Factoring Multidimensional Data to Create a Sophisticated Bayes Classifier

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Abstract
In this paper we derive an explicit formula for calculating the marginal likelihood of a given factorization of a categorical dataset. Since the marginal likelihood is proportional to the posterior probability of the factorization, these likelihoods can be used to order all possible factorizations and select the “best” way to factor the distribution from which the dataset is drawn. The best factorization can then be used to construct a Bayes classifier which benefits from factoring out mutually independent sets of variables.

1 Introduction
We wish to investigate the most efficient way to compute the probability of some variable conditioned on other variables, i.e. to calculate \( P(y \mid x) \). This can be done using the definition of conditional probability which says:

\[
P(y \mid x) = \frac{P(y, x)}{P(x)}.\tag{1}
\]

The denominator in Equation 1 is a scaling factor which doesn’t depend on \( y \), so our focus will be the estimation of \( P(y, x) \), which can also be written as

\[
P(y, x) = P(y)P(x \mid y).\tag{2}
\]

Since we assume \( y \) is a single variable, we can efficiently estimate \( P(y) \), so the problem can also be reduced to estimating \( P(x \mid y) \).

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The simplest approach to computing $P(y, x)$ would be to construct an $N$ dimensional histogram, assuming we have $N - 1$ random variables in $x$, and computing the relative frequency of events ending up in the bin $(y, x)$. This method has the advantage that we don’t have to make any assumptions about the distribution from which the data is drawn. The drawback is that the error on the prediction of $y$ will scale exponentially like $K^{N/2}$, where $K$ is the number of categories or bins for each variable. This makes intuitive sense since for a dataset with a fixed number of samples, the number of bins grows exponentially with the number of variables, and therefore we should expect a large error because the statistics in each bin will be low.

One common solution to this problem is to use a Naive Bayes classifier [1] where all the $X_i$ variables are assumed to be mutually independent conditional on $y$. With this assumption we can rewrite Equation 1 as

$$P(y | x) = \frac{1}{P(x)} P(y) \prod_i P(x_i | y). \quad (3)$$

The error on the prediction in this case only grows like $\sqrt{2N}$. This also makes intuitive sense since we have reduced the calculation from looking up the probability in an $N$ dimensional histogram to a product of $N$ 1-dimensional histograms. However, the accuracy of this estimate will depend on how good the independent approximation is.

In this paper, we propose a solution to this problem by asking how the distribution $P(x | y)$ can be factored. For example, supposing we had just two variables $X_1$ and $X_2$, we can ask whether it can be factored as $P(x_1 | y)P(x_2 | y)$ or whether we need to consider the full probability $P(x_1, x_2 | y)$. To distinguish between these two models, we consider ordering them by the posterior probability of the factorization [2]. For the example just described this involves calculating two probabilities: $P(M_I | D)$ and $P(M_D | D)$, where $M_I$ stands for the independent model which can be factored and $M_D$ stands for the dependent model. In particular, we show that for a categorical distribution, there is a simple analytical solution for computing the marginal likelihood\(^1\) of a given model, i.e. $P(D | M)$ which is proportional to the posterior probability $P(M | D)$ up to a constant scaling factor and some prior over the models.

For the general case of $N$ variables, we have to consider all possible ways to factor $P(x | y)$. This is equivalent to considering all possible groupings of the variables, where within each group the variables are considered to be dependent, but the different groups are treated as independent. For example, all possible groupings of 4 variables are shown in Table 1.

The rest of the paper is organized as follows: in Section 2 we consider the general problem of how to factor a distribution $P(x)$ by computing the marginal likelihood $P(D | M)$ for a given factorization. In Section 3 we explicitly calculate these terms for two binary random variables and then give a formula for the Bayes factor to distinguish between them. Finally, in Section 4 we give concluding remarks.

\(^1\)By marginal likelihood we mean the likelihood of the model independent of the specific parameters governing the model.
Table 1: All possible groupings of 4 variables. Each group represents a different way to factor the probability distribution $P(x_1, x_2, x_3, x_4)$.

2 Calculation

In this section, we consider the general problem of factoring a distribution of $N$ categorical random variables labelled $(X_0, X_1, \ldots, X_N)$. To do so, we choose the “best” factorization where the ordering of the different factorizations is determined by the posterior probability of a given factorization. If we label a given factorization as a model $M$, we wish to compute $P(M \mid D)$ where $D$ stands for the data. This posterior is related to the marginal likelihood $P(D \mid M)$ as follows:

$$P(M \mid D) = \frac{P(D \mid M)P(M)}{P(D)}.$$  

(4)

The first term in the numerator of Equation 4 is the marginal likelihood, the second term in the numerator represents any prior we may have, and the denominator is simply a scaling factor which is not relevant if we only consider ordering the models. So, to order the models we need to compute the marginal likelihood $P(D \mid M)$ and then we can multiply it by any prior we might have (or simply use the likelihood directly if we have no preference for any particular factorization).

We will represent each possible factorization as a particular grouping of the $N$ variables. For example, the possible groupings for 4 random variables are shown in Table 1. For a given factorization $M$, we will label each group within the factorization as $g_i$, where $i$ runs over all the different groups. For example, one possible factorization of 4 random variables is $((X_1, X_2), (X_3), (X_4))$. For this case, the group $(X_1, X_2)$ will be referred to as $g_0$, the next group $(X_3)$ as $g_1$, and $(X_4)$ as $g_2$.

The probability distribution for each group $g_i$, can be specified by the variables $p_{i,j}$ labeling the probability of landing in the $j^{th}$ bin for group $g_i$. When referring to these
probabilities for a general group $g$ we will also sometimes denote these probabilities as $p_{g,j}$. The number of bins in each group is equal to 

$$
\eta_i = \prod_{X \in g_i} |X|.
$$

where $|X|$ is the number of possible values for the random variable $X$. For the previous example, assuming each variable can take on only two discrete values, there would be 4 probabilities for the first group, $p_{0,0}, p_{0,1}, p_{0,2}, p_{0,3}$, two probabilities for the second group $p_{1,0}, p_{1,1}$, and two probabilities for the last group $p_{2,0}, p_{2,1}$. We will sometimes denote these values as vectors, i.e. $\mathbf{p}_0$, $\mathbf{p}_1$, and $\mathbf{p}_2$. When referring to a general group $g$, we will simply write $\mathbf{p}_g$.

We begin by considering the marginal likelihood and expanding it in terms of the probabilities $p_{i,j}$

$$
P(D \mid M) = \int_{p_{0,1}} \int_{p_{0,2}} \cdots \int_{p_{m,n_m}} P(D \mid p_{i,j}, M) P(p_{i,j} \mid M),
$$

where $m$ is equal to the number of groups. The two terms on the right are the full likelihood and the prior for the model parameters $p_{i,j}$ for the factorization $M$.

For the second term in Equation 5, we assume a flat Dirichlet prior for the probabilities within each group,

$$
P(p_{i,j} \mid M) = \prod_{g \in M} \text{Dir}(\mathbf{p}_g, 1). \quad (6)
$$

The Dirichlet distribution is given by the equation:

$$
\text{Dir}(\alpha, \mathbf{x}) = \frac{1}{B(\alpha)} \prod_i x_i^{\alpha_i-1} \quad (7)
$$

where $B$ is the multivariate Beta function given by

$$
B(\alpha) = \frac{\prod_i \Gamma(\alpha_i)}{\Gamma(\sum_i \alpha_i)}. \quad (8)
$$

The first term in Equation 5 is the full likelihood of observing a dataset $D$, which is given by the multinomial distribution

$$
P(D \mid p_{i,j}, M) = \frac{N!}{\prod_i n_i!} \prod_i p_i^{n_i}. \quad (9)
$$

Note that in this last expression, the $i$ variable runs over all possible combinations of the values for the $X$ variables, $n_i$ represents the number of samples with outcome $i$, and $p_i$
The last product in this expression can be written as

$$\text{Dir}(p_g, 1) \prod_i p_{g,i} = \frac{1}{B(1)} \prod_i p_{g,i} = \text{Dir}(p_g, 1 + n) \frac{B(1 + n)}{B(1)}.$$ (12)
Table 3: Table showing the mapping between the values for the random variables $x$ and the numbers in Equation 15.

| $x_1$ | $x_2$ | $n_i$ |
|-------|-------|-------|
| 0     | 0     | $n_1$ |
| 0     | 1     | $n_2$ |
| 1     | 0     | $n_3$ |
| 1     | 1     | $n_4$ |

Plugging this back into Equation 11 we get

$$P(D \mid M) = \int_{p_{0,1}} \int_{p_{0,2}} \cdots \int_{p_{m,n_m}} \frac{N!}{\prod_i n_i!} \prod_{g \in M} \text{Dir}(p_g, 1 + n) \frac{B(1 + n_g)}{B(1)} \quad (13)$$

which simplifies to

$$P(D \mid M) = \frac{N!}{\prod_i n_i!} \prod_{g \in M} \frac{B(1 + n_g)}{B(1)}. \quad (14)$$

Note that the length of the vector $1$ in the denominator of Equation 14 is equal to $\eta_i$ for group $i$, i.e. it has the same length as $p_g$ and $n_g$.

Equation 14 is the main result of this paper which gives an explicit formula for the calculation of the marginal likelihood of a given factorization. There exist efficient routines for calculating the multivariate Beta function, so calculating the marginal likelihood for a given factorization is straightforward. In practice, it is useful to compute the log of Equation 14 when comparing factorizations since otherwise the factorials can produce numbers which do not fit into standard 32 or 64 bit floats and integers.

3 Two Binary Variables

In the simple case of 2 binary random variables, we get the result

$$P(D \mid M_I) = \frac{(n_1 + n_2)!}{n_1! n_2!} \frac{(n_1 + n_3)!}{n_1! n_3!} \frac{(n_2 + n_4)!}{n_2! n_4!} \frac{(n_3 + n_4)!}{n_3! n_4!} \frac{(N + 1)(N + 1)!}{6} \quad (15)$$

$$P(D \mid M_D) = \frac{6}{(N + 3)(N + 2)(N + 1)} \quad (16)$$

where $M_I$ stands for the independent hypothesis, and $M_D$ stands for the dependent hypothesis, the $n_i$ are the numbers of samples with the values shown in Table 3, and $N$ is the total number of samples.

We can use these values to compute the Bayes Factor

$$K = \frac{P(D \mid M_I)}{P(D \mid M_D)} = \frac{(n_1 + n_2)!}{n_1! n_2!} \frac{(n_1 + n_3)!}{n_1! n_3!} \frac{(n_2 + n_4)!}{n_2! n_4!} \frac{(n_3 + n_4)!}{n_3! n_4!} \frac{(N + 3)(N + 2)}{(N + 1)!6}.$$
For values of $K$ less than 1 the data favor the correlated hypothesis, and for values greater than 1 it favors the independent hypothesis.

### 4 Conclusion

We have given an explicit formula for calculating the marginal likelihood of a given factorization of a dataset of categorical random variables. This formula can be used to choose the best way to factor the conditional probability $P(x \mid y)$ and thus gives us a way to construct a Bayes classifier which takes full advantage of mutually independent sets of variables.

Although it is possible in principle sort through all possible factorization using Equation 14, the number of calculations of the multivariate Beta function grows like the size of the powerset of the number of variables. This means that in practice it is prohibitive to sort through all factorizations for more than approximately 30 variables (where one would need to calculate over a billion terms). However, we suspect that for real world data there are ways to considerably reduce the number of factorizations to check by using heuristics.

One particular area where we hope this technique will be of use is in high energy physics analyses. For these analyses it is very common to define a broad range of cuts designed to remove background events and keep events of interest. Although multiple cuts are used, in the end the ultimate goal is often to define a total cut efficiency and sacrifice, i.e. to determine what percentage of background events are successfully cut and what fraction of signal events are “accidentally” cut. If you have a full Monte Carlo simulation of both background and signal it can be relatively easy to do this, but often some of the background events cannot be simulated due to complexity or time constraints. Therefore, it is often necessary to use a combined fit to a sideband and the region of interest to fit for the cut efficiencies. The number of terms in this fit will grow exponentially as the number of cuts increases, and therefore this technique can be used to construct a model of for the cut efficiencies with considerably fewer parameters.

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### References

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[2] Edwin T. Jaynes. *Probability Theory: The Logic of Science*. Cambridge University Press, Cambridge, England, first edition, 2003.