Efficient Bayesian Parameter Estimation in Large Discrete Domains

Nir Friedman
Computer Science Division
University of California
387 Soda Hall, Berkeley, CA 94720
nir@cs.berkeley.edu

Yoram Singer
AT&T Labs, Room A277
180 Park Avenue
Florham Park, NJ 07932-0971
singer@research.att.com

Abstract

In this paper we examine the problem of estimating the parameters of a multinomial distribution over a large number of discrete outcomes, most of which do not appear in the training data. We analyze this problem from a Bayesian perspective and develop a hierarchical prior that incorporates the assumption that the observed outcomes constitute only a small subset of the possible outcomes. We show how to *efficiently* perform *exact* inference with this form of hierarchical prior and compare our method to standard approaches and demonstrate its merits.

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1 Introduction

One of the most important problems in statistical inference is *multinomial* estimation: Given a past history of observations independent trials with a discrete set of outcomes, predict the probability of the next trial. Such estimators are the basic building blocks in more complex statistical models, such as prediction trees [1, 15, 14], hidden Markov models [12] and Bayesian networks [3, 7]. The roots of multinomial estimation go back to Laplace's work in the 18'th century [10].

In Bayesian theory, the classic approach to multinomial estimation is via the use of the *Dirichlet* distribution (see for instance [4]). Laplace's "law of succession" and other common methods can be derived using Bayesian inference with the Dirichlet distribution as a prior distribution. The Dirichlet distribution entertain several properties which become very useful in statistical inference. In particular, estimates derived using Dirichlet priors are *consistent* (the estimate converges with probability one to the true distribution), *conjugate* (the posterior distribution is also a Dirichlet distribution), and can be computed efficiently (all queries of interest have a closed-form solution). Furthermore, theoretical studies of online prediction of individual sequences show that prediction using Dirichlet priors is competitive with *any* other prior distribution (see for instance [9, 2, 5] and the references therein).

Unfortunately, in some key applications, Dirichlet priors are unwieldy. These applications are characterized by several distinct features:

- The set of possible outcomes is very large, and often not known in advance.
- The number of training examples is small compared to the number of possible outcomes.
- The outcomes that have positive probability constitute a relatively small subset of the possible outcomes. However, this subset is not known in advance.

In this situation, a prediction based on a Dirichlet prior, in particular, the uniform distribution, tends to assign most of the probability mass to outcomes that were not seen in the training set.

For example, consider a natural language application, where outcomes are words drawn from an English dictionary, and the problem is predicting the probability of words that follow a particular word, say "Bosnia". If we do not have any prior knowledge, we can consider any word in the dictionary as a possible candidate. Yet, our knowledge of language would lead us to believe that in fact, only few words, such as "Herzegovina", should naturally follow the word "Bosnia". Furthermore, even in a large corpora, we do not expect to see many training examples that involve this phrase. As another example consider the problem of estimating the parameters of a discrete dynamical system. Here the task is to find a distribution over the states that can be reached from a particular state s (possibly after the system receives a particular external control signal). Again, although the number of possible state can be large, we often believe that the set of reachable states, from any state s, is much smaller.

In this paper, we present a Bayesian treatment of this problem using an *hierarchical* prior that averages over an exponential number of hypotheses each of which represents a subset of the feasible outcomes. Such a prior was previously used in a specific context of online prediction using suffix tree transducers [14]. As we show, although this prior involves exponentially many hypotheses, we can *efficiently* perform predictions. Moreover, our approach allows us to deal with countably infinite number of outcomes.

The paper is organized as follows. We start in Section 2 with a short review of Dirichlet priors. In Section 3 we describe the hierarchical prior for multinomial distributions. In Section 4, we examine how to apply our approach to countably infinite sets of outcomes. Section 5 we describe experimental results that show the effectiveness of our approach in language modeling. We conclude in Section 6.

2 Dirichlet priors

Let X be a random variable that can take L possible values from a set Σ. Without loss of generality, let $\Sigma = \{1, \ldots L\}$. We are given a training set D that contains the outcomes of N independent draws $x^1, \ldots, x^N$ of X from an unknown multinomial distribution P^*. We denote by N_i be the number of occurrences of the symbol i in the training data. The *multinomial estimation* problem is to find a good approximation for P^* (which is also a multinomial distribution).

This problem can be stated as the problem of predicting the outcome x^{N+1} given $x^1, \ldots, x^N$. Given a prior distribution over the possible multinomial distributions, the Bayesian estimate is:

$$P(x^{N+1} \mid x^1, \ldots, x^N, \xi) = \int P(x^{N+1} \mid \boldsymbol{\theta}, \xi) P(\boldsymbol{\theta} \mid x^1, \ldots, x^N, \xi) d\boldsymbol{\theta} \qquad (1)$$

where $\boldsymbol{\theta} = \langle \theta_1, \ldots, \theta_L \rangle$ is a vector that describes possible values of the (unknown) probabilities $P^*(1), \ldots, P^*(L)$, and ξ is the "context" variable that denote all other assumptions about the domain. (We consider particular contexts in the next section.)

The posterior probability of $\boldsymbol{\theta}$ can rewritten using Bayes law as:

$$P(\boldsymbol{\theta} \mid x^1, \ldots, x^N, \xi) \propto P(x^1, \ldots, x^N \mid \boldsymbol{\theta}, \xi) P(\boldsymbol{\theta} \mid \xi) = P(\boldsymbol{\theta} \mid \xi) \prod_i \theta_i^{N_i} \qquad (2)$$

The *Dirichlet* distribution is a parametric family that is *conjugates* to the multinomial distribution. That is, if the prior distribution is from this family, so is the posterior. A Dirichlet prior for X is specified by *hyperparameters* $\alpha_1, \ldots, \alpha_L$, and has the form:

$$P(\boldsymbol{\theta} \mid \xi) = \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i \theta_i^{\alpha_i - 1} \quad (\sum_i \theta_i = 1 \text{ and } \theta_i \geq 0 \text{ for all } i)$$

where $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$ is the *gamma* function. Given a Dirichlet prior, the initial prediction for each value of X is

$$P(X^1 = i \mid \xi) = \int \theta_i P(\boldsymbol{\theta} \mid \xi) d\boldsymbol{\theta} = \frac{\alpha_i}{\sum_j \alpha_j}$$

It is easy to see that, if the prior is a Dirichlet prior with hyperparameters $\alpha_1, \ldots, \alpha_L$, then the posterior is a Dirichlet with hyperparameters $\alpha_1 + N_1, \ldots, \alpha_L + N_L$. Thus, we get that the prediction for X^{N+1} is

$$P(X^{N+1} = i \mid x^1, \ldots, x^N, \xi) = \frac{\alpha_i + N_i}{\sum_j (\alpha_j + N_j)}.$$

We can think of the hyperparameters α_i as the number of "imaginary" examples in which we saw outcome i. Thus, the ratio between hyperparameters corresponds to our initial assessment of the relative probability of the corresponding outcomes. The total weight of the hyperparameters represent our confidence (or entrenchment) in the prior knowledge. As we can see, if this weight is large, our estimates for the parameters tend to be further off from the empirical frequencies observed in the training data.

3 A hierarchical prior

We now describe a more structured prior that captures our uncertainty about the set of "feasible" values of X. We define a random variable V that takes values from the set 2^{Σ} of possible subsets of Σ. The intended semantics for this variable, is that if we know the value of V, then $\theta_i > 0$ iff $i \in V$.

Clearly, the hypothesis $V = \Sigma'$ (for $\Sigma' \subseteq \Sigma$) is consistent with training data only if Σ' contains all the indices i for which $N_i > 0$. We denote by Σ^o the set of observed symbols. That is, $\Sigma^o = \{i : N_i > 0\}$, and we let $k^o = |\Sigma^o|$.

Suppose we know the value of V. Given this assumption, we can define a Dirichlet prior over possible multinomial distributions $\boldsymbol{\theta}$ if we use the same hyper-parameter α for each symbol in V. Formally, we define the prior:

$$P(\boldsymbol{\theta}|V) = \frac{\Gamma(|V|\alpha)}{\Gamma(\alpha)^{|V|}} \prod_{i \in V} \theta_i^{\alpha-1} \quad (\sum_i \theta_i = 1 \text{ and } \theta_i = 0 \text{ for all } i \notin V) \tag{3}$$

Using Eq. (2), we have that:

$$P(X^{N+1} = i \mid x^1, \ldots, x^n, V) = \begin{cases} \frac{\alpha + N_i}{|V|\alpha + N} & \text{if } i \in V \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

Now consider the case where we are uncertain about the actual set of feasible outcomes. We construct a two tiered prior over the values of V. We start with a prior over the size of V, and then assume that all sets of the same cardinality have the same prior probability. We let the random variable S denote the cardinality of V. We assume that we are given a distribution $P(S = k)$ for $k = 1, \ldots, L$. We define the prior over sets to be:

$$P(V \mid S = k) = \binom{L}{k}^{-1} \tag{5}$$

We now examine how to compute the posterior predictions given this hierarchical prior. Let D denote the training data $x^1, \ldots, x^N$. Then it is easy to verify that

$$P(X^{N+1} = i \mid D) \quad = \quad \sum_k \frac{\alpha + N_i}{k\alpha + N} \sum_{V, |V| = k, i \in V} P(V \mid D) \tag{6}$$

Let us now examine which sets V actually contribute to this sum.

First, we note that sets that do not contain Σ^o have zero posterior probability, since they are inconsistent with the observed data. Thus, we can examine only sets V that contain Σ^o. Second, as we noted above, $P(D \mid V)$ is the same for all sets of cardinality k that contain Σ^o. Moreover, by definition the prior for all these sets is the same. Using Bayes rule, we conclude that $P(V \mid D)$ is the same for all sets of size k that contain Σ^o. Thus, we can simplify the inner summation in Eq. (6), by multiplying the number of sets in the score of the summation by the posterior probability of such sets.

There are two cases. If $i \in \Sigma^o$, then any set V that has non-zero posterior appears in the sum. Thus, in this case we can write:

$$P(X^{N+1} = i \mid D) = \sum_k \frac{\alpha + N_i}{k\alpha + N} P(S = k \mid D) \qquad \text{if } i \in \Sigma^o$$

If $i \notin \Sigma^o$, then we need to estimate the fraction of subsets of V with non-zero posterior that contain i. This leads to an equation similar to the one above, but with a correction for this fraction. Note, however, that all unobserved outcomes have the same posterior probability. Thus, we can simply divide the mass that was not assigned to the observed outcomes among the unseen symbols.

Notice that the single term in Eq. (3) that depends on N_i can be moved outside the summation. Thus, to make predictions, we only need to estimate the quantity:

$$C(D, L) = \sum_{k=k^o}^{L} \frac{k^o\alpha + N}{k\alpha + N} P(k \mid D)$$

and then

$$P(X^{N+1} = i \mid D) = \begin{cases} \frac{\alpha+N_i}{k^o\alpha+N} C(D, L) & \text{if } i \in \Sigma^o \\ \frac{1}{n-k^o}(1 - C(D, L)) & \text{if } i \notin \Sigma^o \end{cases}$$

We can therefore think of $C(D, L)$ as scaling factor that we apply to the Dirichlet prediction that assumes that we have seen all of the feasible symbols. The quantity $1 - C(D, L)$ is the probability mass assigned to *novel* (i.e., unseen) outcomes.

Using properties of Dirichlet priors we get the following characterization of $C(D, L)$.

Proposition 3.1:

$$P(S = k \mid D) = \frac{m_k}{\sum_{k' \geq k^o} m_k}, \textit{ where } m_k = P(S = k)\frac{k!}{(k - k^o)!} \cdot \frac{\Gamma(k\alpha)}{\Gamma(k\alpha + N)}.$$

Proof: To compute $C(D, L)$, we need to compute $P(S = k \mid D)$. Using Bayes rule, we have that

$$P(k \mid D) = \frac{P(D \mid S = k)P(S = k)}{\sum_{k'} P(D \mid S = k')P(S = k')} \tag{7}$$

By introduction of variables, we have that:

$$P(D \mid S = k) = \sum_{V \supseteq \Sigma^o, |V|=k} P(D \mid V)P(V \mid S = k).$$

Using standard properties of Dirichlet priors, we have that if $\Sigma^o \subseteq V$, then

$$P(D|V) = \frac{\Gamma(|V|\alpha)}{\Gamma(|V|\alpha + N)} \prod_{i \in V^o} \frac{\Gamma(\alpha + N_i)}{\Gamma(\alpha)} \tag{8}$$

Now, using Eq. (8) and (5), we get that if $\Sigma^o \subseteq V$, and $k = |V|$, then

$$P(D \mid V)P(V \mid S = k) = \binom{L}{k}^{-1} \frac{\Gamma(k\alpha)}{\Gamma(k\alpha + N)} \Gamma(\alpha)^{-k^o} \prod_{i \in \Sigma^o} \Gamma(\alpha + N_i). \tag{9}$$

Thus,

$$\begin{aligned} P(D \mid S = k) &= \binom{L - k^o}{k - k^o}\binom{n}{k}^{-1} \frac{\Gamma(k\alpha)}{\Gamma(k\alpha + N)} \Gamma(\alpha)^{-k^o} \prod_{i \in \Sigma^o} \Gamma(\alpha + N_i) \\ &= \left[\frac{(L - k^o)!}{L!} \Gamma(\alpha)^{-k^o} \prod_{i \in \Sigma^o} \Gamma(\alpha + N_i)\right] \frac{k!}{(k - k^o)!} \cdot \frac{\Gamma(k\alpha)}{\Gamma(k\alpha + N)} \end{aligned} \tag{10}$$

Note that the term in the square brackets does not depend on the choice of k. Thus, it cancels out when plug Eq. (10) in Eq.(7). The desired equality follows directly. ∎

From the above proposition we immediately get that

Corollary 3.2:

$$C(D, L) = \frac{\sum_{k=k^o}^{L} \frac{k^o\alpha+N}{k\alpha+N} m_k}{\sum_{k' \geq k^o} m_k}. \tag{11}$$

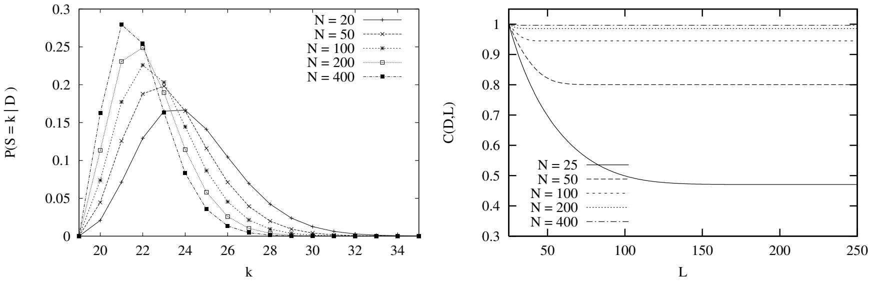

Figure 1: Left: Illustration of the posterior distribution $P(S \mid D)$ for different values of N, with $k^o = 20$, $L = 100$, $\alpha = .25$, and $P(S = k) \propto 0.25^k$. Right: Illustration showing the change in $C(D, L)$ for different values of N, with $k^o = 25$, $\alpha = 1$, and $P(S = k) \propto 0.9^k$.

Note that $P(S = k \mid D)$ and $C(D, L)$ depend only on k^o and N and does not depend on the distribution of counts among the k^o observed symbols. Note that when N is sufficiently larger than k^o (and this depends on the choice of α), then the term $\frac{k!}{(k-k^o)!} \cdot \frac{\Gamma(k\alpha)}{\Gamma(k\alpha+N)}$ is much smaller than 1. This implies that the posterior for larger sets decays rapidly. We can see this behavior on the left hand side of Figure 1 that shows the posterior distribution of $P(S \mid D)$ for different dataset sizes.

4 Unbounded alphabets

By examining the analytic form of $C(D, L)$, we see that the dependency on L is expressed only in the number of terms in the summation. If the terms m_k vanish for large k, then $C(D, L)$ becomes insensitive to the exact size of the alphabet. We can see this behavior on the right hand side of Figure 1, which shows $C(D, L)$ as a function of L. As we can see, when L is close to k^o, then $C(D, L)$ is close to 1. As L grows, $C(D, L)$ asymptotes to a value that depends on N and k^o (as well as α and the prior $P(S = k)$).

This discussion suggests that we can apply our prior in cases where we do not know L in advance. In fact, we can assume that L is unbounded. That is, Σ is isomorphic to $\{1, 2, \ldots\}$. Assume that we assign the prior $P(S = k)$ for each choice of L, and that $\lim_{L\to\infty} P(S = k)$ exists for all k. We define $C(D, \infty) = \lim_{L\to\infty} C(D, L)$. We then use for prediction the term $P(X^{N+1} = i \mid D) = \frac{\alpha+N_i}{k^o\alpha+N} C(D, \infty)$.

For this method to work, we have to ensure that $C(D, \infty)$ is well defined; that is, that the limit exists. Two such cases are identified by the following proposition.

Proposition 4.1: *If $P(S = k)$ is exponentially decreasing in k or if $\alpha \geq 1$ and $P(S = k)$ is polynomially decreasing in k, then $C(D, \infty)$ is well-defined.*

To prove the above proposition we use Stirling's approximation to $\Gamma(\cdot)$ and show that $\lim_{k\to\infty} m_k c^k = 0$ for some constant $c > 1$ (details omitted due to lack of space).

In practice we evaluate $C(D, \infty)$ by computing successive values of (the logarithm of) m_k, until we reach values that are significantly smaller than the largest value beforehand. Since m_k is exponentially decaying, we can ignore the mass in the tail of the sequence. As we can see from the right hand side of Figure 1, there is not much difference between the prediction using a large L, and unbounded one.

5 Empirical evaluation

We have used the proposed estimation method to construct a statistical models for predicting the probability of characters in the context of the previously observed character. Such models, often referred to as bigram models, are of great interest in applications such optical character recognition and text compression.

We tested two of prior distributions for the alphabet size $P_0(S = k)$: an exponential prior, $P_0(S = k) \propto \beta^k$, and a polynomial prior, $P_0(S = k) \propto k^{-\beta}$. The training and test

Method	Perplexity Observed	Novel	Overall
A ($\frac{N_i}{N+r}$)	28.19	141.7	28.20
B (Approximated Good-Turing)	28.15	802.7	28.19
Sparse-Multinomial (Poly)	27.97	3812.9	28.02
Sparse-Multinomial (Exp)	27.97	3913.1	28.03

Table 1: Perplexity results on heterogeneous character data.

material were derived from various archives and included different types of files such C programs, core dumps, and ascii text files. The alphabet for the algorithm consists of all the (ascii and non-ascii) 256 possible characters. The training data consisted of around 170 mega bytes and for testing we used 35 mega bytes.

Each model we compared had to assign a probability to any character. If a character was not observed in the context of the previous character, the new character is assigned the probability of the total mass of novel events. Note that this task is different than common language modeling benchmarks where the probability of each individual word is estimated either using the full context or by "backing off" to a shorter context [8], which is the null context for bigram models.

We compared our approach with two estimation techniques that have been shown to perform well on natural data sets [16]. The first estimates the probability of a symbol i in the context of a given word as $\frac{N_i}{N+r}$ where r is the number of different characters observed at given context (the previous character). The second method, based on an approximation of the Good-Turing estimation scheme [6], estimates the probability of a symbol i as $\frac{(1-f_1/N)N_i}{N}$, where f_1 is the number of different characters that have been observed only once at for the given context. This scheme requires a "fall-back" estimate when $f_1 = n$, as described in more detail in [16]. For evaluation we used the perplexity which is simply the exponentiation of the average log-loss on the test data. Table 1 summarizes the average test-set perplexity for observed characters, novel events, and the overall perplexity. In the experiments we fixed $\alpha = 1/2$ for the parameters of the Dirichlet priors and $\beta = 2$ for the exponentially and polynomially decaying priors of the alphabet size.

One can see from the table that predictions using sparse-multinomials achieve the lowest overall perplexity. (The differences are statistically significant due to the size of the data.) The performance based on the two different priors for the alphabet size is comparable. The results indicate the all the leverage in using sparse-multinomials for prediction is due to more accurate predictions for observed events. Indeed, the perplexity of novel events using sparse-multinomials is much higher than when using either method A or B. Put another way, our approach prefers to "sacrifice" events with low probability (novel events) and suffer high loss in favor of more accurate predictions for frequently occurring events. The net effect is a lower overall perplexity.

6 Discussion

In this paper we presented a Bayesian approach for the problem of estimating the parameters of a multinomial source over a large alphabet. Our method is based on an efficient inference algorithm that is based on hierarchical prior. Among the numerous techniques that have been used for multinomial estimation the one proposed by Ristad [13] is the closest to ours. Though the methodology used by Ristad is substantially different than ours, his method can been seen as a special case of sparse-multinomials with α set to 1 and specific forms for the prior over the alphabet sizes. The main advantage of fixing $\alpha = 1$ is an even simpler inference procedure. The simpler inference procedure demands, however, a price which is loss of flexibility. In addition, our method explicitly represents the posterior distribution. Hence, it is more suitable for tasks, such as stochastic sampling, where an explicit representation of the approximated distribution is required. Our method can be combined with other Bayesian approaches for language modeling such as the one proposed by Mackay and Peto [11].

As briefly discussed in the introduction, there are applications other than language modeling that can make use the proposed modeling scheme. Reinforcement Learning (RL) is an example of such a domain. One of the approaches in RL is to first estimate the parameters of an underlying Markov decision process. However, the number of states of a typical Markov process might be very large. Hence, naive estimation schemes often yield poor results. Instead, one can use sparse multinomials to build a robust estimate for the transition probabilities of each state, despite the fact that the number of times each state was visited might very small. Another possible domain is parameter estimation of large Bayesian networks where one might want to keep the explicit form of posterior distribution for the parameters.

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