Bayesian Blocks in Two or More Dimensions: Image Segmentation and Cluster Analysis

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This paper describes an extension, to higher dimensions, of the Bayesian Blocks algorithm for estimating signals in noisy time series data (Scargle 1998, 2000). The mathematical problem is to find the partition of the data space with the maximum posterior probability for a model consisting of a homogeneous Poisson process for each partition element. For model $\mathcal{M}_n$, attributing the data within region $n$ of the data space to a Poisson process...
with a fixed event rate $\lambda_n$, the global posterior is:

$$P(M_n) = \Phi(N,V) = \frac{\Gamma(N + 1)\Gamma(V - N + 1)}{\Gamma(V + 2)} = \frac{N!(V - N)!}{(V + 1)!}. \quad (1)$$

Note that $\lambda_n$ does not appear, since it has been marginalized, using a flat, improper prior. Other priors yield similar formulas. This expression is valid for a data space of any dimension. It depends on only $N$, the number of data points within the region, and $V$, the volume of the region. No information about the actual locations of the points enters this expression.

Suppose two such regions, described by $N_1, V_1$ and $N_2, V_2$, are candidates for being merged into one. From Eq. (1) construct a *Bayes merge factor*, giving the ratio of posteriors for the two regions merged and not merged, respectively:

$$P(\text{Merge}) = \frac{\Phi(N_1 + N_2, V_1 + V_2)}{\Phi(N_1, V_1) \Phi(N_2, V_2)}. \quad (2)$$

Then collect data points into *blocks* with this *cell coalescence algorithm*:

1. Start with the Voronoi tessellation of the data points
2. Identify each Voronoi cell as a block
3. Iteratively merge the pair of blocks with the largest *merge factor*
4. Halt when the maximum merge factor falls below 1

In many applications it is both required and efficient to place the restriction that only blocks touching each other are allowed to merge. This algorithm partitions the data space into a set of blocks, typically much fewer in number than the data points. Each block has a density equal to the number of data points in it divided by its volume. Then, if desired, high-density blocks adjacent to each other can be collected into *clusters*.

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1 Throughout we use the terms *event* and *data point* synonymously. The event is the occurrence of a datum at a given point in the data space.
This method allows detection of clusters in high-dimensional data spaces, with the following properties:

- The number of clusters is determined, not assumed
- Clusters can have any shape:
  - Avoid the conventional Gaussian assumption
  - Shapes can include both concavities and convexities
  - Blocks and clusters do not even have to be simply connected
- The density profiles within clusters are estimated, not just the locations of the cluster boundaries
- Any slowly varying background is automatically identified
- No binning of the raw data is necessary

2. Statistical Challenges of Modern Astronomy

Certainly in astronomy, and in many other ways, this is the Century of Data. Several new observational programs are severely challenging known techniques for acquiring, archiving, reducing, analyzing, and interpreting astronomical data. The methods described here have been inspired by the need for automated extraction of scientific results from large, synoptic data sets that will be produced by projects such as the Sloan Digital Sky Survey, various other cosmological projects, and – closer to home – the exploration of Mars, the Solar System, and planetary systems in the Sun’s neighborhood.

Automated processing already plays a large role in astronomical data analysis, and will clearly become more and more important. What is not generally agreed on is how far along the path to the final scientific output automatic processing can be taken. In my opinion, artificially intelligent processes will soon become surprisingly practical in this setting.
3. The Data: Points, Counts, Measurements

Consider data obtained to estimate some quantity (as opposed to a
discrete attribute). Such measurements are almost always corrupted by
noise, blurring, and other instrumental effects. The observations may be
in a space of one dimension (e.g., time series, energy spectra), in two
dimensions (e.g. images), or in a space of higher dimension (e.g. galaxy
redshift/position catalogs).

Three types of measurement data can be distinguished. The first is point
data, often called event data in 1D. That is, it consists of discrete points
in the data space under consideration. The density of points detected in a
specific region is taken as an estimate of the true density there. Examples
from NASA’s Compton γ-Ray Observatory: time-tagged photon data,
consisting of lists of photon detection times in units of 2 microseconds; and
sky-image data, consisting of lists of photon positions, energies and times.

While the usual coordinate representation of such points uses real
numbers, in practice the corresponding infinite accuracy and resolution is
not achievable. The coordinate is usually quantized in some unit, small
compared to the total range of observation. In high energy (x- and γ-ray)
time series data, for example, the points are the times of detection of
individual photons; the corresponding quantum is the resolution of the
spacecraft clock, typically in the range of microseconds to milliseconds.

In the second data type the entire observation interval (or area, or
volume) is partitioned into pre-specified bins (or pixels, or cells) and the
number of events in each is recorded. Event data can be converted to this
mode, but in doing so one discards information, reduces the resolution of
the data, and makes the results dependent on the sizes and locations of the
bins. Hence this mode should be used only if event data are not available.

A third type of sequential data is the measurement of some quantity, at
a set of times or points in space. This measurement need not be an event
count, but can be any measurement operation that yields a real number. An
important difference from the event-counting mode arises in the statistical
distribution of the observational errors: counts in bins typically obey a Poisson distribution, whereas here the errors may have any distribution, often assumed normal (Gaussian).

4. The Model: Segmentation Yields Structure

In any analysis involving likelihoods, a key step is the choice of a model representing two separate aspects of the data: the underlying process, or true signal; and the noise process corrupting the observations, thus hiding the true signal. Precisely, we must compute the probability, or likelihood, that the observed data would be obtained, given the model and its parameters. Although we are studying the underlying signal, the likelihood depends also on the data mode, the sampling process, and the nature of the noise and other corruption processes.

Data consisting of independent points are efficiently described by a very simple model, the Poisson process. In such a process the probability that an event will occur in a small element of the data space is just a coefficient times the volume of that element. This coefficient is called the local event rate or Poisson parameter. It need not be constant, but can vary in an arbitrary way over the data space. If this variation is random – a Cox or doubly-stochastic process – it is important to distinguish the two random processes. One describes the occurrence events at a given location, the other how the event rate varies with location. If, as usually assumed, these two processes are independent of each other, even if the event rates at different locations are strongly correlated, the occurrence of events at these locations are independent of each other (i.e., the joint probability is the product of the individual probabilities).

The assumed independence of the data means that the occurrence of one event does not affect the probability of any other event. Hence, a probability referring to separate subsets of the data space is the product of the probabilities of the subsets. A common example of failure of this property – i.e. dependence – is “dead time” in time series data: each photon
is followed by an interval in which the occurrence of a second photon is inhibited.

In general, the Poisson model is surprisingly appropriate for astronomical processes. The model seems extremely specialized but is in fact remarkably general and serves for almost all applications. All we have assumed is that the events are independent, and the local event rate is specified by an arbitrary density function. The main limitation, need for independence of the events, can be relaxed by simply incorporating the dependences into the likelihood function.

The model must specify the Poisson rate as a function of location within the space, either parametrically or nonparametrically. Here we assume one does not have a detailed signal model, indicating nonparametric methods. In particular, consider *piecewise constant representations* of the signal. This very convenient class of model has the following properties

- nonparametric: the number of parameters depends on the number of data points
- general: capable of representing any reasonable signal
- simple: underlying rate is constant on finite intervals
- useful: any physically significant signal property can be computed
  - pulse widths, rise times, decay times, amplitudes
  - background level
- easy to compute: Bayesian changepoint detection is very effective
- easily extended to two dimensional and higher data spaces

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2Rissanen (1989) discusses this seemingly paradoxical definition. Examples are polynomials, Fourier series, and wavelet expansions. The idea is that one is representing the structure generically, in terms of basis functions, the number of which depends on how much information is present – rather than fitting a predefined shape to the data.
• related to classification, cluster detection, and density estimation
• data adaptive, \( i.e. \) responds to local irregularities

One can think of this representation as a density estimator in which blocks take on the role of bins. The sizes and locations of the bins are not fixed, but are determined by the data. The idea is as follows. We partition the data space into subsets, or blocks. The data points within each block are taken to be independent and to obey a Poisson distribution with a constant rate parameter. Different blocks have different event rates. In short, we construct a piecewise constant ("blocky") signal approximation.

Our aim is to detect and characterize all of the signal structure supported by the data \( i.e. \) the statistically significant variations. How best to do this depends on the ultimate purpose of the analysis. Frequently one is interested, not in the true signal shape itself, but in quantities describing local structures \( e.g. \) pulse widths, amplitudes, \( etc. \). Since there are very convenient ways to estimate such parameters directly from blocks, our seemingly crude representation may be perfectly adequate. For such purposes there is no motivation to impose smoothness, although such cosmetic properties are important for visualization of model-data relationships.

Note that we don’t assert that the true event rate changes in a blocky, discontinuous way. The physical signal is presumably continuous, and we represent it as piecewise constant in the spirit of a step-function approximation of a smooth curve \( i.e. \) and not with any hope that this representation is exact in the limit of small steps (\( cf. \) wavelet theory, and see especially the innovative ideas in Donoho 1994a,b). In the interests of accuracy, one might consider models of higher complexity, such as a piecewise linear representation; however, imposing continuity limits the number of free parameters (to be about the same as for piecewise constant models), so the added accuracy is somewhat illusory.

See (Stoyan, Kendall and Mecke 1995) for an excellent discussion of point processes in general, Poisson point processes in particular, and a number of ways that real world data can depart from being Poisson.
5. Algorithms in One Dimension

We begin by considering the one dimensional case (Scargle 1998, 2000). Time series data are usually considered to consist of a signal, the character of which is under investigation, corrupted by observational noise. In this setting, segmentation of the data space into subsets where the signal is taken as constant is a very practical representation for many signals. The very different problem of searching for periodic signals will not be discussed here (see Bretthorst 1988, more recent publications on his web site, and my other contribution to this volume).

Three algorithms for implementing this approach to modeling time series have been described elsewhere (Scargle 1998, 2000), so I omit details. Broadly, the approaches are:

- **Divide and Conquer**: use model comparison to decide whether the interval should be subdivided; apply iteratively to sub-intervals
- **Cell Coalescence**: start from an ultra-fine representation assigning one block to each datum; merge pairs of blocks based on model comparison
- **Markov Chain Monte Carlo**: search the block parameter space, computing the posterior (with all block edge locations and Poisson rate parameters marginalized) as a function of the number of blocks

The first two, *top-down* and *bottom-up*, are greedy algorithms, iterated until the answer to the question “subdivide?” or “merge?” is always “no.” MCMC convergence is more subtle.

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3 A point of occasional confusion is that noise in astronomy and physics has two quite distinct meanings: random observational errors, and random variability intrinsic to the source or physical system. The latter, part of the signal, is often just what one is studying, whereas the observational noise is a corruption, to be eliminated as much as possible.

4 *Greedy algorithms* implement myopic optimization with a “take what you can now, no regard for the future” strategy. On termination of the algorithm the resulting local optimum may be a good approximate solution, but is not guaranteed to be the global optimum.
I have been developing the Cell Coalescence method for astronomical applications, primarily due to its easy generalization to higher dimensions, as we shall now discuss.

6. Structure in Higher Dimensions

This section describes an iterative algorithm for structure analysis based on Bayesian methods. The problem of estimating structure in higher dimensional data spaces is closely related to regression, density estimation (Scott 1992), cluster analysis (Backer 1995), data classification (Gordon 1999), projection pursuit (Friedman and Tukey 1974), etc., depending on the exact nature of the data and the goals of the analysis. Common to all of these approaches is the same situation we have just discussed: the data reflect an underlying signal subject to noise and possibly other corruptions; the signal and the specific noise contributions are unknown, but a statistical model of the noise is known or assumed. The goal is to recover as much information as possible about the signal, making good use of any prior information about the signal and the noise.

Bayesian methods are quite powerful in this arena, due to the natural way prior information and nuisance parameters are handled. In particular, Bayesian methods provide good solutions to problems which apparently plague cluster analysis and related fields (Kaufman and Rousseeuw 1990, Backer 1995, Day 1990): a bewildering variety of ad hoc methods, loss of information in the analysis, and assessing post facto validity of clusters.

6.1. Voronoi Cells

The algorithm I am developing for 2D problems uses the same posterior as in Equations (1)-(2), since their derivations apply to Poisson models for point data in any dimension. However, geometrical considerations for partitioning the data space are considerably harder in 2D. Generalizing the concept of intervals is not very productive, due to the great freedom
one has in the choice for block shapes: ... squares? rectangles? circles? other? What is productive is to follow the cell coalescence idea (above, \S5) and construct small, elementary blocks from which larger blocks can be composed: assemble the macroscopic out of the microscopic.

In the 1D case, the intervals spanned by the midpoints between successive pairs of adjacent data points are the obvious choice for the cells. The mid-point based construction has the following properties:

(1) Cell $i$ contains all points closer to datum $i$ than to any other datum
(2) Forms a partition: Every point in the space lies in one and only one cell
(3) Attached to each cell is a number, $A_i$, namely its area
(4) $\frac{1}{A_i}$ is a measure of the density of data points in the vicinity of datum $i$

Item (1), a constructive definition valid in any dimension, is the space’s Voronoi tessellation (e.g., Stoyan, Kendall and Mecke 1995) determined by the data points. This definition implies (2), i.e. Voronoi cells partition the space. Where points are close together the cell areas are small, and vice versa. Specifically, the reciprocal of the cell area is a convenient measure of local point density. How useful this representation is! With almost no work we already have a detailed, if choppy, density estimation.

Now three definitions. A cell is one of the Voronoi cells, which are in a one-to-one correspondence with the data points. During the iteration we insure that these cells maintain their identity, so there is no problem thinking of cells and data points interchangeably.

A block is a set of one or more merged cells, including both the initial one-cell blocks and the multi-cell blocks that form during the iteration. It is common to restrict mergers to, e.g., only blocks that are touching\footnote{That two blocks are touching can be readily determined by finding a Voronoi cell in one block that has a vertex in common with at least one cell in the other block. The MatLab (© the Math Works, Inc.) routine computing Voronoi tessellations in arbitrary dimensions returns vertex information in a form very convenient for all such computations.}; hence
blocks consist of adjacent cells.

One last definition: At the end of the iteration, we may find that some sets of adjacent blocks stand out from the general background, say by having event rates substantially above background. We call such groups clusters. In the case of galaxies, this corresponds precisely to the notion of galaxy clusters. In the case of photons, this corresponds to the notion of a source. Note that we are interested in density profiles within clusters; for the most part traditional classification and cluster analysis identifies boundaries only.

6.2. The Algorithm: Cell Coalescence

We are now ready to outline the algorithm. The idea is simple: find the partition with the largest total posterior probability

\[ P_{\text{total}} \equiv \prod_{n=1}^{N} \Phi(N_n, V_n), \]

obtained from Eq. (1) applied to each element of the partition, and using the product rule since the elements are assumed independent. In principle we want to maximize this posterior over the set

\[ S_\infty \equiv \{ \mathcal{P} \mid D \text{ is partitioned by } \mathcal{P} \} \]

where \( D \) is the entire data space. This task would be awkwardly complicated and impractically large, so instead we restrict attention to the set

\[ S_0 \equiv \{ \mathcal{P} \mid D \text{ is partitioned by } \mathcal{P} \text{ into blocks of Voronoi cells} \}. \]

There are many ways in which these two sets are different – \((\mathbb{I})\) is highly infinite, \((\mathbb{F})\) is quite finite. But for representing the structural information content of the data points \( S_\infty \) and \( S_0 \) are effectively the same. This is sometimes expressed by saying that the Voronoi tessellation contains all the proximity information in the data, a well known fact in the computer graphics industry.

I have coded and experimented with a very simple search through \( S_0 \), namely a greedy iteration that at each step merges the pair of blocks with the largest value of the merge posterior in Eq. (2):
(0) Initialize: one block (≡ a Voronoi cell) per data point
(1) Compute change in $P(\varphi)$ for merging each pair of adjacent blocks
(2) If largest change is positive, merge that pair and Go To (1)
(3) Else (no pair should be merged) stop.

This greedy algorithm can be criticized because it is not guaranteed to yield the global maximum. To assess this problem, I am exploring alternative procedures which explore more of the parameter space – including randomized algorithms (Motwani and Raghavan 1995), algorithms using more general transformations than just block merges, and combinatorial optimization methods based on dynamic programming (Hubert, Arabie, and Meulman 2001).

6.3. Adopting a Model

There are several ways to determine the model to be adopted. Most simply one can use the model in place when the stopping criterion is triggered. Or, one can select the largest $P(\varphi)$ from the history of the iteration. If the transformations are such that $P(\varphi)$ is monotonically non-decreasing, these two are obviously the same. An alternative is to average all of the models, weighting each one according to its posterior probability – model averaging (see Hoeting, Madigan, Raftery, and Volinsky 1999, and for some software http://www.research.att.com/~volinsky/bma.html). This approach has the advantage of producing a model that is more in accord with the maximum a posteriori (MAP) principle, but the disadvantage that the averaged model is not in the initially defined space of models – namely, piecewise constant Poissonian blocks. Depending on what information one wants from the models, this disadvantage may or may not be important.

$^6$To merge cells $n$ and $m$ simply change cell $n$ according to $N_n = N_n + N_m, V_n = V_n + V_m$ and delete cell $m$. 

6.4. Related Work

Various authors (Ebeling and Wiedenmann 1993, Scargle 2000, Ramella, Boschin, Fadda and Nonino 2001) have considered algorithms that start from the Voronoi tessellation and iteratively merge the Voronoi cells into blocks based on some kind of statistical criterion. Essentially the same problem has been discussed in the literature of automatic data classification (Gordon 1999, Backer 1995), where the concept of merging cells is replaced by a more generalized set of allowed transformations of the partition.

Our ultimate goal is the same as that of classification, the “detection of important relationships and structure within data” (Gordon 1999, §1.2) by finding “a partition in which objects are similar to the other objects belonging to their class and dissimilar to objects belonging to different classes” (Gordon 1999, §3.1). However, we generalize the concept of similarity (most often taken to be simply closeness of the points) to mean that the distributions of the observed points are adequately described by an appropriate statistical model. Other classification criteria, such as homogeneity, lack of heterogeneity, or isolation or separation from the rest of the data, can be subsumed into this more general concept.

7. Information Theoretic Inference

Several foundational issues are pertinent to the above analysis, beginning with the Bayesian definition of probability as a measure of the degree of one’s belief in the truth of the hypothesis (Jaynes 1997). It would be hard to identify two words more fraught with philosophical difficulties than belief and truth.

Science never achieves absolute truth of any hypothesis. Instead it seeks to establish approximate but useful descriptions, models, predictions of future events and measurements, and so on. Belief – by others or of one’s own – is hard to define operationally. The pragmatic point here is that we believe that our model is not true. A discontinuous model can not be a
true representation of a continuous signal. The prior for our model is zero. This leads directly to oblivion. There are ways to deal with this problem within the Bayesian framework, but uneasiness about this point remains.

The vexing concept of the noninformative prior is particularly relevant for the construction of general purpose, turn-key algorithms. Although it is possible to fashion algorithms so that one can plug in the prior that expresses one’s knowledge in any given situation, it is still legitimate to seek an algorithm that makes no prior assumptions, perhaps at the price of some loss of sensitivity, efficiency, or the like.

There are other aspects of the Bayesian data analysis formalism that are muddled by the belief-in-truth interpretation. The founders of Bayesian data analysis made a great step forward in recognizing that deductive logic is inappropriate to scientific thought and research. However, in substituting inductive logic they missed that the problem is not just the kind of logic, but that logic itself is inappropriate to the practice of scientific data analysis.

The notion that science deals with information about the Universe, more than with truths about it, leads to a data analysis approach that substitutes information theoretic quantities for the subjective Bayesian probabilities. In particular information contained in data and models replaces the usual notion of belief in the truth of hypotheses. The resulting framework avoids difficulties associated with noninformative priors, and I believe is more in tune with how data analysis actually proceeds – uncovering and processing information about the Universe.

We use models to extract from data information about the world. There is no learning of absolute truths about the world. We proceed by comparing model predictions with observed data. Evaluating the joint information contained in model and data is a straightforward application of information theory. Elsewhere in this volume, related information theoretic ideas are discussed in the papers “Inductive Logic” by Kevin Knuth, and “Information Theoretic Approach to Bayesian Inference” by Jeffrey Jewell.

We equate two expressions for data-model information – following the
standard derivation of Bayes Theorem by equating two expressions for the joint data-model probability. Start by defining the *mutual information* of two random variables as the relative entropy between their actual joint distribution and what the joint distribution would have been if the variables were independent – *i.e.* the product of the individual distributions:

**Definition: Mutual Information**

Given random variables $X$ and $Y$, with probability distributions $p(x)$ and $p(y)$, and joint probability distribution $p(x, y)$, the mutual information of $X$ and $Y$ is

$$I(X; Y) = \sum_x \sum_y p(x, y) \log \frac{p(x, y)}{p(x)p(y)}$$

that is, the expectation of $\log \frac{p(x, y)}{p(x)p(y)}$ with respect to the full joint distribution $p(x, y)$. The sums in $x$ and $y$ are over the appropriate discrete event spaces, and become integrals for continuous variables.

Cover and Thomas (1991) prove that

$$I(X; Y) = H(X) - H(X|Y)$$

where $H(X)$ is the unconditional entropy of $X$, and $H(X|Y)$ is the entropy of $X$ conditional on $Y$. Noting that $I(X; Y) = I(Y; X)$, using the more mnemonic variable names $D$ for data and $M$ for model, and replacing entropy, $H$, with the negative of information, $-I$, we have

$$I(M|D) = I(D|M) + I(M) - I(D)$$

rather like Bayes Theorem with the identification $I \leftrightarrow \log(P)$. I am experimenting with inference procedures for cluster analysis based on this relationship.

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