Data analysis recipes:
Choosing the binning for a histogram[1]

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Abstract

Data points are placed in bins when a histogram is created, but there is always a decision to be made about the number or width of the bins. This decision is often made arbitrarily or subjectively, but it need not be. A jackknife or leave-one-out cross-validation likelihood is defined and employed as a scalar objective function for optimization of the locations and widths of the bins. The objective is justified as being related to the histogram's usefulness for predicting future data. The method works for data or histograms of any dimensionality.

1 Introduction

There are many situations in experimental science in which one is presented with a collection of discrete measurements $\mathbf{x}_j$ and one must bin those points into a set of finite-sized bins i, with centers $\mathbf{X}_i$ and full-widths $\mathbf{\Delta}_i$, to create a histogram of numbers of points N_i, or the equivalent when the points have non-uniform weights w_j. The problem of binning comes up, for example, when one needs to plot a data histogram, when one needs to perform least-square fitting of a probability distribution function, and when one wants to compute entropies or other measurements on the inferred data probability distribution function.

The choice of bin centers and widths often seems arbitrary. However, there is a non-arbitrary choice, derived below, which emerges when the histogram is thought of as an estimate of the probability distribution function of whatever process generated the data. If the binning is too coarse, the histogram does not give much information about the shape of the probability distribution function. If the binning is too fine, bins become empty and the

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histogram becomes noisy, so it in some sense "overfits" the data. The best binning lies in between these extremes and can be found simply and quickly by a "jackknife" or cross-validation method, that is, by excluding data sub-samples and using the non-excluded data to predict the excluded data. This is not the only data-based binning-choice approach[2], but it is simple and sensible.

In what follows, we are going to consider a data histogram, which we imagine as a set of bins i, with centers $\mathbf{X}_i$ and widths (or multi-dimensional volumes) $\mathbf{\Delta}_i$. Equivalently (and perhaps more usefully), the parameterization of the bins can be described by a set of edges $\mathbf{X}_{(i-1/2)}$ so the centers become $\mathbf{X}_i = \left(\mathbf{X}_{(i-1/2)} + \mathbf{X}_{(i+1/2)}\right)/2$ and the widths become $\mathbf{\Delta}_i = \left|\mathbf{X}_{(i+1/2)} - \mathbf{X}_{(i-1/2)}\right|$. These bins will get filled by a set of (possibly multi-dimensional) data points $\mathbf{x}_j$, leading to each bin i containing a number of data points N_i. We will also make reference to the binning function $i(\mathbf{x})$ which, for a given data value $\mathbf{x}$, returns the bin i.

2 Model probability distribution function

Our best binning is based on the idea that the histogram is a sampling of a probability distribution function and can therefore be thought of as providing an estimate or model of that probability distribution function.

One possible (approximate) probabilistic model for the data is that they are drawn from a probability distribution function such that, in each bin of the histogram we are making, the probability is constant and proportional to the number of actual data points that landed (by chance) in that bin. This model has the limitation that bins that happen (by chance) to be empty will be assigned zero probability; when a new datum happens to arrive (by chance) inside one of those previously empty bins, it will be assigned a vanishing likelihood and render the probabilistic model false at (arbitrarily) high confidence.

A more well-behaved (approximate) probabilistic model is that the prob-

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[2]see, for example, Knuth, K. H., "Optimal data-based binning for histograms," arXiv:physics/0605197, and references cited therein.

ability $p(i)$ that a data point land in bin i is

$$p(i) = \frac{N_i + \alpha}{\sum_k [N_k + \alpha]} \quad , \tag{1}$$

where α is a dimensionless "smoothing" constant of order unity (to be set later). Here, so long as there are a finite number of bins, the probability is non-zero in every bin. The associated (approximate, model) probability distribution function is

$$\tilde{f}(\mathbf{x}) = \frac{p(i(\mathbf{x}))}{\boldsymbol{\Delta}_{i(\mathbf{x})}} \quad , \tag{2}$$

where $i(\mathbf{x})$ is the function that returns the bin i for any value $\mathbf{x}$. Note that the function $\tilde{f}(\mathbf{x})$ is normalized by construction;

$$\int \tilde{f}(\mathbf{x}) \, d\mathbf{x} = 1 \quad . \tag{3}$$

In general, the data points will not all be treated equally, but in fact each data point $\mathbf{x}_j$ will come with a weight w_j, and each bin i will contain total weight W_i. The only change this makes is in the inferred probability $p(i)$, which becomes

$$p(i) = \frac{W_i + \alpha}{\sum_k [W_k + \alpha]} \quad , \tag{4}$$

where now the smoothing constant α will be of order the mean weight w_j.

3 Jackknife likelihood

Imagine now that a new datum is recorded and happens to fall in bin i. The (logarithmic) likelihood of this new datum (according to the approximate model) is just $\ln \tilde{f}(\mathbf{x})$. If the binning is extremely fine ($\boldsymbol{\Delta}_i$ small), then most bins will be empty and assigned identical probabilities. If the binning is extremely coarse ($\boldsymbol{\Delta}_i$ large), then although most bins will have high probabilities, they will not have large values of $\tilde{f}(\mathbf{x})$ because they will have large widths. In either case, the predictive power of the model probability distribution function $\tilde{f}(\mathbf{x})$ is low. For most well-behaved continuous (true) probability distribution functions, there is a finite binning at which the likelihoods of new data are maximized.

With a finite data set, a "jackknife" or leave-one-out cross-validation likelihood L can be defined to be the total weighted (logarithmic) likelihood of each data point $\mathbf{x}_j$ as computed from the model probability distribution function $\tilde{f}(\mathbf{x})$ computed from all the data points *other than* point j.

$$L = \sum_j w_j \, \ln \left(\frac{W_{i(\mathbf{x}_j)} + \alpha - w_j}{\mathbf{\Delta}_{i(\mathbf{x}_j)} \left[\sum_k [W_k + \alpha] - w_j \right]} \right) \quad , \tag{5}$$

where, again, $i(\mathbf{x}_j)$ is the function that returns the bin i containing the data point $\mathbf{x}_j$.

In the simple case of no weighting (or, equivalently, $w_i = 1$ for all i), this jackknife likelihood can be written as

$$L = \sum_i N_i \, \ln \left(\frac{N_i + \alpha - 1}{\mathbf{\Delta}_i \left[\sum_k [N_k + \alpha] - 1 \right]} \right) \quad , \tag{6}$$

where the sum over data points has been converted into a sum over bins, because the latter is generally far faster.

The "best" binning parameters $\mathbf{X}_i$, $\mathbf{\Delta}_i$ and α are those that maximize the jackknife likelihood L. This defines a non-arbitrary choice of binning. The choice is also motivated; it is the choice that best predicts future data, under the assumption that the existing data are representative.

4   Examples

As a simple test, consider equal-width (all Δ_i equal) binnings of a set of (one-dimensional) measurements x_j (galaxy colors in this case), in a fixed range $x_{\min} < x < x_{\max}$. In this simple situation, the binning only has two parameters: the number N of bins (which, given the color range, fixes the bin positions $\mathbf{X}_i$ and common widths $\mathbf{\Delta}_i \equiv \mathbf{\Delta}$) and the smoothing α. The binning function $i(x)$ is then simply

$$i(x) = \text{floor} \left(\frac{x - x_{\min}}{\Delta} - \delta \right) \quad , \tag{7}$$

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where

$$\Delta \equiv \frac{x_{\max} - x_{\min}}{N} \quad . \tag{8}$$

Figure 1 shows the results of a grid search in this parameter space for the optimum binning for the $^{0.1}[g - r]$ colors of a large number of galaxies, and the same for a smaller subsample.

There is nothing special (except simplicity) about the one-dimensional case. Figure 2 shows the results of a grid search for the optimal two-dimensional equal-width binning for two quantities (the $^{0.1}[g - r]$ colors and Sérsic indices n of the same set of galaxies). In the two-dimensional case, the optimal binning is coarser (because the space is "bigger").

5   Discussion

I have shown that when a histogram of data needs to be made, there *is* a non-arbitrary choice of binning. Some qualitative observations follow.

- The optimal bin widths get smaller as the number of data points goes up or as the features in the (true) probability distribution function get narrower.

- The results are more sensitive to the smoothing parameter α when the number of empty or near-empty bins becomes significant.

- The jackknife likelihood makes discontinuous jumps as the bin edges cross individual data points. For this reason, the likelihood does not have well-defined derivatives. Some care must be taken that the optimization technique does not depend on having a differentiable likelihood function.

- There is nothing special about one-dimensional or two-dimensional distribution functions; this is easily generalized to n-dimensional distributions. However, it takes a lot of data points to measure a distribution function in n dimensions when n is large; I understand that the required number of data points scales worse than e^n [need ref].

- There is nothing special about equal-width binning; I simply chose this to make the optimization problem easily tractable and the results easily presentable.

- This method makes no reference to the *errors* or *uncertainties* on the measurements $\mathbf{x}_j$. Effectively, I have assumed that the errors are small relative to any real features in the probability distribution function. In practice, it is rarely useful to have more than a few bins per the width of your error distribution, if all the points have similar uncertainties.

- There is often an additional choice about what minimum and maximum data values to allow for histogramming. This choice also ought to be made in a non-arbitrary fashion if there are data points that will be excluded by the choice.

- Finally, there is nothing special about the "tophat" binning model used in the above examples. Everything can be generalized to smoothly overlapping bins, in which points are assigned fractionally to multiple bins. In general, smoother binning models make for more well-behaved derivatives of the jackknife likelihood and therefore more straightforward optimization. This can also all be generalized to kernel-smoothing techniques for density estimation, which ought to be made the subject of a separate note.
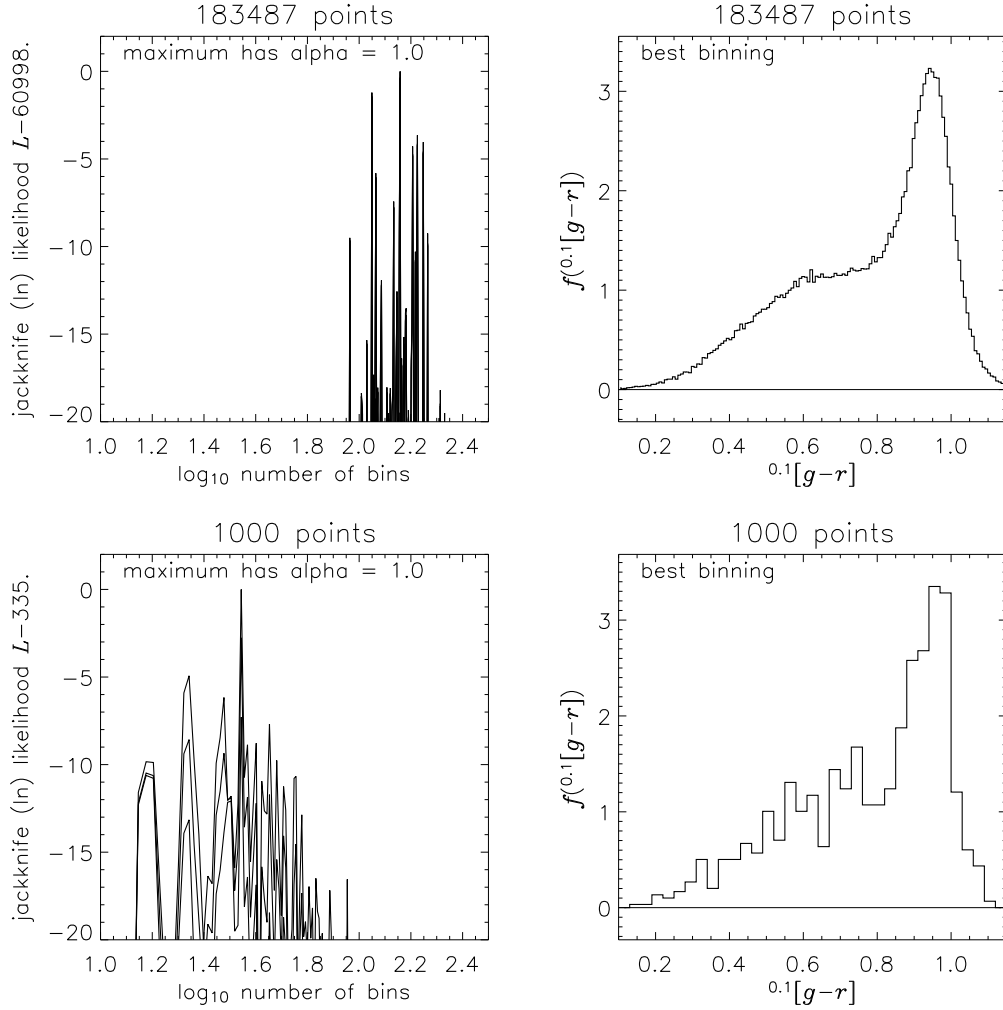
Figure 1: Constant-width binning of a set of measured galaxy colors. The top-left panel shows grid searches in binsize for the eight possible combinations of smoothing $\alpha = (10, 1, 0.1, 0.01)$ and binning phase $\delta = (0, 0.5)$ (see text for definitions). The top-right panel shows the data binned with the maximum-likelihood binning parameters. The bottom panels show the same, but for a randomly chosen subsample.
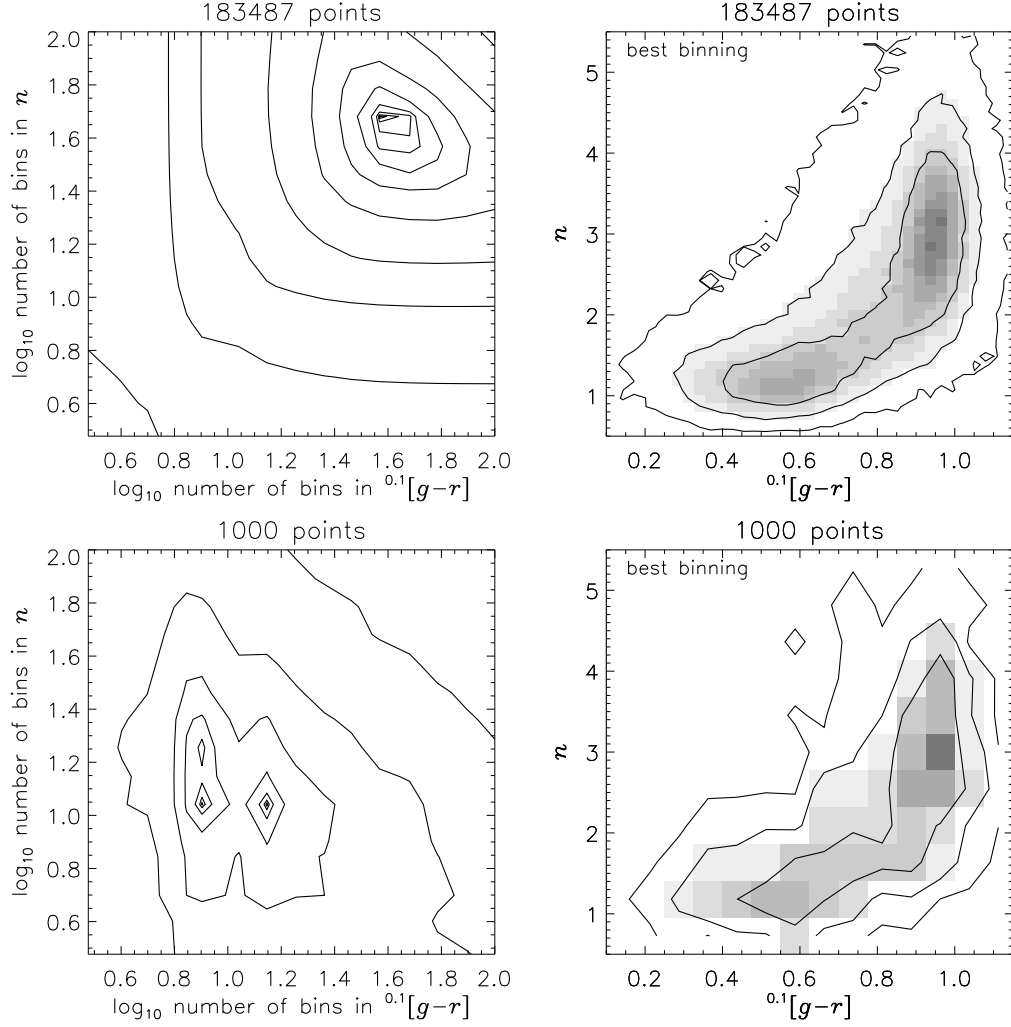
Figure 2: Two-dimensional constant-width binning of a set of measured galaxy colors and radial profile shapes (as parameterized by the Sérsic index n). The top-left panel shows a grid search in the two binsizes, with smoothing fixed at $\alpha = 1.0$ and both phases fixed at $\delta = 0$. The top-right panel shows the data binned with the maximum-likelihood binning parameters, plus contours at 2, 10, 25, 50, and 75 percent of the maximum value. The bottom panels show the same, but for a randomly chosen subsample.