Cascaded High Dimensional Histograms: A Generative Approach to Density Estimation

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Abstract

We present tree- and list- structured density estimation methods for high dimensional binary/categorical data. Our density estimation models are high dimensional analogies to variable bin width histograms. In each leaf of the tree (or list), the density is constant, similar to the flat density within the bin of a histogram. Histograms, however, cannot easily be visualized in higher dimensions, whereas our models can. The accuracy of histograms fades as dimensions increase, whereas our models have priors that help with generalization. Our models are sparse, unlike high-dimensional histograms. We present three generative models, where the first one allows the user to specify the number of desired leaves in the tree within a Bayesian prior. The second model allows the user to specify the desired number of branches within the prior. The third model returns lists (rather than trees) and allows the user to specify the desired number of rules and the length of rules within the prior. Our results indicate that the new approaches yield a better balance between sparsity and accuracy of density estimates than other methods for this task.

Keywords: Density Estimation, Decision Trees, Histogram, Interpretable Modeling.

1. Introduction

A histogram is a piecewise constant density estimation model. There are good reasons that the histogram is among the first techniques taught to any student dealing with data (Chakrabarti et al., 2006): (i) histograms are easy to visualize, (ii) they are accurate as long as there are enough data in each bin, and (iii) they have a logical structure that most people find interpretable. A downside of the conventional histogram is that all of these properties fail in high dimensions, particularly for binary or categorical data. One cannot easily visualize a conventional high dimensional histogram. For binary data this would require us to visualize a high dimensional hypercube. In terms of accuracy, there may not be enough data in each bin, so the estimates would cease to be accurate. In terms of interpretability, for a high dimensional histogram, a large set of logical conditions ceases to be an interpretable representation of the data, and can easily obscure important relationships between variables. Considering marginals is often useless for binary variables, since there are only two bins (0 and 1). The question is how to construct a piecewise constant

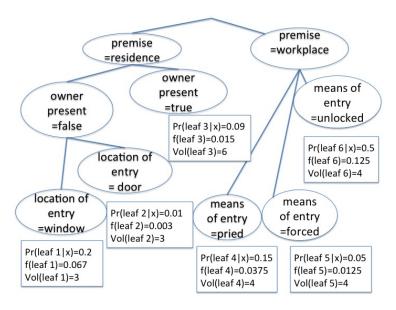


Figure 1: A sparse tree to represent the grain data set. Probability of belonging to the leaf, the densities (f) and volume (Vol) are specified in the sparse tree.

density estimation model (like a histogram) that has the three properties mentioned above: (i) it can be visualized, (ii) it is accurate, (iii) it is interpretable.

In this paper we present three cascaded (tree- or list- structured) density estimation models. These are similar to variable bin-width histograms, (e.g., see Wand (1997); Scott (1979)), though our approaches use only a subset of the variables. A leaf (that is, a histogram bin) is defined by conditions on a subset of variables (e.g. "the second component of x is 0" and "the first component of x is 1"), and the density is estimated to be constant with each leaf.

Let us give an example to illustrate how each bin is modeled to be of constant density. Let us say we are modeling the population of burglaries (housebreaks) in a city. We might want to create a density model to understand how common or unusual the particular details of a crime might be (e.g., do we see crimes like this every month, or is this relatively uncommon?). A leaf (histogram bin) in our model might be the following: if premise is residence, $owner\ present$ is false, $location\ of\ entry$ is window, then p(state) is 0.20. This means that the total density in the bin where these conditions hold is 0.20, that is, for 20% of burglaries, the three conditions are met. Let us say we have an additional variable $means\ of\ entry$ with outcomes pried, forced, and unlocked, indicating how the criminal entered the premise. Each of these outcomes would be equally probably in the leaf, each with probability 0.20/3=.067. We described just one bin above, whereas a full tree could be that of Figure 1.

Bayesian priors control the shape of the tree. This helps with both generalization and interpretability. For the first method, the prior parameter controls the number of leaves. For the second method, the prior controls the desired number of branches for nodes of the tree. For the third method, which creates lists (one-sided trees), the prior controls the desired number of leaves and also the length of the leaf descriptions.

This generative structure aims to fix the three issues with conventional histograms: (i) visualization: we need only write down the conditions we used in the tree- or list-shaped cascade to visualize the model. (ii) accuracy: the prior encourages the cascade to be smaller, which means the bins are larger, and generalize better. (iii) interpretability: the prior encourages sparsity, and encourages the cascade to obey a user-defined notion of interpretability.

Density estimation is a classic topic in statistics and machine learning. Without using domain-specific generative assumptions, the most useful techniques have been nonparametric, mainly variants of kernel density estimation (KDE) (Akaike, 1954; Rosenblatt et al.. 1956; Parzen, 1962; Cacoullos, 1966; Mahapatruni and Gray, 2011; Nadaraya, 1970; Rejtö and Révész, 1973; Wasserman, 2006; Silverman, 1986; Devroye, 1991). KDE is highly tunable, not domain dependent, and can generalize well, but does not have the interpretable logical structure of histograms. Similar alternatives include mixtures of Gaussians (Li and Barron, 1999; Zhuang et al., 1996; Ormoneit and Tresp, 1995, 1998; Chen et al., 2006; Seidl et al., 2009), forest density estimation (Liu et al., 2011), RODEO (Liu et al., 2007) and other nonparametric Bayesian methods (Müller and Quintana, 2004) which have been proposed for general purpose (not interpretable per se) density estimation. (Jebara, 2012) provides a Bayesian treatment of latent directed graph structure for non-iid data, but does not focus on sparsity. Pólya trees are generated probabilistically for real valued features and could be used as priors (Wong and Ma, 2010). The most similar paper to ours is on density estimation trees (DET) (Ram and Gray, 2011). DETs are constructed in a top-down greedy way. This gives them a disadvantage in optimization, often leading to lower quality trees. They also do not have a generative interpretation, and their parameters do not have a physical meaning in terms of the shape of the trees (unlike the methods defined in this work).

2. Models

For all the three models, we will need the following notation. There are p features. We express the path to a leaf as the set of conditions on each feature along the path. For instance, for a particular leaf (leaf t in Figure 2), we might see conditions that require the first feature $x_{.1} \in \{4, 5, 6\}$ and the second feature $x_{.2} \in \{100, 101\}$. Thus the leaf is defined by the set of all outcomes that obey these conditions, that is, the leaf could be

$$x \in \{x_{.1} \in \{4, 5, 6\}, x_{.2} \in \{100, 101\}, x_{3.}, x_{.4}, \dots, x_{.p} \text{ are any allowed values}\}.$$

This implies there is no restriction on $x_3, x_{.4}, \ldots, x_{.p}$ for observations within the leaf. Notationally, a condition on the j^{th} feature is denoted $x_{.j} \in \sigma_j(l)$ where $\sigma_j(l)$ is the set of allowed values for feature j along the path to leaf l. If there are no conditions on feature j along the path to l, then $\sigma_j(l)$ includes all possible outcomes for feature j. Thus, leaf l includes outcomes x obeying:

$$x \in \{x_{.1} \in \sigma_1(l), x_{.2} \in \sigma_2(l), \dots, x_{.p} \in \sigma_p(l)\}.$$

For categorical data, the volume of a leaf l is defined to be $\mathbb{V}_l = \prod_{j=1}^p |\sigma_j(l)|$. We give an example of this computation next.

VOLUME COMPUTATION EXAMPLE

The data are categorical. Possible outcomes for $x_{.1}$ are $\{1, 2, 3, 4, 5, 6, 7\}$. Possible outcomes for $x_{.2}$ are $\{100, 101, 102, 103\}$. Possible outcomes for $x_{.3}$ are $\{10, 11, 12, 13, 14, 15\}$. Possible outcomes for $x_{.4}$ are $\{8, 9, 10\}$.

Consider the tree in Figure 2. We compute the volume for leaf l. Here, $\sigma_1(l) = \{4, 5\}$

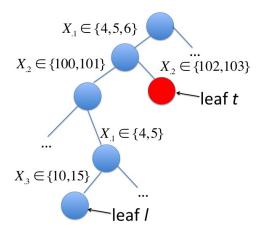


Figure 2: Example of computation of volume.

since l requires both $x_{.1} \in \{4, 5, 6\}$ and $x_{.1} \in \{4, 5\}$. $\sigma_2(l) = \{100, 101\}$, $\sigma_3(l) = \{10, 15\}$, and $\sigma_4(l) = \{8, 9, 10\}$ because there is no restriction on $x_{.4}$. So

$$\mathbb{V}_{l} = \prod_{j} |\sigma_{j}(l)| = 2 \cdot 2 \cdot 2 \cdot 3 = 24.$$

Our notation handles only categorical data for ease of exposition but can be extended to handle ordinal and continuous data. For ordinal data, the definition is the same as for categorical but σ_j can (optionally) include only continguous values (e.g. $\{3,4,5\}$ but not $\{3,4,6\}$). For continuous variables, σ_j is the "volume" of the continuous variables, for example, for node condition $x_{.j} \in (0,0.5), \sigma_j = 0.5 - 0$.

In the next three subsections, we present the leaf-based modeling approach, branch-based modeling approach, and an approach to construct density rule lists.

2.1 Model I: Leaf-based Cascade Model

We define prior and likelihood for the tree-based model. To create the tree we will optimize the posterior over possible trees.

Prior:

For this model, the main prior on tree T is on the number of leaves K_T . This prior we choose to be Poisson with a particular scaling (which will make sense later on), where the Poisson is centered at a user-defined parameter λ . Notation N_{K_T} is the number of trees

with K_T leaves. The prior is:

$$P(\text{Number of leaves in } T = K_T | \lambda) \propto N_{K_T} \cdot \text{Poisson}(K_T, \lambda)$$

= $N_{K_T} e^{-\lambda} \frac{\lambda^{K_T}}{K_T!}$.

Thus λ allows the user to control the number of leaves in the tree. The number of possible trees is finite, thus the distribution can be trivially normalized.

Among trees with K_T leaves, tree T is chosen uniformly, with probability $1/N_{K_T}$. This means the probability to choose a particular tree T is Poisson:

$$P(T|\lambda) \propto P(T|K_T)P(K_T|\lambda) \propto \frac{1}{N_{K_T}}N_{K_T}e^{-\lambda}\frac{\lambda^{K_T}}{K_T!} = e^{-\lambda}\frac{\lambda^{K_T}}{K_T!}$$

 $\propto \text{Poisson}(K_T, \lambda).$

We place a uniform prior over the probabilities for a data point to land in each of the leaves. To do this, we start from a Dirichlet distribution with equal parameters $\alpha_1 = \ldots = \alpha_{K_T} = \alpha \in \mathbb{Z}^+$ where hyperparameter $\alpha > 1$. We denote the vector with K_T equal entries $[\alpha, ..., \alpha]$ as α_{K_T} . We draw multinomial parameters $\theta = [\theta_1, ..., \theta_{K_T}]$ from $\text{Dir}(\alpha_{K_T})$.

Thus, the first part of our model is as follows, given hyperparameters λ and α :

Number of leaves in T: $K_T \propto \text{scaled Poisson}(\lambda)$, i.e., $N_{K_T} \cdot \text{Poisson}(K_T, \lambda)$ Tree shape : $T \propto \text{Uniform over trees with } K_T \text{ leaves}$

Prior distribution over leaves: $\theta \propto \text{Dir}(\alpha_{K_T})$.

As usual, the prior can be overwhelmed given enough data.

Likelihood:

Let n_l denote the number of points captured by the l-th leaf, and denote \mathbb{V}_l to be the volume of that leaf, defined above. The probability to land at any specific value within leaf l is $\frac{\theta_l}{\mathbb{V}_l}$. The likelihood for the full data set is thus

$$P(X|\boldsymbol{\theta},T) = \prod_{l=1}^{K_T} \left(\frac{\theta_l}{\mathbb{V}_l}\right)^{n_l}.$$

Posterior:

The posterior can be written as follows, where we have substituted the distributions from the prior into the formula. Here, $B(\boldsymbol{\alpha}_{K_T}) = \frac{\prod_{l=1}^{K_T} \Gamma(\alpha_l)}{\Gamma(\sum_{l=1}^{K_T} \alpha_l)} = \frac{(\Gamma(\alpha))^{K_T}}{\Gamma(K_T\alpha)}$ is the multinomial beta

function which is also the normalizing constant for the Dirichlet distribution.

$$\begin{split} &P(T|\lambda, \boldsymbol{\alpha}, X) \\ &\propto \int_{\boldsymbol{\theta}: \text{simplex}} P(K_T|\lambda) \cdot P(T|K_T) \cdot P(\boldsymbol{\theta}|\boldsymbol{\alpha}_{K_T}) \cdot P(X|\boldsymbol{\theta}, T) d\boldsymbol{\theta} \\ &\propto \int_{\boldsymbol{\theta}: \text{simplex}} P(T|\lambda) \left[\frac{1}{B(\boldsymbol{\alpha}_{K_T})} \left(\prod_{l=1}^{K_T} \theta_l^{\alpha-1} \right) \right] \left[\prod_{l=1}^{K_T} \left(\frac{\theta_l}{\mathbb{V}_l} \right)^{n_l} \right] d\boldsymbol{\theta} \\ &\propto P(T|\lambda) \frac{1}{B(\boldsymbol{\alpha}_{K_T})} \left(\prod_{l=1}^{K_T} \left(\frac{1}{\mathbb{V}_l} \right)^{n_l} \right) \int_{\boldsymbol{\theta}: \text{simplex}} \prod_{l=1}^{K_T} \boldsymbol{\theta}^{n_l + \alpha - 1} d\boldsymbol{\theta} \\ &\propto P(T|\lambda) \frac{B(n_1 + \alpha, \dots, n_{K_T} + \alpha)}{B(\boldsymbol{\alpha}_{K_T})} \prod_{l=1}^{K_T} \frac{1}{\mathbb{V}_l^{n_l}} \\ &\propto P(T|\lambda) \frac{\Gamma(K_T \alpha)}{\Gamma(n + K_T \alpha)} \prod_{l=1}^{K_T} \frac{(n_l + \alpha - 1)!}{(\alpha - 1)!} \mathbb{V}_l^{-n_l}, \end{split}$$

where $P(T|\lambda)$ is simply $Poisson(K_T, \lambda)$ as discussed earlier. For numerical stability, we maximize the log-posterior which is equivalent to maximizing the posterior.

For the purposes of prediction, we are required to estimate the density that is being assigned to leaf l. This is calibrated to the data, simply as:

$$\hat{f} = \frac{n_l}{n \mathbb{V}_l}$$

where n is the total number of training data points and n_l is the number of training data points that reside in leaf l. The formula implicitly states that the density in the leaf is uniformly distributed over the features whose values are undetermined within the leaf (features for which σ_i contains all outcomes for feature j).

2.2 Model II: Branch-based Cascade Model

In the previous model, a Dirichlet distribution is drawn only over the leaves. In this model, a Dirichlet distribution is drawn at every internal node to determine branching. Similar to the previous model, we choose the tree that optimizes the posterior.

Prior:

The prior is comprised of two pieces: the part that creates the tree structure, and the part that determines how data propagates through it.

Tree Structure Prior: For tree T, we let $B_T = \{b_i | i \in I\}$ be a multiset, where each element is the count of branches from a node of the tree. For instance, if in tree T, the three nodes have 3 branches, 2 branches, and 2 branches respectively, then $B_T = \{3, 2, 2\}$. We let N_{B_T} denote the number of trees with the same multiset B_T . Note that B_T is unordered, so $\{3, 2, 2\}$ is the same multiset as $\{2, 3, 2\}$ or $\{2, 2, 3\}$.

Let I denote the set of internal nodes of tree T and let L denote the set of leaves. We let \mathbb{V}_l denote the volume at leaf l.

In the generative model, a Poisson distribution with parameter λ is used at each internal node in a top down fashion to determine the number of branches. Iteratively, for node i, the number of branches, b_i , obeys $b_i \sim \text{Poisson}(\lambda)$. Hence, at any node i, with probability $\exp(-\lambda)\frac{\lambda^{b_i}}{b_i!}$, there are b_i branches from node i. This implies that with probability $\exp(-\lambda)$, the node is a leaf. In summary,

$$P(\text{Multiset of branches } = B|\lambda) \propto N_B \left[\prod_{i \in I} e^{-\lambda} \frac{\lambda^{b_i}}{b_i!} \right] \left[\prod_{l \in L} e^{-\lambda} \right].$$

Among trees with multiset B, tree T is chosen uniformly, with probability $\frac{1}{N_B}$. This means the probability to choose a particular tree is:

$$P(T|\lambda) \propto P(T|B_T)P(B_T|\lambda) \propto \frac{1}{N_{B_T}} N_{B_T} \left[\prod_{i \in I} e^{-\lambda} \frac{\lambda^{b_i}}{b_i!} \right] \left[\prod_{i \in I} e^{-\lambda} \right] = \left[\prod_{i \in I} e^{-\lambda} \frac{\lambda^{b_i}}{b_i!} \right] \left[\prod_{i \in I} e^{-\lambda} \right]. \tag{1}$$

Tree Propagation Prior: After the tree structure is determined, we need a generative process for how the data propagate through each internal node. We denote θ_l as the probability to land in leaf l. We denote $\widetilde{\theta}_{ij}$ as the probability to traverse to node j from internal node i. Notation $\boldsymbol{\theta}$ is the vector of leaf probabilities (the θ_l 's), $\widetilde{\boldsymbol{\theta}}$ is the set of all $\widetilde{\theta}_{ij}$'s, and $\widetilde{\boldsymbol{\theta}}_i$ is the set of all internal node transition probabilities from node i (the $\widetilde{\theta}_{ij}$'s).

We compute $P(\widetilde{\boldsymbol{\theta}}_i|\alpha,T)$ for all internal nodes i of tree T. At each internal node, we draw a sample from a Dirichlet distribution with parameter $[\alpha,\ldots,\alpha]$ (of size equal to the number of branches b_i of i) to determine the proportion of data, $\widetilde{\boldsymbol{\theta}}_{i,j}$, that should go along the branch leading to each child node j from the internal parent node i. Thus, $\widetilde{\boldsymbol{\theta}}_i \sim \text{Dir}(\boldsymbol{\alpha})$ for each internal node i, that is:

$$P(\widetilde{\boldsymbol{\theta}}_i|\boldsymbol{\alpha},T) = \frac{1}{B_{b_i}(\boldsymbol{\alpha})} \prod_{j \in C_i} \widetilde{\boldsymbol{\theta}}_{ij}^{\alpha-1},$$

where $B_k(\boldsymbol{\alpha})$ is the normalizing constant for the Dirichlet distribution with parameter α and k categories, and C_i are the indices of the children of i. Thus,

$$P(\widetilde{\boldsymbol{\theta}}|\boldsymbol{\alpha},T) = \prod_{i} P(\widetilde{\boldsymbol{\theta}}_{i}|\boldsymbol{\alpha},T) = \prod_{i} \frac{1}{B_{b_{i}}(\boldsymbol{\alpha})} \prod_{j \in C_{i}} \widetilde{\boldsymbol{\theta}}_{ij}^{\alpha-1}.$$
 (2)

Thus, the prior is $P(T|\lambda) \cdot P(\widetilde{\boldsymbol{\theta}}|\alpha, T)$, where $P(T|\lambda)$ is in (1) and $P(\widetilde{\boldsymbol{\theta}}|\alpha, T)$ is in (2). In summary, the prior of our model is as follows, given hyperparameters λ and α :

Multiset of branches:
$$B_T \propto N_{B_T} \left[\prod_{i \in I} e^{-\lambda} \frac{\lambda^{b_i}}{b_i!} \right] \left[\prod_{l \in L} e^{-\lambda} \right].$$

Tree shape : $T \sim \text{Uniform over trees with branches } B_T$.

Prior distribution over each branch: $\widetilde{\boldsymbol{\theta}}_i \sim \operatorname{Dir}(\alpha)$.

Likelihood:

The density within leaf l is uniform and equal to

$$P(X = x | X \in \text{leaf } l) = \begin{cases} \frac{1}{\mathbb{V}_l}, & x \in \text{leaf } l, \\ 0, & \text{otherwise.} \end{cases}$$

We denote the set P_l as the set of branches in the path from the root of the tree to the leaf l. The probability of X taking on value x (permitting that x is an allowed outcome in leaf l) is thus:

$$P(X = x, X \in \text{leaf } l) = P(X = x | X \in \text{leaf } l) \cdot P(X \in \text{leaf } l)$$
$$= \frac{1}{\mathbb{V}_l} \cdot \theta_l = \frac{\prod_{(\hat{i}, \hat{c}) \in P_l} \widetilde{\theta}_{\hat{i}, \hat{c}}}{\mathbb{V}_l}.$$

Denote the set of children of node i by C_i and the number of data points in node c as n_c . It is true that:

$$\prod_{l \in L} \left(\prod_{(\hat{i}, \hat{c}) \in P_l} \widetilde{\theta}_{\hat{i}, \hat{c}} \right)^{n_l} = \prod_{i \in I} \prod_{c \in C_i} \widetilde{\theta}_{i, c}^{n_c}.$$

The equality stems from two distinct ways of counting the branches that a particular data point passes through from the root to the leaf. The first way of counting is to start from the leaf and count backwards from the leaf to the root (depth first). The second way of counting is by examining each internal node (breadth first).

Hence the likelihood of a particular data set can be written:

$$P(X|\widetilde{\boldsymbol{\theta}},T) = \prod_{l \in L} \left(\frac{\prod_{(\hat{i},\hat{c}) \in P_l} \widetilde{\boldsymbol{\theta}}_{\hat{i},\hat{c}}}{\mathbb{V}_l} \right)^{n_l} = \frac{\prod_{i \in I} \prod_{c \in C_i} \widetilde{\boldsymbol{\theta}}_{i,c}^{n_c}}{\prod_{l \in L} \mathbb{V}_l^{n_l}}.$$

Posterior:

The posterior is proportional to the prior times the likelihood terms. Here we are integrating over the $\widetilde{\theta}_i$ terms for each of the internal nodes i.

$$\begin{split} &P(T|\lambda,\alpha,X) \\ &\propto \int P(B_T|\lambda) \cdot P(T|B_T) \cdot P(\widetilde{\boldsymbol{\theta}}|\alpha,T) \cdot P(X|\widetilde{\boldsymbol{\theta}},T) d\widetilde{\boldsymbol{\theta}} \\ &\propto \left[\prod_{l \in L} \left(\frac{e^{-\lambda}}{\mathbb{V}_l^{n_l}} \right) \right] \left(\prod_{i \in I} e^{-\lambda} \frac{\lambda^{b_i}}{b_i!} \frac{1}{B_{b_i}(\alpha,\ldots,\alpha)} \int_{\widetilde{\boldsymbol{\theta}}_i \in \text{simplex}} \prod_{c \in C_i} \widetilde{\boldsymbol{\theta}}_{i,c}^{\alpha-1} \widetilde{\boldsymbol{\theta}}_{i,c}^{n_c} d\widetilde{\boldsymbol{\theta}}_i \right) \\ &= e^{-\lambda(|I| + |L|)} \left(\prod_{i \in I} \frac{\lambda^{b_i}}{b_i!} \frac{1}{B_{b_i}(\alpha,\ldots,\alpha)} \int_{\widetilde{\boldsymbol{\theta}}_i \in \text{simplex}} \prod_{c \in C_i} \widetilde{\boldsymbol{\theta}}_{i,c}^{n_c + \alpha - 1} d\widetilde{\boldsymbol{\theta}}_i \right) \prod_{l \in L} \left(\frac{1}{\mathbb{V}_l^{n_l}} \right) \\ &= e^{-\lambda(|I| + |L|)} \lambda^{\sum_{i \in I} b_i} \left(\prod_{i \in I} \frac{1}{b_i!} \frac{B_{b_i}(\alpha + n_{c_1},\ldots,\alpha + n_{c_{b_i}})}{B_{b_i}(\alpha,\ldots,\alpha)} \right) \prod_{l \in L} \left(\frac{1}{\mathbb{V}_l^{n_l}} \right) \\ &= e^{-\lambda(|I| + |L|)} \lambda^{|L| + |I| - 1} \left(\prod_{i \in I} \frac{1}{b_i!} \frac{B_{b_i}(\alpha + n_{c_1},\ldots,\alpha + n_{c_{b_i}})}{B_{b_i}(\alpha,\ldots,\alpha)} \right) \prod_{l \in L} \left(\frac{1}{\mathbb{V}_l^{n_l}} \right) \end{split}$$

where $c_1, \ldots, c_{b_i} \in C_i$ in the second last expression. We used the equation $\sum_{i \in I} b_i = |L| + |I| - 1$ for a tree in the last line.

We use a specialized simulated annealing method to search for the maximum a posteriori tree. Our algorithm moves among neighboring trees and records the best tree that has been found so far. The description of this method is in the appendix.

Possible Extension: We can include an upper layer of the hierarchical Bayesian Model to control (regularize) the number of features d that are used in the cascade out of a total of p dimensions. This would introduce an extra multiplicative factor within the posterior of $\begin{pmatrix} p \\ d \end{pmatrix} \gamma^d (1-\gamma)^{p-d}$, where γ is a parameter between 0 and 1, where a smaller value favors a simpler model.

$$\begin{pmatrix} p \\ d \end{pmatrix} \gamma^d (1 - \gamma)^{p-d} e^{-\lambda(|I| + |L|)} \lambda^{|I| + |L| - 1}$$

$$\left(\prod_{i \in I} \frac{1}{b_i!} \frac{B_{b_i}(\alpha + n_{c_1}, \dots, \alpha + n_{c_{b_i}})}{B_{b_i}(\alpha, \dots, \alpha)} \right) \prod_{l \in L} \left(\frac{1}{\mathbb{V}_l^{n_l}} \right).$$

2.3 Model III: Leaf-based Density Rule List

Rather than producing a general tree, an alternative approach is to produce a rule list. A rule list is a one-sided tree. Rule lists are easier to optimize than trees. Each tree can be expressed as a rule list; however, some trees may be more complicated to express as a rule list. By using lists, we implicitly hypothesize that the full space of trees may not be necessary and that simpler rule lists may suffice.

An example of a density rule list is as follows:

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if x obeys a_1 then \operatorname{density}(x) = f_1
else if x obeys a_2 then \operatorname{density}(x) = f_2
:
else if x obeys a_m then \operatorname{density}(x) = f_m
else \operatorname{density}(x) = f_0.
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The antecedents $a_1,...,a_m$ are chosen from a large pre-mined collection of possible antecedents, called A. We define A to be the set of all possible antecedents of size at most H, where the user chooses H. The size of A is:

$$|A| = \sum_{j=0}^{H} A_j,$$

where A_j is the number of antecedents of size j,

$$A_{j} = \sum_{ \begin{cases} t_{1}, t_{2}, \dots, t_{j} \in \{1, \dots, p\} \\ \text{s.t. } t_{1} > t_{2} \dots > t_{j} \end{cases}} \prod_{i=1}^{j} q_{t_{i}},$$

where feature i consists of q_i categories.

Generative Process:

We now sketch the generative model for the tree from the observations x and antecedents A. Prior parameters λ and η are used to indicate preferences over the length of the density list and the number of conjunctions in each sub-rule a_i .

Define $a_{< j}$ as the antecedents before j in the rule list if there are any. For example $a_{< 3} = \{a_1, a_2\}$. Similarly, let c_j be the cardinalities of the antecedents before j in the rule list. Let d denote the rule list. The generative model is as follows, following the exposition of Letham et al. (2015):

- 1. Sample a decision list length $m \sim P(m|A, \lambda)$.
- 2. For decision list rule j = 1, ..., m: Sample the cardinality of antecedent a_j in d as $c_j \sim P(c_j|c_{< j}, A, \eta)$. Sample a_j of cardinality c_j from $P(a_j|a_{< j}, c_j, A)$.
- 3. For observation i = 1, ..., n: Find the antecedent a_j in d that is the first that applies to x_i . If no antecedents in d applies, set j = 0.
- 4. Sample parameter $\boldsymbol{\theta} \sim \text{Dirichlet } (\boldsymbol{\alpha})$ for the probability to be in each of the leaves, where $\boldsymbol{\alpha}$ is a user-chosen vector of size m+1, usually where all elements are the same. $f_i = \frac{\theta_i}{\mathbb{V}_i}$, where \mathbb{V}_i is the volume.

Prior:

The distribution of m is the Poisson distribution, truncated at the total number of preselected antecedents:

$$P(m|A,\lambda) = \frac{\lambda^m/m!}{\sum_{j=0}^{|A|} (\lambda^j/j!)}, m = 0, \dots, |A|.$$

When |A| is huge, we can use the approximation $P(m|A,\lambda) \approx \lambda^m/m!$, as the denominator of the previous term would be close to 1.

We let $R_j(c_1, \ldots, c_j, A)$ be the set of antecedent cardinalities that are available after drawing antecedent j, and we let $P(c_j|c_{< j}, A, \eta)$ be a Poisson truncated to remove values for which no rules are available with that cardinality:

$$P(c_j|c_{< j}, A, \eta) = \frac{(\eta^{c_j}/c_j!)}{\sum_{k \in R_{j-1}(c_{< j}, A)} (\eta^k/k!)}, \ c_j \in R_{j-1}(c_{< j}, A).$$

We use a uniform distribution over antecedents in A of size c_i excluding those in a_i ,

$$P(a_j | a_{< j}, c_j, A) \propto 1, \quad a_j \in \{a \in A \setminus a_{< k} : |a| = c_j\}.$$

The cascaded prior for the antecedent lists is thus:

$$P(d|A, \lambda, \eta) = P(m|A, \lambda) \cdot \prod_{j=1}^{m} P(c_j|c_{< j}, A, \eta) \cdot P(a_j|a_{< j}, c_j, A).$$

The prior distribution over the leaves $\boldsymbol{\theta} = [\theta_1, \dots, \theta_m, \theta_0]$ is drawn from $Dir(\boldsymbol{\alpha}_{m+1})$.

$$P(\boldsymbol{\theta}|\alpha) = \frac{1}{B_{m+1}(\alpha, \dots, \alpha)} \prod_{l=0}^{m} \theta_l^{\alpha-1}$$

It is straightforward to sample an ordered antecedent list d from the prior by following the generative model that we just specified, generating rules from the top down.

Likelihood:

Similar to the first model, the probability to land at any specific value within leaf l is $\frac{\theta_l}{\mathbb{V}_l}$. Hence, the likelihood for the full data set is:

$$P(X|\boldsymbol{\theta},d) = \prod_{l=0}^{m} \left(\frac{\theta_l}{\mathbb{V}_l}\right)^{n_l}.$$

Posterior:

The posterior can be written as

$$\begin{split} &P(d|A,\lambda,\eta,\alpha,X) \\ &\propto \int_{\boldsymbol{\theta} \in \text{simplex}} P(d|A,\lambda,\eta) \cdot P(\boldsymbol{\theta}|\alpha) \cdot P(X|\boldsymbol{\theta},d) d\boldsymbol{\theta} \\ &= P(d|A,\lambda,\eta) \int_{\boldsymbol{\theta} \in \text{simplex}} \frac{1}{B_{m+1}(\alpha,\cdots,\alpha)} \prod_{l=0}^{m} \theta_l^{\alpha-1} \left(\frac{\theta_l}{\mathbb{V}_l}\right)^{n_l} d\boldsymbol{\theta} \\ &= P(d|A,\lambda,\eta) \frac{\prod_{l=0}^{m} \Gamma(n_l+\alpha) \mathbb{V}_l^{-n_l}}{\Gamma(\sum_{l=0}^{m} (n_l+\alpha))}. \end{split}$$

where the last equality uses the standard Dirichlet-multinomial distribution derivation.

To search for optimal rule lists that fit the data, we use local moves (adding rules, removing rules, and swapping rules) and use the Gelman-Rubin convergence diagnostic applied to the log posterior function.

A technical challenge that we need to address in our problem is the computation of the volume of a leaf. Volume computation is not needed in the construction of a decision list classifier like that of Letham et al. Letham et al. (2015) but it is needed in the computation of density list. There are multiple ways to compute the volume of a leaf of a rule list. The first set of approaches do not require the overhead of creating a complicated data structure, and thus might be better for smaller problems.

Approach 1: create uniform data over the whole domain, and count the number of points that satisfy the antecedents. This approach would be expensive when the domain is huge but easy to implement for smaller problems.

Approach 2: use an MCMC sampling approach to sample uniformly the whole domain space. This approach is again not practical when the domain size is huge as the number of samples required will increase exponentially due to curse of dimensionality.

Approach 3: use the inclusion-exclusion principle to directly compute the volume of each leaf. Consider computing the volume of the *i*-th leaf. Let V_{a_i} denote the volume induced by the rule a_i , that is the number of points in the domain that satisfy a_i . To belong to that leaf, a data point has to satisfy a_i and not $a_{< i}$. Hence the volume of the *i*-th leaf is equal to the volume obeying a_i alone, minus the volume that has been used by earlier rules. Hence,

we have the following:

$$\begin{split} \mathbb{V}_i &= V_{a_i \wedge \bigwedge_{k=1}^{i-1} a_k^c} \\ &= V_{a_i} - V_{a_i \wedge (\bigvee_{k=1}^{i-1} a_k)} \\ &= V_{a_i} - V_{(\bigvee_{k=1}^{i-1} a_i \wedge a_k)} \\ &= V_{a_i} - \sum_{k=1}^{i-1} (-1)^{k+1} \sum_{1 \leq j_1 \leq \dots j_k \leq n} V_{a_i \wedge a_{j_1} \dots \wedge a_{j_k}}, \end{split}$$

where the last expression is due to the inclusion-exclusion principle and it only involves the volume resulting from conjunctions. The volume resulting from conjunctions can be easily computed from data. Without loss of generality, suppose we want to compute the volume of $V_{a_1 \wedge ... \wedge a_k}$, for each feature that appears, we examine if there is any contradiction. For example if feature 1 is present in both a_1 and a_2 and they specify feature 1 to take different values, then we have found a contradiction and the volume should be 0. Suppose this is not the case, then the volume is equal to the product of the number of distinct categories of all the features that are not used. By using the inclusion-exclusion principle, we reduce the problem to just computing a volume of conjunctions, however, computing these volumes requires a clever data structure. This would be suitable for larger problems but might slow down computations for smaller problems.

3. Experiments

Our experimental setup is as follows. We considered five models: the leaf-based cascaded histograms, the branch-based cascaded histograms, the leaf-based density list, regular histograms and density estimation trees (DET) (Ram and Gray, 2011). To our knowledge, this essentially represents the full set of logical, high dimensional density estimation methods. To ascertain uncertainty, we split the data in half 5 times randomly and assessed test log-likelihood and sparsity of the trees for each method. A model with fewer bins and higher test likelihood is a better model.

For the histogram, we treated each possible configuration as a separate bin. DET was designed for continuous data, which meant that the computation of volume needed to be adapted – it is the number of configurations in the bin (rather than the lengths of each bin multiplied together). The DET method has two parameters, the minimum allowable support in a leaf, and the maximum allowable support. We originally planned to use a minimum of 0 and a maximum of the size of the full dataset, but the algorithm often produced trivial models when we did this. We tried also values $\{0,3,5\}$ for the minimum values and $\{10,n,\lfloor\frac{n}{2}\rfloor\}$ where n is the number of training data points, and reported results for the best of these. For the leaf-based cascade model, the mean of the Poisson prior was chosen from the set $\{5,8\}$ using nested cross validation. For the branch-based cascade model, the parameter to control the number of branches was chosen from the set $\{2,3\}$. γ was fixed to be 0.5, and α was set to be 2 for the experiment. For the leaf-based density list model, the parameters λ, η and α were chosen to be 3, 1 and 1 respectively.

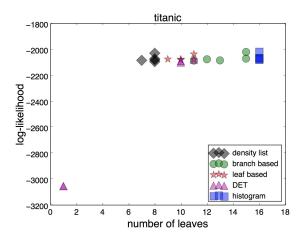


Figure 3: The scatter plot for titanic.

3.1 An Experiment on the Titanic Data Set

The Titanic dataset has an observation for each of the 2201 people aboard the Titanic. There are 3 features: gender, whether someone is an adult, and the class of the passenger (first class, second class, third class, or crew member). A cascade would help us understand the set of people on board the Titanic.

Figure 3 shows the results, both out-of-sample likelihood and sparsity, for each model, for each of the 5 folds. The histogram method had high likelihood, but also the most leaves (by design). The other methods performed similarly, arguably the leaf-based density list method performed slightly better in the likelihood-sparsity tradeoff. DET produced a trivial tree for one of the splits. In general, we will see similar results on other datasets: the histogram produces too many bins, the leaf-based density list model and leaf-based cascade perform well, and DET has inconsistent performance (possibly due to its top-down greedy nature, or the fact that DET approximately optimizes Hellinger distance rather than likelihood.) Figure 4 shows one of the density cascades generated by the leaf-based method. The reason for the top split is clear: the distributions of the males and females were different, mainly due to the fact that the crew was mostly male. There were fewer children than adults, and the volume of crew members was very different than the volume of 1st, 2nd, and 3rd class passengers. Figure 5 shows one of the density lists generated by our model. It shows that male crew and third class male adults have higher density.

3.2 Crime Dataset

The housebreak data used for this experiment were obtained from the Cambridge Police Department, Cambridge, Massachusetts. The motivation is to understand the common types of modus operandi (M.O.) characterizing housebreaks, which is important in crime analysis. The data consist of 3739 separate housebreaks occurring in Cambridge between 1997 and 2012 inclusive. We used 6 categorical features.

1. Location of entry: "window," "door," "wall," and "basement."

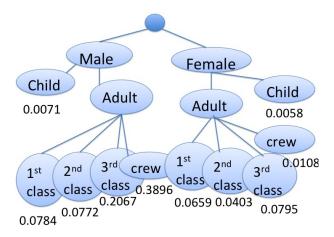


Figure 4: Tree representing titanic.

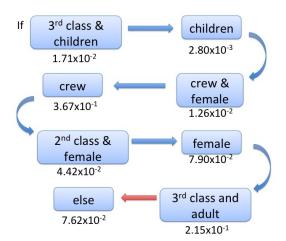


Figure 5: List representing titanic. Each arrow represents an "else if' statement. This can be directly compared to the cascade in Figure 4. Slight differences in estimates between the two models occurred because we used different splits of data for the two figures. The estimates were robust to the change in data.

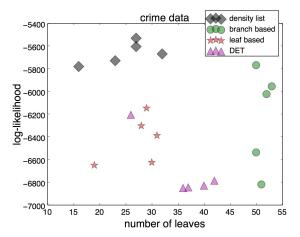


Figure 6: the scatter plot for Cambridge Police Department dataset.

- 2. Means of entry: "forceful" (cut, broke, cut screen, etc.), "open area," "picked lock," "unlocked," and "other."
- 3. Whether the resident is inside.
- 4. Whether the premise is judged to be ransacked by the reporting officer.
- 5. "Weekday" or "Weekend."
- 6. Type of premise. The first category is "Residence" (including apartment, residence/unk., dormitory, single-family house, two-family house, garage (personal), porch, apartment hallway, residence unknown, apartment basement, condominium). The second category is "non-medical, non-religious work place" (commercial unknown, accounting firm, research, school). The third group consists of halfway houses, nursing homes, medical buildings, and assisted living. The fourth group consists of parking lots and parking garages, and the fifth group consists of YWCAs, YMCAs, and social clubs. The last groups are "storage," "construction site," "street," and "church" respectively.

The experiments show that DET and our approaches are competitive for the crime data set. (The histogram's results involve too many bins to fit on the figure.)

Let us discuss one of the trees obtained from the leaf-based cascade method where we have set the mean of the Poisson distribution to be chosen from the set $\{20,30\}$. The tree is in Figure 12. It states that most burglaries happen at residences – the non-residential density has values less than 1×10^{-4} . Given that a crime scene is a residence, most crimes happened when the resident was not present. If the premise is a residence and the resident was present for the housebreak, the burglary is more likely to happen on a weekday, in which case most burglaries involve forceful means of entry (density = 9.16×10^{-3}). When the premise is a residence and the resident was not present, the location of entry is usually either a window or a door. Given this setting:

1. If the means of entry is forceful, most crime happens on weekdays, and in that case it is almost twice as likely that the means of entry is through a door (density=0.15)

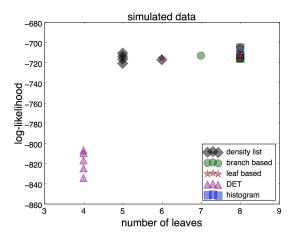


Figure 7: Performance vs sparsity on sparse tree data set.

compared to a window (density=0.078). If the crime happened on a weekend, it is more likely for the crime scene not to be ransacked (density= 5.50×10^{-2}) as compared to being ransacked (density= 2.41×10^{-3}).

- 2. If the means of entry is either an open area or a lock is picked, it is more likely to be on a weekday (density= 2.48×10^{-3}) compared to a weekend (density= 7.30×10^{-3}).
- 3. If the means of entry is none of the above, it is almost three times more likely to happen on a weekday (density= 3.60×10^{-3}) compared to a weekend (density= 1.07×10^{-3}).

These types of results can be useful for crime analysts to assess whether a particular modus operandi is unusual. A density list for these data is presented in Figure 13.

4. Empirical Analysis

Each subsection below is designed to provide insight into how the models operate.

4.1 Sparse Tree Dataset

We generated a dataset that arises from a tree with 6 leaves, involving 3 features. The data consists of 1000 data points, where 100 points are tied at value (1,2,1), 100 points are at (1,2,2), 100 points are at (2,1,1), 400 points are at (2,1,2), and 300 points are at (2,2,2). The correct tree is in Figure 8.

We trained the models on half of the dataset and tested on the other half. Figure 7 shows the scatter plot of out-of-sample performance and sparsity. This is a case where the DET failed badly to recover the true model. It produced a model that was too sparse, with only 4 leaves. The leaf-based cascade method recovered the full tree from Figure 8 and we present the tree in Figure 9. The output for the corresponding density list is presented in Figure 10.

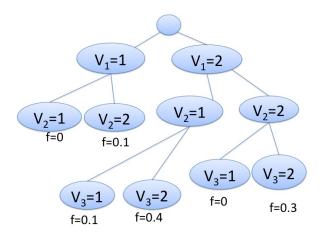


Figure 8: Tree diagram for sparse tree data set.

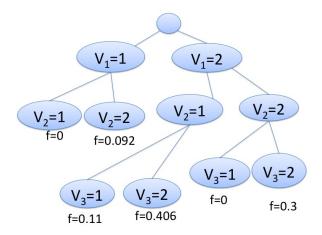


Figure 9: Output for leaf-based model that recovers the data structure.

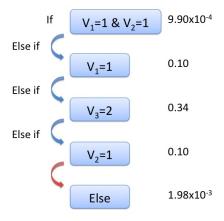


Figure 10: List output for sparse tree data set.

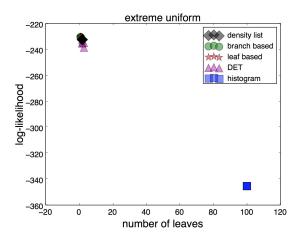


Figure 11: Performance vs sparsity on uniform data.

4.2 Extreme Uniform Dataset

We generated a 1-dimensional data set that consists of 100 data points. The data are simply all unique integers from 1 to 100. This is a case where the histogram badly fails to generalize. Figure 11 shows the result.

The leaf-based and branch-based models both return the solution that consists of a single root node, implying that the data are in fact uniformly distributed, or at least that we do not have evidence to further split on the single node. The density list output is close to uniform as well. DET is competitive as well, though it does not return the trivial tree. The histogram totally fails, since the test data and training data do not overlap at all.

5. Consistency

A consistent model has estimates that converge to the real densities as the size of the training set grows. Consistency of conventional histograms is well studied for example, Abou-Jaoude (1976); Devroye and Györfi (1983). More generally, consistency for general rectangular partitions has been studied by Zhao et al. (1991); Lugosi et al. (1996). Typical consistency proofs, (e.g., Devroye et al. (1996); Ram and Gray (2011)) require the leaf diameters to become asymptotically smaller as the size of the data grows. In our case if the ground truth density is a tree, we do not want our models to asymptotically produce smaller and smaller bin sizes, we would rather they reproduce the ground truth tree. This means we require a new type of consistency proof.

Definition 1: Density trees have a single root and there are conditions on each branch. A density value, f_l is associated with each leaf l of the tree.

Definition 2: Two trees, T_1 and T_2 are *equivalent* with respect to density f if they assign the same density values to every data point on the domain, $f_{T_1}(x) = f_{T_2}(x)$, for all x. We denote the class of trees that are equivalent to T as $[T]_f$.

Theorem 1: Let Θ be the set of all density trees. Consider these conditions:

- 1. $T_n \in \arg \max_T \text{Obj}(T)$. The objective function can be decomposed into $\text{Obj}(T) = \ln q_n(T|X) + \ln g_n(T|X)$ where $\arg \max_T [\ln q_n(T|X) + \ln g_n(T|X)] \equiv \arg \max_T \ln g_n(T|X)$ as $n \to \infty$.
- 2. $\ln g_n(T|X)$ converges in probability, for any tree T, to the empirical log-likelihood that is obtained by the maximum likelihood principle, $\hat{l}_n(T|X) = \frac{1}{n} \sum_{i=1}^n \ln \hat{f}_n(x_i|T)$.
- 3. $\sup_{T\in\Theta} |\hat{l}_n(T|X) l(T)| \xrightarrow{P} 0 \text{ where } l(T) = \mathbb{E}_x(\ln(f(x|T))).$
- 4. $T_{\text{MLE}}^* \in \arg \max_T l(T)$ is unique up to equivalence among elements of $[T_{\text{MLE}}^*]_f$.

If these conditions hold, then the trees T_n that we learned, $T_n \in \arg\max_T \operatorname{Obj}(T)$, obey $T_n \in [T^*_{\operatorname{MLE}}]_f$ for n > M for some M.

The first condition and the second condition are true any time we use a Bayesian model. They are also true any time we use regularized empirical likelihood where the regularization term's effect fades with the number of observations. Note that the third condition is automatically true by the law of large numbers. The last condition is not automatically true, and requires regularity conditions for identifiability. The result states that our learned trees are equivalent to maximum likelihood trees when there are enough data. The proof is presented in Appendix C.

6. Conclusion

We have presented a Bayesian approach to density estimation using cascaded piecewise constant estimators. These estimators have nice properties: their prior encourages them to be sparse, which permits interpretability. They do not have the pitfalls of other nonparametric density estimation methods like density estimation trees, which are top-down greedy. They are consistent, without needing to asymptotically produce infinitesimally small leaves. Practically, the approaches presented here have given us insight into a real data set (the housebreak dataset from the Cambridge Police) that we could not have obtained reliably in any other way.

Acknowledgments

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Appendix A. Simulated Annealing Algorithm

At each iteration we need to determine which neighboring tree to move to. To decide which neighbor to move to, we fix a parameter $\epsilon > 0$ beforehand, where ϵ is small. At each time, we generate a number from the uniform distribution on (0,1), then:

- 1. If the number is smaller than $\frac{1-\epsilon}{4}$, we select uniformly at random a parent which has leaves as its children, and remove its children. This is always possible unless the tree is the root node itself in which case we cannot remove it and this step is skipped.
- 2. If the random number is between $\frac{1-\epsilon}{4}$ and $\frac{1-\epsilon}{2}$, we pick a leaf randomly and a feature randomly. If it is possible to split on that feature, then we create children for that leaf. (If the feature has been used up by the leaf's ancestors, we cannot split.)
- 3. If the random number is between $\frac{1-\epsilon}{2}$ and $\frac{3(1-\epsilon)}{4}$, we pick a node randomly, delete its descendants and split the node into two nodes containing subsets of the node's outcomes. Sometimes this is not possible, for example if we pick a node where all the features have been used up by the node's ancestors, or if the node has only one outcome. In that case we skip this step.
- 4. If the random number is between $\frac{3(1-\epsilon)}{4}$ and $(1-\epsilon)$, we choose two nodes that share a common parent, delete all their descendants and merge the two nodes.
- 5. If the random number is more than 1ϵ , we perform a structural change operation where we remove all the children of a randomly chosen node of the tree.

The last three actions avoid problems with local minima. The algorithms can be warm started using solutions from other algorithms, e.g., DET trees. We found it useful to occasionally reset to the best tree encountered so far or the trivial root node tree. Ordinal data are treated differently than binary categorical data in that merges and splits in Steps 3 and 4 are done on neighboring ordinal values.

Appendix B. Evaluation Metric

We discuss evaluation metrics for use in out-of-sample testing and parameter tuning with nested cross-validation. The natural evaluation metric is the likelihood of the trained model calculated on the test data. Hellinger distance is an alternative (Hellinger, 1909), however, we prefer likelihood for two reasons. (i) To compute the Hellinger distance, it is assumed that the real distribution is known, when in reality it is not known. (ii) Hellinger distance would

be approximated by $2 - \frac{2}{n} \sum_{i=1}^{n} \sqrt{\frac{\hat{f}(x_i)}{f(x_i)}}$ (Liu et al., 2007) where f is not known in practice. The estimate of the Hellinger distance often comes out negative, which is nonsensical. An alternative is to use a least square criterion (see Loader, 1999). We consider the risk for tree h:

$$L(h) = \int (\hat{f}_n(x) - f(x))^2 dx$$

= $\int (\hat{f}(x))^2 dx - 2 \int \hat{f}_n(x) f(x) dx + \int f^2(x) dx$.

Since the true density is not known, the third term cannot be evaluated, is a constant, and thus can be ignored. The first two terms can be estimated using a leave one out estimator:

$$\hat{J}(h) = \int \left(\hat{f}_n(x)\right)^2 dx - \frac{2}{n} \sum_{i=1}^n \hat{f}_{(-i)}(x_i)$$

where the second term's f(x) vanishes because x is drawn from density distribution f. We desire this value to be as negative as possible. We know that $\hat{f}(x_i) = \frac{n_l}{nV_l}$ if $i \in l$ where l is a leaf. We approximate $\hat{f}_{(-i)}$ using the assumption that the tree does not change structurally when one point is removed:

$$\hat{f}_{(-i)}(x_i) \approx \frac{n_l - 1}{(n-1)V_l} = \frac{n(n_l - 1)}{(n-1)n_l} \hat{f}(x_i) = \frac{n(n_l - 1)}{(n-1)n_l} \hat{f}_l.$$

Hence, we simplify $\hat{J}(h)$ as follows:

$$\hat{J}(h) = \int \left(\hat{f}_n(x)\right)^2 dx - \frac{2}{n} \sum_{l \in L} (n_l) \hat{f}_{(-i)}(x_i)$$

$$\approx \int \left(\hat{f}_n(x)\right)^2 dx - 2 \sum_{l \in L} \frac{n_l - 1}{(n - 1)} \hat{f}_l$$

$$= \sum_{l \in L} \hat{f}_l^2 V_l - 2 \sum_{l \in L} \frac{n_l - 1}{(n - 1)} \hat{f}_l$$

$$= \sum_{l \in L} \left(\hat{f}_l V_l - \frac{2(n_l - 1)}{(n - 1)}\right) \hat{f}_l$$

$$= \sum_{l \in L} \left(\frac{n_l}{n} - \frac{2(n_l - 1)}{(n - 1)}\right) \hat{f}_l.$$

The formula can be used as an alternative evaluation metric of which the more negative it is, the better the model fit the data. It can be viewed as a weighted sum of likelihood over the leaves.

Appendix C. Proof for Theorem 1

From definition of T_n , T_n is an optimal value of the log-objective function and hence it is also an optimal solution to g_n as n is sufficiently large due to the first condition. We have that

$$\ln \mathrm{Obj}(T_n|X) - \ln \mathrm{Obj}(T_{\mathrm{MLE}}^*|X) \ge 0$$

by definition of T_n as the maximizer of Obj. Because Obj becomes close to g_n , we have that

$$\ln g_n(T_n|X) - \ln g_n(T_{\text{MLE}}^*) \ge 0 \tag{3}$$

as n is sufficiently large.

From Condition 2, we know that $\ln g_n(T|X) - \hat{l}_n(T|X) \xrightarrow{P} 0$ and from Condition 3, we have $\hat{l}_n(T|X) - l(T) \xrightarrow{P} 0$. Adding this up using the fact that convergence in probability is preserved under addition, we know that $\ln g_n(T|X) \xrightarrow{P} l(T)$.

Hence by taking the limit of (3) as n grows, we have that $\lim_{n\to\infty} l(T_n|X) \geq l(T_{\text{MLE}}^*)$. Since T_{MLE}^* is optimal for l(T) by definition, and by Condition 4, we conclude that T_n stays in $[T_{\text{MLE}}^*]$ when n is sufficiently large.

Appendix D. Optimal Density for the Likelihood Function

Denote the pointwise density estimate at x to be $\hat{f}_{n,x} = \frac{n_x}{n}$. Denote the density estimate for all points within leaf l similarly as $\hat{f}_{n,l} = \frac{\sum_{j \in \text{leaf } l} n_j}{nV_l}$.

The true density from which the data are assumed to be generated is denoted D. We assume that D arises from a tree over the input space (otherwise we would be back to standard analysis, where the proof is well-known).

Lemma 1: Any tree achieving the maximum likelihood on the training data has pointwise density equal to $\hat{f}_n(x)$. This means for any l in the tree and for any x, $\hat{f}_{n,l}(x) = \hat{f}_{n,x}(x)$.

Proof:

We will show that the pointwise histogram becomes better than using the tree if the tree is not correct. This is in some sense a version of a well-known result that the maximum likelihood is the pointwise maximum likelihood. We will show:

$$\prod_{j \in \text{leaf } l} \hat{f}_{n,j}^{n_j} \ge \hat{f}_{n,l}^{\sum_{j \in \text{leaf } l} n_j}.$$

By taking logarithms, this reduces to

$$\sum_{j \in \text{leaf } l} n_j \log \hat{f}_{n,j} \ge \sum_{j \in \text{leaf } l} n_j \log \hat{f}_{n,l}$$

$$\sum_{j \in \text{leaf } l} n_j \log \left(\frac{n_j}{n}\right) \ge \sum_{j \in \text{leaf } l} n_j \log \left(\frac{\sum_{m \in \text{leaf } l} n_m}{nV_l}\right)$$

$$\sum_{j \in \text{leaf } l} n_j \log n_j \ge \sum_{j \in \text{leaf } l} n_j \log \left(\frac{\sum_{m \in \text{leaf } l} n_m}{V_l}\right)$$

$$\sum_{j \in \text{leaf } l} n_j \log \left(\frac{n_j}{\sum_{m \in \text{leaf } l} n_m}\right)$$

$$\ge \sum_{m \in \text{leaf } l} n_j \log \left(\frac{1}{\sum_{m \in \text{leaf } l} V_m}\right)$$

$$\sum_{j \in \text{leaf } l} \frac{n_j}{\sum_{m \in \text{leaf } l} n_m} \log \left(\frac{n_j}{\sum_{m \in \text{leaf } l} n_m}\right)$$

$$\ge \sum_{j \in \text{leaf } l} \frac{n_j}{\sum_{m \in \text{leaf } l} n_m} \log \left(\frac{1}{\sum_{m \in \text{leaf } l} V_m}\right).$$

We know the last equation is true since this is just Gibb's inequality. Hence we have proven that the statement is true.

To avoid singularity, we separately consider the case when one of the $\hat{f}_{n,j} = 0$. For a particular value of q, if $\hat{f}_{n,q} = 0$, then $n_q = 0$ by definition. Hence, if we include a new

x within the leaf that has no training examples, we will find that the left hand side term of (4) remains the same but since the volume increases when we add the new point, the quantity on the right decreases. Hence the inequality still holds.

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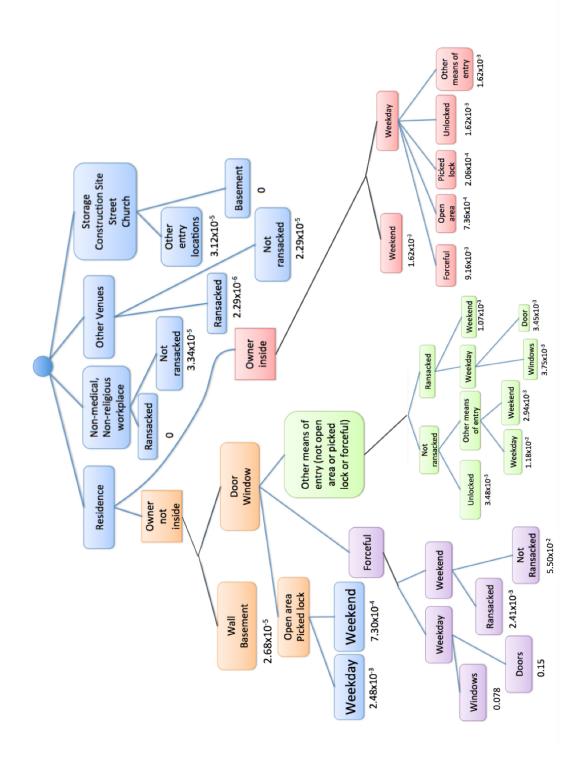


Figure 12: Tree representing the crime data set.

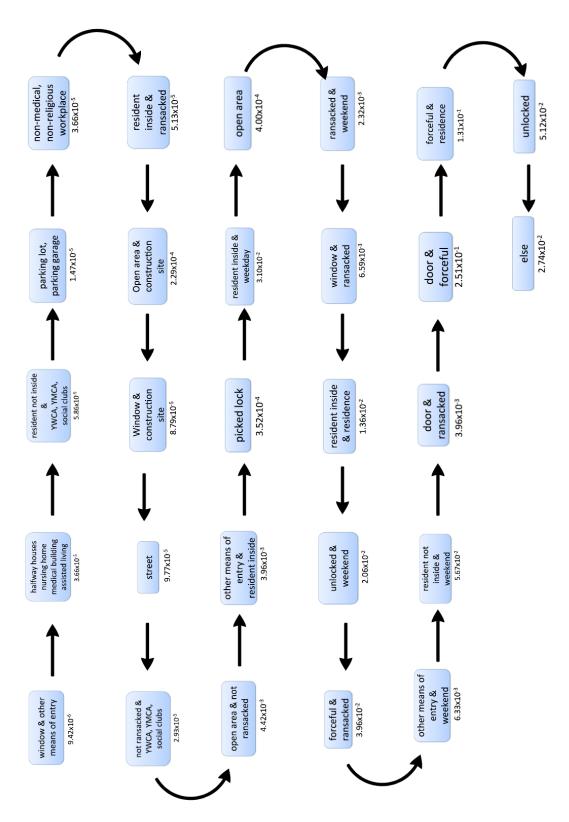


Figure 13: List representing the crime data set. Each arrow represent an "else if" statement.