rate for detecting change-points.

The prior can be determined empirically as a function of the false-positive rate through simple toy studies. By generating many pseudo-data distributions and applying the Bayesian Block algorithm with a large range of prior values, one can determine the desired prior value for a given false-positive rate. In general, the number of change-points is insensitive to a large range of reasonable values for \(\lambda\).

The codes used to implement Bayesian Blocks in this paper is modified from the AstroML python package.

III. ILLUSTRATIONS

Our first illustration is the sharp peak in the distribution of the invariant mass \(M_{\mu\mu}\) of muon pairs produced at a hadron collider; this resonance is the Z boson. The example shown in Fig. 1 is produced using simulated events. In a typical application one compares collider data (represented by black dots with error bars) to a simulation (represented here by the light-blue histogram) expecting to see good agreement. If, for example, the momentum scale calibration for the data is not quite correct, one will observe a shift in one distribution with respect to the other. Consequently, the ratio of the two histograms will display a characteristic S-shape. The clarity of the ratio of the two histograms is of central importance in this type of diagnostic study. For the sake of this illustration, we have one set of simulated data with no modification, and a second, independent sample in which the invariant mass values are shifted by 1%. There are 10,000 events in the “data” sample, and \(\approx 680,000\) events in the “simulation” sample.

The left plot in Fig. 1 shows a typical choice of binning and the right plot shows the binning obtained with the
Bayesian Block algorithm. Each plot shows the distribution on a logarithmic scale and the ratio of the two histograms on a linear scale. The red shaded regions show the statistical uncertainties for the ratio. The standard plot is unsatisfactory because the statistical fluctuations below $M_{\mu\mu} \approx 60$ GeV and above $M_{\mu\mu} \approx 125$ GeV are too large to allow any quantitative conclusions to be drawn about the tails of these distributions. Furthermore, the fairly sharp shape of the peak near 90 GeV is not very clear and the ratio plot has only a hint of the S-shaped curve. The Bayesian-Block plot, in contrast, shows a sharp peak and a very clear S-shape, and the statistical fluctuations in the tails are somewhat reduced. Since the widths of the Bayesian Blocks plot are not uniform, we normalize each bin by its width. We also normalize the standard histogram by bin width. The Bayesian Block algorithm produced 20 bins, so we used 20 bins for the standard histogram. In this illustration, the Bayesian-Block algorithm produces a superior visualization of the distribution and of the differences between the two samples.

Our second illustration is the distribution of the transverse momentum $p_T$ of a reconstructed jet produced in association with a vector boson; this distribution is known to fall rapidly as $p_T$ increases and is characterized by a long, sparsely-populated, high-energy tail. Comparisons of data and Monte Carlo simulations can be unsatisfactory when a uniform binning is employed.

The two double-log plots in Fig. 2 show histograms produced with a typical uniform linear binning and a binning determined by the Bayesian Blocks algorithm. The uniform binning histogram is overly coarse in the low-momentum region, potentially obscuring any interesting features or disagreements of the data with the simulation. Conversely, the high-momentum region is binned too finely, and the ratio plot (lower panel) in the lower panel is difficult to interpret due to large statistical uncertainties. The Bayesian Block binning histogram suffers from none of these defects, again producing a much more instructive and visually appealing plot.
FIG. 1: Comparison of simulated Drell-Yan distributions.

(a) Fixed-width binning.

(b) Bayesian Block binning.

FIG. 2: Comparison of simulated Jet momentum distributions.

(a) Fixed-width binning.

(b) Bayesian Block binning.
IV. BUMP HUNTING

A. Overview

The Bayesian Block algorithm provides us with a non-parametric, theory-agnostic approach to categorizing one-dimensional data into multiple bins. Typically in particle physics, a fully-reconstructed particle signal is defined as an peaked excess on top of some smoothly-varying background distribution. Using the Bayesian Block algorithm, the background distribution alone would lead to regular and relatively wide bins, but if there is a localized excess due to a signal, then the Bayesian Block algorithm should assign some number of change points surrounding the signal region. The following example illustrates these considerations with a toy data set.

The decay channel $H \rightarrow \gamma\gamma$ is one of the golden channels for the Higgs boson discovery and analysis at the LHC. The distribution of the invariant mass of the two photons $M_{\gamma\gamma}$ consists of a smoothly-falling background spectrum with a Gaussian-like signal peak centered at $M_{\gamma\gamma} \approx 125 \text{ GeV}$. We generated a toy dataset mimicking the background and signal features using the Delphes detector simulation [11] – see Fig 3.

In order to analyze the utility of the Bayesian Block algorithm for finding the Higgs peak, toy data sets are needed. The simulated background distribution ($100 \leq M_{\gamma\gamma} \leq 180 \text{ GeV}$) was fit to a third-order polynomial (Fig. 4a) and the signal distribution was fit to a Gaussian-like signal peak centered at $M_{\gamma\gamma} \approx 125 \text{ GeV}$. We generated a toy dataset mimicking the background and signal features using the DELPHES detector simulation [11] – see Fig 3.

![Fig. 3: Monte Carlo simulation of the diphoton mass distributions for background (blue histogram) and signal (green histogram)](image)

B. Application of Bayesian Blocks

The naive application of the Bayesian Block algorithm to a sample of background and signal data is shown in Fig. 6a. Even though the number of signal events injected correspond to a very significant deviation from the background-only distribution ($p_{\text{local}} < 1 \times 10^{-7}$), it is difficult to discern a signal peak in the uniform binning case. The Bayesian Block algorithm produces a set of change points whose locations are different than in the background-only case (Fig. 5a) but they do not easily isolate the signal. The majority of the signal is combined with the adjacent low-mass background events. The falling background and rising signal causes the algorithm to misidentify the location of the beginning of the signal, and instead treats that region as roughly uniform.

While the naive implementation of the Bayesian Block algorithm to background + signal events does not have the desired effect of isolating the signal events, the information contained in the background-only and signal-only change points can be leveraged to produce a hybrid binning scheme. The new set of change points is the union of the background-only and signal-only change points (as shown in Fig. 5), along with the removal of any background-only change points that are located within the bounds of the signal-only region. The results of this hybrid binning scheme on both the background-only and background + signal datasets are shown in Fig. 6b. This scheme successfully isolates the signal events and the presence of the signal has an obvious visual impact in the histogram.

C. Hypothesis Testing

In building a histogram based on the hybrid binning scheme we have made minimal assumptions about the shape of the background and the signal; this histogram is an example of a nonparametric density estimator. As such it avoids issues associated with the assumed functional forms of background and signal pdfs. To what extent does an hypothesis test retain the statistical power of a typical analytical fit?

We compare the statistical significance obtained with the hybrid binning to that obtained by fitting the $M_{\gamma\gamma}$ distribution to the analytical functions depicted in Fig. 5. The amplitude of the signal function is defined by the parameter $A$; we took all other shape parameters for
the background and signal to be fixed. This treatment leads to the greatest possible statistical power. The analytical fits were performed with a maximum likelihood method and a test statistic was defined based on the negative log-likelihood, NLL:

\[ q_0 = -2 \left( \text{NLL}_{A=\hat{A}} - \text{NLL}_{A=0} \right) \]

where \( \hat{A} \geq 0 \) is the value of \( A \) that minimizes NLL. Since \( q_0 \) satisfies the criteria for Wilks’ Theorem and consequently can be modeled as a \( \chi^2 \) distribution \cite{12}, we define a \( Z \) score according to \( Z = \sqrt{q_0} \).

The hybrid set of bin edges will be referred to as the “template shape”. In order to compute the average \( Z \) score, a set of 1000 toy datasets is generated. The Bayesian Block template shape and the parametric functions are fit to each dataset. The exact bin edges used for the template fit are those defined in Section IV B. A comparison of the \( Z \) scores from the Bayesian Block template shape and the analytical function is shown in Fig. 7.

The average \( Z \) scores for the Bayesian Block template fit and the unbinned analytic fit are 5.35 and 5.57, respectively. In this example, the statistical power of the hybrid binning scheme is nearly as good as that of the unbinned maximum likelihood fit, which itself is optimal. These results are very encouraging, as they imply that the Bayesian Blocks template can be almost as effective at hypothesis testing as a completely unbinned method, and does not require any prior knowledge of a paramet-
Bayesian Blocks (red line) and uniform binning (blue histogram) for the background + signal toy data

FIG. 6: Application of Bayesian Blocks algorithm to toy background + signal data

Application of the hybrid Bayesian Block algorithm. The green line shows background + signal while the blue histogram shows background only

FIG. 7: Distributions of Z scores for single-parameter fits to toy distributions

V. LOOKING FOR A BROAD EXCESS

A. Overview

Analyses that focus on unearthing new physics in the tails of distributions stand to benefit from an adaptive binning approach. An example of such an analysis is the search for microscopic black holes performed by the CMS Collaboration [13]. The mass of the black hole is sensitive to the details of the underlying theoretical model, so the search strategy is based on a relatively inclusive event-based observable, namely, the sum of the total transverse energy of all final state particles in an event, $S_T$. The signal corresponds to a broad distribution at high values of $S_T$.

For the purpose of illustrating the benefit of choosing a Bayesian Blocks binning, we assume the simplest model of a semi-classical black hole production that decays isotropically into several energetic final state particles. Such black holes can form at the LHC if gravity is rendered sufficiently strong by the presence of large extra dimensions (as posited in the ADD model) or a warped extra dimension (as appears in the Randall Sundrum model). These black holes have large cross sections and can be detected despite the presence of a substantial background coming from standard model processes characterized by many hadronic jets.

With the aim of mimicking the CMS analysis, we consider distributions of $S_T$ for various particle multiplicities, where a “particle” is a lepton, a photon, or a hadronic jet. We model the multijet background using an empirical pdf:

$$f_B(x) = \frac{A(1 + x)^\alpha}{x^{\beta \gamma + \ln x}}$$

(7)

where $\alpha$, $\beta$, and $\gamma$ are free parameters determined in a fit to distributions of $S_T$ [13] ($A$ is a normalization constant), and $x$ is $S_T$. This pdf is used to generate sets of $S_T$ values for the multijet background, and the number of values approximates the total number of data points in Fig. 3 of Ref. [13].

In order to determine the values of the free parameters in Eq. (7) the pdf is fit to a Monte Carlo data set that was generated to mimic the $S_T$ (multiplicity $\geq 2$) distribution. This function is also compared with the $S_T$ (multiplicity $\geq 8$) distribution in order to determine that the function is indeed a reasonable choice. The re-
results of the fit and comparison are shown in Fig. 8. As in Section IV, this functional form is considered the ‘true’ underlying pdf used to generate all further toy data set in this study. Each data set will contain 136 events, equal to the total number of events in the $S_T$ (multiplicity $\geq 8$) distribution. The range of the pdf is defined to be $2800 < S_T < 13000$ GeV.

FIG. 8: Data generated to mimic the $S_T$ distributions found in Ref. [13]. The $S_T$ multiplicity 2 distribution is fit with Eq. 7 and the resulting values for the free parameters are listed on the plot. The function is rescaled and compared with the $S_T$ multiplicity 8 distribution.

The signal models are characterized by very high values of $S_T$, largely beyond the highest values obtained in standard model multijet processes. For this study, they are modeled as wide Gaussian distributions in $S_T$. The mean values range from 4750 to 8380 GeV, and the standard deviations range from 970 to 1660 GeV.

B. Application of Bayesian Blocks

The Bayesian Block algorithm is applied to a toy data set generated from the pdf defined in Eq. 7. The results of the Bayesian Blocks binning and a uniform binning of width 100 GeV are shown in Fig 9. For this particular toy data set, the Bayesian Block algorithm determined four separate bins, bound by the first and last generated data point. Because the possible signal events can exist at very high $S_T$, an additional bin is appended starting at the final Bayesian Block bin edge and ending at the maximum energy of 13000 GeV.

As in Section IV, the binning produced with a background-only distribution is suboptimal for describing a potential signal. Again we construct a hybrid binning scheme, leveraging some information from the signal models. To do so, we generate a simulated data set derived from each signal pdf, with the number of events equal to the number of data events. This is essentially the opposite of the assumption that there is no significant signal contribution; instead, all events are signal and there is no background. The result of the Bayesian Blocks binning and a uniform binning of 100 GeV width is shown in Fig 10.

FIG. 9: Bayesian Blocks and uniform binning for a background-only $S_T$ toy distribution.

The resultant ‘hybrid’ binning is shown in Fig 11. The bin edges for this distribution are simply the union of the bin edges for the background-only and signal-only distributions, with an additional appended bin from the final bin edge and 13000 GeV. The simulated data in this plot was generated by combining the 136 background events with the 136 signal events used to generate the individual binning schemes.

In the following examples, the ‘simulated data’ are the 136 generated events shown previously in Fig. 9. The ‘simulated background’ consists of 100,000 events generated from the same distribution, and then reweighted to correspond to the number of data events. The statistical uncertainty is therefore dominated by the ‘simulated data’. Fig 12c Fig. 12e and Fig. 12e show the data and
background distributions for a uniform, a background-only Bayesian Blocks, and a hybrid binning scheme, respectively. The agreement between the data and background is apparent in both of the Bayesian Blocks cases, and it is immediately obvious that there is no significant signal contribution. The same cannot be said of the uniform binning scheme, where the statistical fluctuations obfuscate any potential signal that could be hiding in the data.

Fig. 12b, Fig. 12d, and Fig. 12f show almost identical distributions, with the addition of 8 signal events to the data. As in the previous figures, the deviation from the background is immediately apparent with the Bayesian Block schemes, and very difficult to discern in the case of uniform binning. The hybrid binning scheme also has sufficient granularity in the high $S_T$ region to discern some shape information with regards to the signal, as opposed to lumping all signal events in a single large bin.

C. Hypothesis Testing

We investigate the statistical power of the histogram constructed from the Bayesian Blocks algorithm by computing 95% confidence level upper limits on the signal amplitude and compare these results to limits produced by using histograms with uniform bins, and also with the unbinned dataset. The unbinned dataset uses the true analytical functions to determine the background and signal distributions, and therefore must produce the statistically optimal upper limits.

The 95% confidence level upper limits are calculated using Monte Carlo methods. A collection of 3000 toy datasets are generated for each signal model, and the signal strength parameters for the various binning methods are determined by fitting each dataset with the appropriate function or template. In addition to the binned and unbinned methods described above, a cut-and-count method is also employed. This method simply integrates over all events larger than a given minimum $S_T$ value, and determines the signal strength based on the expected signal and background contributions for that selection. The minimum $S_T$ value is optimized separately for each mass point.

Fig. 13 shows the results of calculating the upper limits on signal strength for a series of signal masses. As expected, the cut-and-count method produces the weakest limit, as it essentially ignores shape information in the $S_T$ distribution. Conversely, the unbinned method sets the strongest limit, because it is based on perfect knowledge of the underlying pdfs. The 100 GeV binning closely follows the unbinned method, because it is binned finely enough to closely mimic the unbinned method. The two Bayesian Blocks methods fall between the unbinned and the cut-and-count methods. The hybrid method out-performs the background-only binning method, as it leverages more signal shape information.
FIG. 12: Comparisons of various binning schemes for the purpose of detecting deviations in the tail of a distribution. The figures on the left are background-only distributions. The figures on the right contain background and 8 injected signal events.
FIG. 13: Upper limits on the signal amplitude computed at the 95% CL for binned and unbinned cases.
VI. SUMMARY AND CONCLUSIONS

We have shown that histograms specified with the Bayesian Blocks algorithm have certain advantages over typical histograms in high energy physics. First, the flexible binning allows for a better balance of statistical precision across a spectrum: sparse parts of distributions automatically have larger bins, and dense parts have smaller bins. The binning is statistically optimal in a well-defined sense. Plots comparing two very similar distributions, especially the ratio of two similar distributions, are cleaner and easier to interpret, as illustrated by the plots in Figs. 1 and 2.

The second and more important advantage of histograms formed with Bayesian Block algorithm is their use as non-parametric probability density functions when searching for new physics. We constructed two test cases. The first is modeled after the discovery of the Higgs boson in the $H \rightarrow \gamma \gamma$ channel and the other is modeled after the search for black holes. The statistical power of the Bayesian Block histograms nearly matches that of a traditional unbinned maximum likelihood fit. The advantage of the Bayesian Blocks histograms is that they do not involve any arbitrary choices; they are determined by the minimization of an objective function based essentially on the Poisson distribution. By using histograms constructed with the Bayesian Blocks algorithm, one can sidestep concerns that a particular choice of analytical function leads to a bias, with only a small cost in statistical power.

This paper serves to introduce the Bayesian Blocks algorithm to the high energy physics community. Theoretical background can be found in the references, and applications await further data analysis elsewhere.

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