Bayesian Blocks: Divide and Conquer, MCMC, and Cell Coalescence Approaches

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Abstract. Identification of local structure in intensive data — such as time series, images, and higher dimensional processes — is an important problem in astronomy. Since the data are typically generated by an inhomogeneous Poisson process, an appropriate model is one that partitions the data space into cells, each of which is described by a homogeneous (constant event rate) Poisson process. It is key that the sizes and locations of the cells are determined by the data, and are not predefined or even constrained to be evenly spaced. For one-dimensional time series, the method amounts to Bayesian changepoint detection. Three approaches to solving the multiple changepoint problem are sketched, based on: (1) divide and conquer with single changepoints, (2) maximum posterior for the number of changepoints, and (3) cell coalescence. The last method starts from the Voronoi tessellation of the data, and thus should easily generalize to spaces of higher dimension.

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I INTRODUCTION: THE DATA ANALYSIS PROBLEM

Developments in detector technology for high energy astrophysics\(^2\) have led to observation systems capable of reporting accurate arrival times for individual photons. These times, while not binned, are quantized in microsecond-scale units I like to call “ticks” – since they are in fact generated by the ticking of the computer clock on-board the spacecraft. In the approximation where the ticks are short compared to time scales of interest, we very accurately have a Poisson process. Note that, depending on the nature of the variability of the process, different mathematical models apply, as indicated in the table below.

| Nature of Variability | Mathematical Model Process |
|-----------------------|----------------------------|
| Constant              | Homogeneous Poisson        |
| Deterministic         | Inhomogeneous Poisson      |
| Random                | Doubly Stochastic Poisson  |
|                       | (Cox Process)              |

A number of mathematical references \([20,36,1,2,40]\) describe the nature of spatial Poisson processes. Time series are the \(1D\) special case, consisting of streams of numbers representing photon detection times. In this context, the Poisson distribution is so accurate that it is hardly an approximation. Statisticians seem to have a hard time understanding this point. I believe the culprit is the fact that the Poisson process is usually taught as the limit of a binomial process or the like. Technically, our data do comprise a finite Bernoulli lattice \([40]\), since typically more than one event cannot be recorded at a given tick. (See \([8]\) for an interesting discussion of a lattice theory of quantum fields.) But the rates in units of events\(^3\) per tick are so

\(^2\) The term *high energy astrophysics* is used loosely for both the study of astronomical objects which produce and emit large amounts of energy, and for observations of radiation consisting of high-energy photons, *e.g.* X-rays and gamma-rays. Often the two meanings coincide.

\(^3\) We use the term *event* for photon detections, or other data points.
low that the probability of such multiple events is very low.

In practice, the most significant imperfection is a departure, not from the assumed distribution, but from the assumption of independence of the process at different times. Photon detectors always have a finite dead time — an interval after the detection of one event during which another photon cannot be recorded, either because the detector mechanism itself is temporarily paralyzed, or the data system is too busy processing the event. This yields interdependencies in the detection of photons close together in time.

The discrete nature of photon counting data is most often considered a challenge. Many analysts first bin their data and then apply standard methods. Further, the notion is rife that not only are bins necessary, but that they must be large and contain enough events to produce a “statistically significant sample.” This is wrong and wasteful. Analysis can be carried out directly on the event data. It is my belief that the discreteness and utter simplicity of the fundamental event — a photon was detected or it wasn’t — are a big advantage. This simplicity and the fact that the observational errors accurately follow a distribution with essentially no free parameters mean that the posterior marginalization can be carried out exactly, at least for some of the nuisance parameters [see Eqs. (4) and 5].

Happily, the simplicity of the basic events allows almost immediate generalization of one-dimensional results to data spaces of higher dimension. Simple examples are cases where the photons, in addition to being timed, are also tagged with spectral and spatial information — i.e. energies of photons and their location on the sky. Processes that sample the density of events in spaces of various dimension (denoted $D$) include:

- time series ($D = 1$)
- other sequential data ($D = 1$; e.g., genetic sequences)
- images ($D = 2$)
- time sequences of images ($D = 3$)
- time sequences of spectra ($D = 2$)
- points in parameter spaces (any $D$)

The corresponding data types have in common that they comprise sets of points in some well defined space. Since the underlying process defines the intensity of some physical quantity over the space, we call these intensive data. The actual data can consist of a list of points, or the number of points in pre-selected bins (e.g. image pixels), or other data modes. A problem of broad interest is the detection of local structures in such data. Pulses, or other time-domain structures in time

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4) The Poisson rate parameter is pretty closely nailed at the local event rate.

5) I use the term local to distinguish features of limited extent from global features, such as periodic signals extending over the whole of the data space.
series data, features in images and clusters in parameter spaces of various dimension (classification) are examples.

For one-dimensional time series, the method of *Bayesian Blocks* approximates the signal as a piecewise constant Poisson process [35]. Generalizing this representation to a space, denoted $S$, of arbitrary dimension, the basic problem can be phrased as the following relatively straightforward Bayesian Maximum a posteriori (MAP) problem:

Consider all partitions of $S$ into subvolumes, or *cells*. Model the event rate within each cell as a homogeneous Poisson Process.

**Among all such partitioned models, which is the most likely?**

We determine the parameters in order of how fundamental they are to the nature of the model. The piecewise constant Poisson nature of the model is assumed, so the most fundamental parameter is $N_{cp}$, the number of changepoints. This is determined by marginalizing all of the other parameters – the locations of the changepoints and the Poisson rates between them. Then the locations of the changepoints are determined. Finally, the block event rates are determined; trivially, the MAP value is just the ratio of $N$, the number of events in the cell, to $V$, its volume.

The resulting evidence in favor of this model for a single cell, called the *marginal likelihood*, and defined below in Eq. (4), is a simple function of $V$ and $N$ [below, Eqs. (4) and (5), and also see [35]]. For binned data and other data modes, and for other distributions than the Poisson one assumed here, the likelihood is similarly an explicit function of the same two parameters. We assume the cells are independent, so the total likelihood is the product of the likelihoods of the cells (see Section III).

### II EXACT BAYES FACTORS

For the multiple changepoint problem we need to evaluate the posterior probability for piecewise constant models, given the data. An important simplification is that the marginal likelihoods and posterior probabilities for such models factor into the product of the same quantities for each independent segment of the model. We refer to these segments as *blocks* in 1D contexts, and as *cells* in higher dimensions. This section gives the computation of the posterior for a single cell, which can then be used in various ways – such as the evaluation of Bayes factors for comparison of two or more models. The general form of Bayes factor comparing two models $M_1$ and $M_2$, given data $D$ {c.f. [15], eq. (6.4)} is:

$$
\text{Bayes factor}(M_2; M_1) = \frac{p(D|M_2)}{p(D|M_1)} = \frac{\int p(\lambda_2|M_2)p(D|\lambda_2, M_2)d\lambda_2}{\int p(\lambda_1|M_1)p(D|\lambda_1, M_1)d\lambda_1}
$$

(1)
where \( p(\lambda|M) \) is the prior on \( \lambda \) and \( p(D|\lambda, M) \) is the likelihood. Given the discussion above, it is easy to compute the appropriate factor for a Poisson model with rate parameter \( \lambda \) (units: events per unit volume) for a set of events in some block or cell. The Poisson Likelihood, obtained by multiplying likelihoods for individual sample bins, is

\[
L(N|\lambda, V) = e^{-V\lambda} \lambda^N
\]  

(2)

The usual Poisson factorial does not appear because the number of counts in a tick is 0 or 1. Marginalizing \( \lambda \) using the conjugate Poisson prior (\cite{15}; Section 2.7, p. 49-50)

\[
p(\lambda) = \frac{\beta^\alpha}{\Gamma(\alpha)} e^{-\beta \lambda} \lambda^{\alpha-1},
\]

(3)

the contribution to the Bayes factor for a cell – often called the marginal likelihood – is

\[
P(M|D) = \int_0^\infty p(\lambda)L(N|\lambda, V)d\lambda = \frac{\beta^\alpha}{\Gamma(\alpha)} \frac{\Gamma(N+\alpha)}{(V+\beta)^{N+\alpha}}.
\]

(4)

Based on a prior assigning a uniform distribution to the probability of occurrence of a single event, the marginal likelihood

\[
P(M|D) = \frac{\Gamma(N+1)\Gamma(V-N+1)}{\Gamma(V+2)},
\]

(5)

was derived in \cite{35}. A function of the same two sufficient statistics, \( N \) and \( V \), it behaves similarly to the marginal likelihood in Eq. (4), but was found less accurate in simulation studies such as the one discussed below.

III THREE APPROACHES TO THE MULTIPLE CHANGEPPOINT PROBLEM

We now have to evaluate the above marginal likelihood for each segment of a piecewise homogeneous Poisson model consisting of successive, independent6 blocks of data, and cobble the results together. The next section describes three ways to do this. The first two seem effective in 1D, but have problematical extensions to higher dimensions. The third was inspired by its simplicity in 2D and 3D. All three methods are demonstrated on the same synthetic 1D data.

A An Iterative Approach: Top Down

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6) That is, due to a fundamental property of the Poisson distribution, random variables corresponding to counts in successive blocks (or different cells in general) are independent. This fact should not be confused with independence of the actual Poisson rates, which in general does not hold.
As detailed in [35], the formulas above allow easy computation of the Bayes factor comparing (1) the two-block model in which the interval is segmented into two parts at a changepoint, with (2) a single Poisson model for the whole interval. The decision whether to keep an interval unsegmented or to divide it into two subintervals is based on comparison of the corresponding marginal likelihoods. Let \( \Phi(N,V) \) stand for the marginal likelihood corresponding to a Poisson model for a volume of size \( V \) containing \( N \) events, such as one of the two functions given above. Then an interval should be broken in two if
\[
\Phi(N_i,V_i)\Phi(N_{i+1},V_{i+1}) - \Phi(N,V) > 0 ,
\]
where the putative changepoint divides the interval of size \( V \) into two parts, of size \( V_i \) and \( V_{i+1} = V - V_i \), containing \( N_i \) and \( N_{i+1} = N - N_i \) events, respectively. This criterion is easily computed as a function of the location of the changepoint. The interval is then segmented at the point that maximizes the expression in Eq. (6). This divide and conquer scheme is applied first to the whole data interval, and then iteratively to any subintervals found at the previous step. When this criterion favors segmentation of no further intervals, computation halts.

Figure 1 shows the results for synthetic data generated by a piecewise constant Poisson process, between eleven known changepoints. I used a modified form of the Blocks function popularized by David Donoho, Iain Johnstone, and the WaveLab project [3] as a sample function with many discontinuities that can be detected using wavelet methods (see Fig. 1 in [27]). The original function has blocks of negative amplitude, which will not do as Poisson rates. Hence I added a constant, \( 3 \frac{1}{2} \), to the classic Blocks function, and then generated points obeying the Poisson distribution.

The three panels show three divide and conquer iterations. It can be seen that the various changepoint locations are found rather accurately, albeit with the single changepoint algorithm. In the early steps the posterior has multiple peaks at the various changepoints, but only the highest one is used at each step. There is a tendency for changepoints determined early in the process to be less accurate. These errors are not corrected as the iteration proceeds, but the algorithm could be modified to do so.

### B Maximum Posterior for \( N_{cp} \) via MCMC

It is clear that the above method is not rigorous, in that it does not solve for all of the changepoints simultaneously. It is relatively straightforward, however, to remedy this with a more rigorous, but also more computationally intensive scheme. If there are multiple changepoints, say \( N_{cp} \) in number, the full posterior is just the product of the posteriors of all the subintervals. The marginalization of all the locations of the changepoints requires evaluating the \( N_{cp} \)-dimensional integral\(^7\) of the posterior over all values of the changepoint locations.

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\(^7\) In practice, this is a finite sum, e.g. over a bin index or an event index.
Results obtained in this way, using a simple Markov Chain Monte Carlo (MCMC) method, are surprisingly good. Figure 2 shows the block representation of the same data as in Figure 1, obtained from a simple MCMC evaluation of the marginal likelihood as a function of the number of changepoints. The maximum posterior was at 16 changepoints (17 blocks), compared to the correct value of 11. The “extra” blocks are narrow, and while they do not look pretty, they will not much affect derived quantities (such as pulse widths, rise times, etc).

The good performance with only a few iterations may be due to a combination of several factors:

- the well behaved nature of the data
  - low dynamic range of the signal
  - well behaved backgrounds
  - exact Poisson statistics for the observational uncertainties
- a simple, exact Likelihood; only one parameter
- the fact that the posterior does not have to be computed accurately to distinguish one value of $N_{cp}$ from another
- the useful characteristics of the final model are not that sensitive to $N_{cp}$

Nevertheless, when the number of changepoints and the number of data points are large, the computation is quite long. Since there is little global communication, in the sense that the location of a change point in one part of the observation interval affects that of one elsewhere, breaking the data up into smaller intervals is an effective way to speed up the overall computation.

C Cell Coalescence (Bottom Up)

Based on preliminary tests, a new algorithm may be a significant improvement over either of the above approaches. It begins with a fine-grained segmentation, namely the Voronoi tessellation of the data points, and merges these many cells to form fewer, larger ones. The outline of the algorithm is simple:
Bayesian Cell Coalescence

(0) Initial Segmentation: Voronoi Tessellation of the Events
(1) Compute Bayes Factor for Merging Each Pair of Adjacent Cells
(2) Identify Largest Bayes Factor (at \( i \))
(3) If Largest Bayes Factor is < 1, HALT!
(4) Otherwise Merge Pair of Cells with Largest Bayes Factor:
   - \( N_i \leftarrow N_i + N_{i+1} \)
   - \( V_i \leftarrow V_i + V_{i+1} \)
   - Delete Cell \( i + 1 \)
(5) Go to 1

While there is no rigorous justification for this procedure, one has the sense that it should come reasonably close to obtaining the optimal solution. At each step in the iteration the local event rate in a cell is \( \frac{N}{V} \), the number of events in the cell divided by its volume. The rate estimates for the initial cells, \( \frac{1}{V} \), are reasonable estimates of the fine-grain, local event rate if these cells are assigned roughly their surrounding volume, extending approximately halfway to neighboring points. An obvious choice for the initial partition is thus the Voronoi tessellation \([40,19]\) of the data points. The Voronoi cell for a data point consists of all the space closer to that point than to any other data point.

The Voronoi tessellation of a set of points on an interval (1D) is trivial: it is simply the set of intervals spanned by pairs of midpoints between successive data points. Many algorithms exist for computing Voronoi tessellations in higher dimensions \([21,13,32,11]\), allowing one to address problems such as cluster detection in parameter spaces, and identification of structures in images. Since the marginal posteriors discussed above are valid for piecewise constant Poisson data in any dimension, the methods demonstrated here for 1D should apply in general.

The decision whether to merge two cells or to halt, Step (3), is based on comparison of the Bayes factors. Using the same notation as above, in Eq. (6), cells \( i \) and \( i + 1 \) are merged if

\[
\Phi(N_i + N_{i+1}, V_i + V_{i+1}) - \Phi(N_i, V_i)\Phi(N_{i+1}, V_{i+1}) > 0
\]

and kept separate otherwise. When this criterion favors the merging of no further cells, computation halts.
Figure 3 demonstrates the application of this algorithm to the same synthetic data as in the previous two examples. The top panel depicts the state part way into the iterations, but is not far from the initial Voronoi tessellation, one Voronoi cell for each data point. Successive panels show the evolution of the representation as the cells merge into fewer, larger ones. In the last panel, the halting criterion mentioned above has just terminated the iteration. It can be seen that most of the changepoints are accurately detected. Several though are missed.

IV RELATED WORK

It is well known that Bayesian methods are well-suited to finding changepoints (e.g. [30,34]; see also Appendix C of [16]). In [42] methods similar to those described here are used to find changepoints in binned data, to an accuracy better than the bin size. A number of recent publication are relevant to this problem [37,17,18,42,6,34,38,39,31,7] and [22–29]. More recently, Raftery and colleagues have developed similar methods, mainly for 2D problems. In [5] the Voronoi sites are fiducial markers for the cells, not the tessellation defined by the individual data points. Other approaches are described in [14,4,10,41,33]. Bayesian methods are also useful for segmentation of autoregressive models, with applications to speech processing [9].

After this article was completed, I became aware that NASA’s Chandra X-ray Observatory, is using an unbinned source detection technique much like cell coalescence, and starting from the same Voronoi tessellation [12]. Source cells are merged with a percolation process based on a sample estimate of the density distribution.

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FIGURE 1. Block representations based on the divide and conquer algorithm. The piecewise homogeneous Poisson data were generated from a modification of Donoho's Blocks function. The actual changepoints used to generate the data are shown as vertical lines at the bottom, and the changepoints determined on the first three steps of the iteration are dashed lines.
FIGURE 2. Block representations based on the MCMC algorithm. The piecewise homogeneous Poisson data were generated from a modification of Donoho’s Blocks function. The actual change-points used to generate the data are shown as vertical dashed lines. Spurious, narrow blocks have been emphasized (e.g. the one at about $t = 0.76$).
FIGURE 3. Block representations using the Cell Coalescence algorithm. The top panel shows the overly fine segmentation in the early stages of the iteration. In successive panels the process is converging toward a coarser representation. The bottom panel shows the first stage at which the Bayes factor contraindicates merging of all of the remaining blocks. The actual changepoints used to generate the data are shown as vertical dotted lines.