# Algorithms and Hardness for Estimating Statistical Similarity

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#### Abstract

We study the problem of computing statistical similarity between probability distributions. For distributions P and Q over a finite sample space, their statistical similarity is defined as  $S_{\text{stat}}(P,Q) := \sum_x \min(P(x),Q(x))$ . Statistical similarity is a basic measure of similarity between distributions, with several natural interpretations, and captures the Bayes error in prediction and hypothesis testing problems. Recent work has established that, somewhat surprisingly, even for the simple class of product distributions, exactly computing statistical similarity is #P-hard. This motivates the question of designing approximation algorithms for statistical similarity. Our primary contribution is a Fully Polynomial-Time deterministic Approximation Scheme (FPTAS) for estimating statistical similarity between two product distributions. To obtain this result, we introduce a new variant of the Knapsack problem, which we call the Masked Knapsack problem, and design an FPTAS to estimate the number of solutions of a multidimensional version of this problem. This new technical contribution could be of independent interest. Furthermore, we also establish a complementary hardness result. We show that it is NP-hard to estimate statistical similarity when P and Q are Bayes net distributions of in-degree 2.

### 1 Introduction

Given two distributions P and Q over a finite sample space, their statistical similarity (denoted  $S_{\text{stat}}(P,Q)$  is defined as:

$$S_{\text{stat}}(P,Q) := \sum_{x} \min(P(x), Q(x)). \tag{1}$$

Statistical similarity serves as a fundamental measure in machine learning and statistical inference. We defer a detailed discussion of motivating applications to Section 1.1.

When the sample space is small, computing  $S_{\rm stat}$  is trivial. However, for high-dimensional distributions, this computation presents significant challenges. Surprisingly, recent work [BGM<sup>+</sup>23] has established that computing  $S_{\rm stat}$  is #P-hard even for the simple class of product distributions. This hardness result is striking given that product distributions represent one of the most basic distribution classes, where each dimension is independent.

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The hardness of this elementary case raises fundamental questions about the computational nature of statistical similarity: What are the boundaries between tractable and intractable computation? Can we develop efficient approximation algorithms for cases of practical interest?

Our work initiates a principled investigation of approximating statistical similarity, systematically identifying both tractable and intractable cases. Our primary contribution is a Fully Polynomial-Time deterministic Approximation Scheme (FPTAS) for estimating  $S_{\rm stat}$  between product distributions. Our technical approach introduces novel algorithmic techniques. To obtain the FPTAS for product distributions, we develop a new variant of the knapsack counting problem, which we call the Masked Knapsack problem. We establish an FPTAS for the multidimensional version of this problem, a result that may be of independent interest.

To complement this algorithmic result, we establish sharp computational boundaries by proving that approximating  $S_{\text{stat}}$  becomes NP-hard even for slightly more general distributions. Specifically, we show that the problem is NP-hard to approximate for Bayes net distributions with in-degree 2.

#### 1.1 Motivating Applications

Statistical similarity plays a central role across multiple domains in machine learning and statistics. We examine three key applications of statistical similarity: Its connection to Bayes error in prediction problems, its role in characterizing optimal decision rules in hypothesis testing, and its interpretation through coupling theory. These applications not only demonstrate the theoretical significance of  $S_{\rm stat}$  but also motivate our investigation of efficient algorithms for its computation.

Statistical similarity arises naturally in the analysis of prediction problems through the notion of Bayes error. Consider a binary prediction problem defined by a distribution P over  $X \times \{0, 1\}$ , where X is a finite feature space. When a classifier  $g: X \to \{0, 1\}$  attempts to predict the label, it incurs a 0-1 prediction error measured as  $\mathbf{Pr}_{(x,y)\sim P}[g(x) \neq y]$ . The Bayes optimal classifier, which outputs 1 if and only if P(x|1) > P(x|0), achieves the minimum possible error  $R^*$ , known as the Bayes error. This error represents a fundamental lower bound that no classifier can surpass.

This connection manifests through a precise mathematical relationship: For any prediction problem, the Bayes error exactly equals the statistical similarity between its scaled likelihood distributions. Specifically, if we denote the prior probabilities P(0) and P(1) by  $\alpha_0$  and  $\alpha_1$  respectively, then  $R^* = S_{\text{stat}}(\alpha_0 P(X|0), \alpha_1 P(X|1))$  (a proof is given in Appendix A), where  $\alpha_i P(X|i)$  represents the sub-distribution obtained by scaling P(X|i) with  $\alpha_i$ .

The relationship between statistical similarity and optimal decision-making extends beyond prediction problems to the domain of hypothesis testing [LR08, Nie14]. This setting is particularly relevant to our computational focus, as it deals with known distributions representing null and alternate hypotheses. A recent result [KA24] establishes how statistical similarity between product distributions determines the optimal error in hypothesis testing [PSNK14, BK15].

To illustrate this connection, consider a hypothesis testing game where a random bit  $Y \in \{0,1\}$  is drawn with bias  $p_1$  (letting  $p_0 = 1 - p_1$ ), followed by an i.i.d. sequence  $X_1, \ldots, X_n$  where each  $X_i \in \{0,1\}$  satisfies  $\mathbf{Pr}[X_i = 1|Y = 1] = \psi_i$  and  $\mathbf{Pr}[X_i = 1|Y = 0] = \eta_i$  for parameters  $\psi, \eta \in (0,1)^n$ . The optimal decision rule  $f^{\mathsf{OPT}}: \{0,1\}^n \to \{0,1\}$  that minimizes  $\mathbf{Pr}[f^{\mathsf{OPT}}(X) \neq Y]$  achieves an error rate of  $S_{\mathsf{stat}}(p_1 \mathsf{Bern}(\psi), p_0 \mathsf{Bern}(\eta))$ , where  $\mathsf{Bern}(\psi)$  denotes the product distribution of individual  $\mathsf{Bern}(\psi_i)$  distributions.

These theoretical connections have significant practical implications. Since Bayes error represents the theoretically optimal performance limit, statistical similarity serves as a benchmark for the evaluation of machine learning models. This capability has spurred extensive research in

estimating Bayes error and statistical similarity [FH75, Dev85, NXH19, TWV<sup>+</sup>21, IYC<sup>+</sup>23].

Statistical similarity can be interpreted through coupling theory. For distributions P and Q,  $S_{\text{stat}}(P,Q)$  equals the maximum probability of equality achievable by any coupling (X,Y) where  $X \sim P$  and  $Y \sim Q$ . Coupling theory, introduced by Doeblin [Doe38], has led to important results in computer science and mathematics [Lin02, LPW06, MT12]. This connection highlights the significance of statistical similarity to broader audience.

Finally, statistical similarity admits a characterization in the form of statistical distance (also known as total variation distance)  $d_{\text{TV}}$ , defined as  $d_{\text{TV}}(P,Q) := \max_{S \subseteq D} (P(S) - Q(S)) = \frac{1}{2} \sum_{x \in D} |P(x) - Q(x)|$ . The identity  $S_{\text{stat}}(P,Q) = 1 - d_{\text{TV}}(P,Q)$ , known as Scheffé's identity, establishes a duality.

#### 1.2 Paper Organization

We present some necessary background material in Section 2. We then present a survey of related work in Section 3. Section 4 describes our primary contributions, and an overview of proof techniques. Section 5 is dedicated to the algorithmic result: An FPTAS to estimate the statistical similarity between product distributions. The proof of NP-hardness of estimating the statistical similarity between in-degree 2 Bayes net distributions is provided in Section 6. Section 7 gives concluding remarks. Appendix A discusses the connections between Bayes error and statistical similarity. In Appendix B, we present the pseudocode for all of our procedures.

#### 2 Preliminaries

We use [n] to denote the set  $\{1, \ldots, n\}$ . We will use log to denote  $\log_2$ . The following notion of a deterministic approximation algorithm is important in this work.

**Definition 1.** A function  $f: \{0,1\}^* \to \mathbb{R}$  admits a fully polynomial-time approximation scheme (FPTAS) if there is a deterministic algorithm  $\mathcal{A}$  such that for every input x (of length n) and  $\varepsilon > 0$ , the algorithm  $\mathcal{A}$  outputs a  $(1 + \varepsilon)$ -multiplicative approximation to f(x), i.e., a value that lies in the interval  $[f(x)/(1+\varepsilon), (1+\varepsilon)f(x)]$ . The running time of  $\mathcal{A}$  is poly $(n, 1/\varepsilon)$ .

A related notion is that of an additive approximation in which we are interested in ensuring that the output of algorithm  $\mathcal{A}$  is within the range  $[f(x) - \varepsilon), f(x) + \varepsilon]$ .

A Bernoulli distribution with parameter p is denoted by Bern(p). A product distribution is a product of independent Bernoulli distributions. A product distribution P over  $\{0,1\}^n$  can be described by n Bernoulli parameters  $p_1, \ldots, p_n$  where each  $p_i \in [0,1]$  is the probability that the i-th coordinate equals 1 (such a P is usually denoted by Bern $(p_1, \ldots, p_n)$  or  $\bigotimes_{i=1}^n \text{Bern}(p_i)$ ). For any  $x \in \{0,1\}^n$ , the probability of x with respect to the product distribution P is given by  $P(x) = \prod_{i \in S_x} p_i \prod_{i \in [n] \setminus S_x} (1-p_i)$  whereby  $S_x \subseteq [n]$  is such that  $i \in S_x$  if and only if  $x_i = 1$ .

Let  $\ell$  be the maximum number of bits required to represent any Bernoulli parameter  $p_i$ . Then the number of bits need to represent a product distribution over n variables is  $n\ell$ .

**Definition 2.** Given two distributions P and Q over a finite sample space D, the statistical similarity between P and Q is

$$S_{\mathrm{stat}}(P,Q) := \sum_{x \in D} \min(P(x), Q(x)).$$

Statistical similarity can be proved to be equal to the complement of statistical distance, which is commonly called total variation distance and denoted by  $d_{\text{TV}}$ . See below.

**Definition 3.** For distributions P, Q over a sample space D, the total variation (TV) distance between P and Q is

$$d_{\text{TV}}(P, Q) := \sum_{x \in D} \max(0, P(x) - Q(x)).$$

**Proposition 4** (Scheffé's identity, see also [Tsy09]). Let P, Q be distributions over a sample space D. Then

$$S_{\text{stat}}(P,Q) = 1 - d_{\text{TV}}(P,Q)$$
.

*Proof.* We have that

$$S_{\text{stat}}(P, Q) = \sum_{x \in D} \min(P(x), Q(x))$$

$$= \sum_{x \in D} \min(P(x), P(x) + Q(x) - P(x))$$

$$= \sum_{x \in D} P(x) + \sum_{x \in D} \min(0, Q(x) - P(x))$$

$$= 1 - \sum_{x \in D} \max(0, P(x) - Q(x))$$

$$= 1 - d_{\text{TV}}(P, Q).$$

We shall also require the notion of *sub-distribution* defined as follows: P is a sub-distribution over a sample space D, if there exists  $0 < \alpha \le 1$  and a distribution P' over D such that for every  $x \in D$ ,  $P(x) = \alpha P'(x)$ . If P' is a product distribution, then P is called a sub-product distribution. The notion of statistical similarity can be extended to sub-distributions.

#### 2.1 Counting Problems

A function f from  $\{0,1\}^*$  to nonnegative integers is in the class #P if there is a polynomial-time nondeterministic Turing machine M so that for any x the value of f(x) is equal to the number of accepting paths of M(x). For functions whose range is not  $\mathbb{N}$ , it is standard to define the notion of #P-membership via normalization (by some efficiently computable integer).

The following result establishes the hardness of computing statistical similarity.

**Theorem 5** ([BGM<sup>+</sup>23]). Exactly computing  $S_{\text{stat}}$  between product distributions is #P-hard.

#### 2.1.1 #MASKEDKNAPSACK

The standard #KNAPSACK problem is the following computational problem: Given weights  $a_1, \ldots, a_n$  and capacity b, compute the number of  $x \in \{0,1\}^n$  so that  $\sum_{i=1}^n a_i x_i \leq b$ .

In this paper, we introduce the following "masked" version of #KNAPSACK.

**Definition 6** (#MASKEDKNAPSACK). #MASKEDKNAPSACK is the following counting problem. An instance K for the problem is specified by a set of weights  $a_1, \ldots, a_n$ , a capacity b, and a mask vector  $u = (u_1, \ldots, u_n) \in \{0, 1\}^n$ . We say that  $x = x_1 \ldots, x_n \in \{0, 1\}^n$  is a solution to K if  $\sum_{j=1}^n a_j (x_j \oplus u_j) \leq b$ . The computational problem is: given an instance K, count the number of solutions to K. The sum  $\sum_{i=1}^n a_i + b$  is called the *total weight* of the instance.

Note that when the mask vector u is all 0 vector, the #MASKEDKNAPSACK is #KNAPSACK. We will need a multidimensional version of MASKEDKNAPSACK.

**Definition** 7 (Multidimensional #MASKEDKNAPSACK). An m-dimensional #MASKEDKNAPSACK instance K is specified by m many #MASKEDKNAPSACK instances  $K_1, \ldots, K_m$  over n variables. A binary vector x is a solution to K, if it is a solution to all  $K_i$ 's. The computational problem is: given an instance K, count the number of solutions of K.

#### 3 Related Work

Statistical similarity is a fundamental measure with deep connections to machine learning, hypothesis testing, and algorithmic applications. Estimating the Bayes error has been a topic of continued interest in the machine learning community [FH75, Dev85, NXH19, TWV<sup>+</sup>21, IYC<sup>+</sup>23]. These works focus on the setting where distributions are only accessible through samples rather than explicitly specified, leading to techniques distinct from those needed in our setting of explicitly represented distributions.

The computational complexity of statistical similarity was established through Scheffé's identity  $(S_{\text{stat}}(P,Q)+d_{\text{TV}}(P,Q)=1)$  and the result of [BGM<sup>+</sup>23], showing that exact computation is #P-hard even for product distributions. This hardness naturally leads to the study of approximation algorithms, with multiplicative approximation being stronger than additive approximation for measures bounded in [0, 1].

For distributions samplable by Boolean circuits, additive approximation of statistical similarity is complete for SZK (Statistical Zero Knowledge) [SV03], while the problem becomes tractable for distributions that are both samplable and have efficiently computable point probabilities [BGMV20].

While recent work has made significant progress on multiplicative approximation of statistical distance (also known as total variation distance), including an FPRAS [FGJW23] and an FPTAS [FLL24] for product distributions, these results do not directly translate to statistical similarity. This is because multiplicative approximation of statistical distance does not yield multiplicative approximation of its complement (statistical similarity), necessitating new algorithmic techniques for statistical similarity. Similarly, the NP-hardness result for multiplicatively approximating statistical distance between Bayes nets [BGM+23] does not immediately imply hardness for statistical similarity.

It is perhaps worth remarking that technical barrier in translating multiplicative approximation of statistical distance to statistical similarity is rather fundamental, i.e., it is not possible in general to use an efficient multiplicative approximation algorithm for a function f in order to design an efficient multiplicative approximation algorithm for 1-f. In particular, even if there is an efficient multiplicative approximation algorithm f, approximating 1-f could be NP-hard. For instance, let f be a function that takes as input a Boolean DNF formula  $\phi$  and outputs the probability that a random assignment satisfies  $\phi$ . It is known that there is a randomized multiplicative approximation algorithm for estimating f [KLM89]. However, a multiplicative approximation algorithms (RP = NP). This is because the complement of a DNF formula is a CNF formula, and there is no efficient randomized multiplicative approximation for estimating the acceptance probability of CNF formulas unless RP = NP.

The connection between statistical similarity and hypothesis testing has been explored in several works. While [KA24] provides analytical bounds on statistical similarity for product distributions in the context of hypothesis testing, these bounds do not yield multiplicative approximation algorithms.

### 3.1 The Need for New Techniques for $S_{\text{stat}}$

A curious reader may wonder about the need for new techniques to arrive at our results in light of prior work on the multiplicative approximation of  $d_{\text{TV}}$ . In particular, while multiplicative approximation of  $d_{\text{TV}}$  does not lead to multiplicative approximation of  $S_{\text{stat}}$ , it is worth asking whether techniques employed in these aforementioned works can be extended to  $S_{\text{stat}}$ . We now discuss the limitations of these techniques.

The prior work [FGJW23] on multiplicative approximation of  $d_{\text{TV}}$  uses the notion of coupling between distributions that is mentioned in the introduction. Let P and Q be two product distributions over  $\{0,1\}^n$  specified by their Bernoulli parameters  $\{p_i\}_{i=1}^n$  and  $\{q_i\}_{i=1}^n$  for the n dimensions respectively. Then their TV distance is the minimum probability of seeing  $X \neq Y$  for any coupling (X,Y) such that  $X \sim P$  and  $Y \sim Q$ . A natural candidate for this minimum coupling would be the product of locally minimum couplings: that is distribution C over  $\{00,01,10,11\}^n$  where the i-th dimension  $C_i$  is the best coupling between  $\text{Bern}(p_i)$  and  $\text{Bern}(q_i)$ . Unfortunately, it can be shown that there exists examples where the optimal coupling O can get a still smaller probability and C is not optimal. Nevertheless, it turns out that one can multiplicatively approximate the ratio  $A = \Pr_O[X \neq Y] / \Pr_C[X \neq Y]$ . The FPRAS for  $d_{\text{TV}}(P,Q)$  follows since it is easy to exactly compute  $\Pr_C[X \neq Y]$ . Towards this, we define a distribution  $\Pi(w) = \Pr_C[X = w \mid X \neq Y]$  and  $f(w) = \Pr_O[X \neq Y \land X = w] / \Pr_O[X \neq Y \land X = w]$ . Then it can be shown that the expectation of f(w) under  $w \sim \Pi$  is exactly A and that  $f(w) \in [0,1]$  and  $A \in [1/n,1]$ . Therefore, we can design and FPRAS for estimating A using standard Monte-Carlo sampling.

We face a barrier while executing this idea for  $S_{\text{stat}}$  approximation. First, note that for  $S_{\text{stat}}$ , we need to approximate the ratio  $A' = \mathbf{Pr}_O[X = Y] / \mathbf{Pr}_C[X = Y]$ . Then, we may define a distribution  $\Pi'(w) = \mathbf{Pr}_C[X = w \mid X = Y]$  and  $f'(w) = \mathbf{Pr}_O[X = Y \land X = w] / \mathbf{Pr}_C[X = Y \land X = w]$  similarly, where O is the minimum coupling and C is the product of locally minimum couplings as before. However, now we see that  $f'(w) \in [1, \infty)$ , an extreme example being  $P = \text{Bern}(1) \otimes \text{Bern}(0)$  and  $Q = \text{Bern}(1/2) \otimes \text{Bern}(1/2)$  where both f'(w) and A' diverge to infinity, making the Monte-Carlo sampling approach infeasible.

#### 4 Our Results

Our first contribution is the design of a deterministic polynomial-time approximation scheme to estimate the statistical similarity between product distributions.

**Theorem 8.** There is an FPTAS for estimating  $S_{\text{stat}}(P,Q)$  when P and Q are product distributions.

Remark 9. As discussed in the introduction, the Bayes error is characterized by the similarity between sub-distributions. Indeed, the techniques that we use to establish the above result can be extended to the case when P and Q are sub-product distributions. We also stress that our algorithm is deterministic, not randomized.

A natural question is whether this result can be extended to more general distributions such as Bayes net distributions. Our second result is a hardness result.

**Theorem 10.** Given two probability distributions P and Q that are defined by Bayes nets of in-degree two, it is NP-complete to decide whether  $S_{\text{stat}}(P,Q) \neq 0$  or not. Hence the problem of multiplicatively estimating  $S_{\text{stat}}$  is NP-hard.

One of our technical contributions is the introduction of #MaskedKnapsack problem and an FPTAS for this problem. This new problem and the FPTAS could be of interest to a broader audience.

In fact, Theorem 8 is proved via a reduction to 2-dimensional #MASKEDKNAPSACK.

**Theorem 11.** There is an FPTAS A for m-dimensional #MASKEDKNAPSACK on n variables, when m is a constant. The running time of A is  $O\left((n/\varepsilon)^{O(1)}\right)\log W$ , whereby  $\varepsilon$  is the desired error parameter and W is the maximum total weight among the #MASKEDKNAPSACK instances.

#### 4.1 Technical Overview

The FPTAS for product distributions is obtained by a reduction to 2-dimensional #MASKEDKNAPSACK. However, in order to do this we introduce an intermediate problem called #MINPMFATLEAST.

**Definition 12** (#MINPMFATLEAST). Given product distributions P and Q over  $\{0,1\}^n$  and  $C \ge 0$ , compute the number of  $x \in \{0,1\}^n$  such that  $\min(P(x),Q(x)) \ge C$ .

We first show that approximating  $S_{\rm stat}$  between product distributions reduces to approximating  $\#{\rm MinPMFATLEAST}$ , as stated below.

**Proposition 13.** For any  $\delta > 0$ , computing a  $(1 + \delta)$ -multiplicative approximation to  $S_{\text{stat}}(P,Q)$  for product distributions P,Q can be efficiently reduced to computing a  $(1 + \varepsilon)$ -multiplicative approximation to polynomially-many #MINPMFATLEAST instances over P and Q, where  $\varepsilon = \Theta(\delta)$ .

Thus, if there is an FPTAS algorithm for #MINPMFATLEAST, then there is an FPTAS for estimating  $S_{\text{stat}}$  between product distributions.

Next we prove that #MINPMFATLEAST (exactly) reduces to the 2-dimensional #MASKEDKNAPSACK problem in polynomial time.

**Proposition 14.** #MINPMFATLEAST reduces to 2-dimensional #MASKEDKNAPSACK.

Finally, we design an FPTAS for multidimensional #MASKEDKNAPSACK when m is a constant. For this we use the read-once branching program approach to designing deterministic polynomial-approximation algorithm for Knapsack counting problems. For making this approach work, we prove a new *rounding* result for MASKEDKNAPSACKinstances along the lines of the work of Dyer [Dye03].

## 5 FPTAS for Statistical Similarity

In this section, we design an FPTAS for estimating  $S_{\rm stat}$  between product distributions. The proof is divided into several subsections. Section 5.1 gives a reduction from estimating  $S_{\rm stat}$  to #MINPMFATLEAST. Section 5.2 gives a reduction from #MINPMFATLEAST to 2-dimensional #MASKEDKNAPSACK. Section 5.3 gives an FTPAS for multidimensional #MASKEDKNAPSACK. Finally, Section 5.4 combines the reductions to obtain the final result, Theorem 8.

#### 5.1 Reduction from Statistical Similarity to #MINPMFATLEAST

We prove Proposition 13.

Proof of Proposition 13. Let P and Q be two product distributions. We will reduce

$$S_{\text{stat}}(P,Q) = \sum_{x \in \{0,1\}^n} \min(P(x), Q(x))$$

to a collection of polynomially many #MINPMFATLEAST instances over P and Q.

Let  $m_{\min}$  and  $m_{\max}$  denote the minimum and maximum nonzero values of  $\min(P(x), Q(x))$  over all x. By our assumption on the bit representation of the parameters  $p_i, q_i$ , we get that  $m_{\min} \geq m_0 := \left(2^{-\ell}\right)^n = 2^{-\ell n}$ . Moreover,  $m_{\max} \leq 1$ . Let  $V \geq 1$  be a number so that  $\min(P(x), Q(x))/m_0 \leq V$  for all x. Therefore,  $V \leq m_{\max}/m_0 \leq 1/m_0 = 2^{\ell n}$ . In fact, let us set  $V := 2^{\ell n}$ . Let  $Y_x := \min(P(x), Q(x))/m_0$  and note that  $Y_x$  lies in [1, V).

We will divide the interval [1, V) into sub-intervals that are multiples of  $(1 + \varepsilon)$  for some  $\varepsilon$  that is within a linear factor of  $\delta$  which we will fix later. More precisely, let

$$[1, V) = \bigcup_{i=0}^{u-1} \left[ (1+\varepsilon)^i, (1+\varepsilon)^{i+1} \right)$$

be a set of sub-intervals for  $0 \le i \le u - 1 = \lceil \log_{1+\varepsilon} V \rceil - 1 \le \operatorname{poly}(\ell, n, 1/\varepsilon)$ . For any  $0 \le i \le u - 1$ , let  $n_i$  denote the number of  $x \in \{0, 1\}^n$  such that  $Y_x$  is in  $\left[1, (1 + \varepsilon)^i\right)$ . That is,

$$n_i := \left| \left\{ x \mid Y_x \in \left[ 1, (1 + \varepsilon)^i \right) \right\} \right|.$$

Let the average contribution of  $Y_x$  in the range  $[(1+\varepsilon)^{i-1}, (1+\varepsilon)^i)$  be  $B_i$ . That is,  $B_i := \sum Y_x/(n_i-n_{i-1})$ , where the sum is over all  $Y_x$  in the interval  $[(1+\varepsilon)^{i-1}, (1+\varepsilon)^i)$ . Then we have the following equation:

$$\frac{S_{\text{stat}}(P,Q)}{m_0} = n_1 B_1 + (n_2 - n_1) B_2 + (n_3 - n_2) B_3 + \dots + (n_u - n_{u-1}) B_u.$$
 (2)

Since  $(1+\varepsilon)^{i-1} \leq B_i < (1+\varepsilon)^i$ , the following estimate d is a  $(1+\varepsilon)$ -approximation of the RHS of Equation (2):

$$d := n_1(1+\varepsilon) + (n_2 - n_1)(1+\varepsilon)^2 + \ldots + (n_u - n_{u-1})(1+\varepsilon)^u.$$
(3)

By reorganizing the terms of Equation (3), we get

$$d = ((1+\varepsilon)^{u} - (1+\varepsilon)^{u-1}) (n_{u} - n_{u-1}) + ((1+\varepsilon)^{u-1} - (1+\varepsilon)^{u-2}) (n_{u} - n_{u-2}) + \dots + (1+\varepsilon)n_{u}.$$
(4)

Therefore it suffices to estimate  $n_u - n_j$  for every  $1 \le j \le u - 1$ . (We know that  $n_u = 2^n$ .) By definition,  $t_j := n_u - n_j$  counts the number of  $x \in \{0, 1\}^n$  such that  $Y_x \ge (1 + \varepsilon)^j$ . Note that

$$Y_x \ge (1+\varepsilon)^j \Leftrightarrow \min(P(x), Q(x)) \ge (1+\varepsilon)^j m_0.$$

That is,  $t_j$  counts the number of  $x \in \{0,1\}^n$  such that  $\min(P(x),Q(x)) \geq (1+\varepsilon)^j m_0$ . If we estimate each  $t_j$  up to a  $(1+\varepsilon)$ -multiplicative approximation, this in turn would give us a  $(1+\varepsilon)$ -multiplicative approximation for d by Equation (4), and for that matter a  $(1+\varepsilon)^2$ -multiplicative approximation for  $S_{\text{stat}}(P,Q)$  by Equation (2). Hence, if we set  $\varepsilon := \Omega(\delta/2)$  so that  $(1+\varepsilon)^2 \leq (1+\delta)$ , we get the desired approximation ratio of  $(1+\delta)$  for  $S_{\text{stat}}(P,Q)$ .  $\square$ 

Remark 15. We note that the above proof goes through even when P and Q are sub-product distributions. In this case the #MINPMFATLEAST instances are over sub-distributions P and Q.

### 5.2 Reduction from #MINPMFATLEAST to #MASKEDKNAPSACK

We prove Proposition 14.

Proof of Proposition 14. In order to show this proposition we introduce another computational problem #PMFATLEAST: Given a product distribution P on n variables and a C > 0, compute the number of  $x \in \{0,1\}^n$  so that  $P(x) \geq C$ . We show that this problem reduces to #MASKEDKNAPSACK. Now, given an instance P,Q and C of #MINPMFATLEAST, for any  $x \in \{0,1\}^n$ ,  $\min(P(x),Q(x)) \geq C$  if and only if  $P(x) \geq C$  and  $Q(x) \geq C$ . It will follow that #MINPMFATLEAST reduces to 2-dimensional #MASKEDKNAPSACK.

Let P be a product distribution with Bernoulli parameters  $p_1, \ldots, p_n$  and C > 0. Given this instance, we will construct a #MASKEDKNAPSACK instance  $K_P$  so that for any  $x \in \{0,1\}^n$ , it is the case that  $P(x) \geq C$  if and only x is a solution to  $K_P$ .

Let

$$a_i := \max\left(\frac{p_i}{1 - p_i}, \frac{1 - p_i}{p_i}\right), \ b_i := \min(p_i, 1 - p_i).$$

For any  $x \in \{0,1\}^n$  define sets  $T_P(x)$  as follows:

$$T_P(x) := \left\{ i \in [n] \mid p_i \ge \frac{1}{2}, \ x_i = 1 \text{ or } p_i < \frac{1}{2}, \ x_i = 0 \right\}.$$

For all  $x \in \{0,1\}^n$ , let  $S_x$  be such that  $i \in S_x$  if and only if  $x_i = 1$  (that is, x is the characteristic vector of  $S_x$ ).

We require the following claim.

Claim 16. It is the case that

$$P(x) = \prod_{i \in S_x} p_i \prod_{i \notin S_x} (1 - p_i) = \left(\prod_{i=1}^n b_i\right) \left(\prod_{i \in T_P(x)} a_i\right).$$

*Proof.* Recall that

$$a_i := \max\left(\frac{p_i}{1 - p_i}, \frac{1 - p_i}{p_i}\right), \qquad b_i := \min(p_i, 1 - p_i).$$

Thus for  $p_i \ge 1/2$ , we have  $a_i = \frac{p_i}{1-p_i}$  and  $b_i = 1 - p_i$  and for  $p_i < 1/2$ , we have  $a_i = \frac{1-p_i}{p_i}$  and  $b_i = p_i$ . Moreover,

$$T_P(x) := \left\{ i \in [n] \mid p_i \ge \frac{1}{2}, \ x_i = 1 \text{ or } p_i < \frac{1}{2}, \ x_i = 0 \right\}.$$

Therefore,

$$P(x) = \prod_{i \in S_x} p_i \prod_{i \notin S_x} (1 - p_i)$$

$$= \prod_{i \in S_x, p_i \ge 1/2} p_i \prod_{i \in S_x, p_i < 1/2} p_i \prod_{i \notin S_x, p_i \ge 1/2} (1 - p_i) \prod_{i \notin S_x, p_i < 1/2} (1 - p_i)$$

$$= \prod_{i \in S_x, p_i \ge 1/2} \frac{p_i}{1 - p_i} (1 - p_i) \prod_{i \in S_x, p_i < 1/2} p_i \prod_{i \notin S_x, p_i \ge 1/2} (1 - p_i) \prod_{i \notin S_x, p_i < 1/2} \frac{1 - p_i}{p_i} p_i$$

$$= \prod_{i \in S_x, p_i \ge 1/2} \frac{p_i}{1 - p_i} (1 - p_i) \prod_{i \notin S_x, p_i < 1/2} \frac{1 - p_i}{p_i} p_i \prod_{i \in S_x, p_i < 1/2} p_i \prod_{i \notin S_x, p_i \ge 1/2} (1 - p_i)$$

$$= \prod_{i \in S_x, p_i \ge 1/2} a_i b_i \prod_{i \notin S_x, p_i < 1/2} a_i b_i \prod_{i \in S_x, p_i < 1/2} b_i \prod_{i \notin S_x, p_i \ge 1/2} b_i$$

$$= \prod_{i \in T_P(x)} a_i \prod_{i \in [n]} b_i.$$

Thus the inequality  $P(x) \geq C$  is equivalent to

$$\left(\prod_{i=1}^{n} b_i\right) \left(\prod_{i \in T_P(x)} a_i\right) \ge C,$$

or

$$\prod_{i \notin T_P(x)} a_i \le \frac{\left(\prod_{i=1}^n a_i\right) \left(\prod_{i=1}^n b_i\right)}{C}.$$

Crucially, since  $a_i \geq 1$  for all i, in order to make the product a sum, we can take log on both sides, yielding

$$\sum_{i \notin T_P(x)} \log a_i \le \log \frac{\left(\prod_{i=1}^n a_i\right) \left(\prod_{i=1}^n b_i\right)}{C}.$$

At this point, the expressions look *similar* to a KNAPSACK constraint. While we do not know how to cast them as standard KNAPSACK constraint, we can frame them as a MASKEDKNAPSACK constraint as follows.

Let y(x) be the characteristic vector of  $[n] \setminus T_P(x)$  and let  $y(x)_i$  denote the  $i^{th}$  bit of y(x). Then the above inequality can be written as

$$\sum_{i=1}^{n} (\log a_i) y(x)_i \le \log \frac{(\prod_{i=1}^{n} a_i) (\prod_{i=1}^{n} b_i)}{C}.$$

Define the mask vector  $u_P$  as follows:  $u_P = u_{P,i}, \dots, u_{P,n}$  is such that  $u_{P,i} = 1$  if and only if  $p_i \ge 1/2$ . Then from the definition of  $T_P$  and  $u_P$ , we have the following claim.

**Claim 17.** For any  $x \in \{0,1\}^n$ ,  $y(x) = x \oplus u_P$ , where  $\oplus$  is the bitwise XOR operation.

Hence the above inequality can be written as

$$\sum_{i=1}^{n} (\log a_i) (x_i \oplus u_{P,i}) \le \log \frac{(\prod_{i=1}^{n} a_i) (\prod_{i=1}^{n} b_i)}{C}.$$

Thus, for an instance P, C of #PMFATLEAST we can construct an #MASKEDKNAPSACK instance  $K_P$  that is specified by the weights  $\log a_1, \ldots, \log a_n$ , capacity  $\log \frac{\left(\prod_{i=1}^n a_i\right)\left(\prod_{i=1}^n b_i\right)}{C}$ , and the mask  $u_P$ . From the above inequality it follows that, for all  $x \in \{0,1\}^n$ ,  $P(x) \geq C$  if and only if x is a solution to instance  $K_P$ . Note that this reduction runs in linear time.

Now, to complete the proof of Proposition 14, we reduce #MINPMFATLEAST to 2-dimensional #MASKEDKNAPSACK. Let P,Q and C be the instance of #MINPMFATLEAST. Construct two #MASKEDKNAPSACK instances  $K_P$  and  $K_Q$  following the above reduction. Then for any  $x \in \{0,1\}^n$ ,  $\min(P(x),Q(X)) \geq C \Leftrightarrow (P(x) \geq C \text{ and } Q(x) \geq C) \Leftrightarrow x$  is a solution to both  $K_P$  and  $K_Q$ .

Remark 18. We again point that the above reduction goes through when P and Q are subproduct distributions. Let P' and Q' be product distributions and  $P = \alpha P'$  and  $Q = \beta Q'$  for constants  $\alpha, \beta$ . Note that  $\min(P(x), Q(x)) \geq C$  if and only  $P(x) \geq C$  and  $Q(x) \geq C$  if and only of  $P'(x) \geq C/\alpha$  and  $Q'(x) \geq C/\beta$ . Thus x is a solution to  $\min(P(x), Q(x)) \geq C$  if and only if it is a solution to  $K_{P'}$  and  $K_{Q'}$ .

#### 5.3 Counting Masked Knapsack Solutions

This algorithm is based on the techniques from [GKM10] and [Dye03].

#### 5.3.1 Branching Programs

A (W, n) read-once branching program (ROBP) M is a (n+1)-layered DAG with a single source (in the first layer) and two sinks (in the last layer) and each intermediate node has at most W vertices. One of the sink nodes is labeled 1 (accepting) and the other is labeled 0 (rejecting). Each node has two outgoing edges labeled 0 and 1. We say that such a branching program accepts a string  $z \in \{0,1\}^n$  (denoted M(z)=1) if the path from the source node along the edges labeled by z reaches the sink node 1. A monotone (W,n)-ROBP is a (W,n)-ROBP such that in each of its layers L, the nodes of L are totally ordered under some relation  $\prec$ , and whenever  $u \prec v$  for some nodes u and v, it is the case that the set of partial accepting paths that start at u are a subset of the set of partial accepting paths that start at v. An implicit description of a monotone ROBP is a description according to which one can efficiently check the relative order of two nodes under  $\prec$  (within any layer), and given a node u one can efficiently compute its neighbors.

The following notion of small-space sources was introduced by [KRVZ11].

**Definition 19** ([KRVZ11]). A width-w small-space source is described by a (w, n)-read-once branching program D with an additional probability distribution  $p_v$  on the outgoing edges associated with vertices  $v \in D$ . Samples from the source are generated by taking a random walk on D according to the  $p_v$ 's and outputting the labels of the edges traversed.

We require the following useful claims by [GKM10]. Claim 20 is an application of dynamic programming.

Claim 20 ([GKM10]). Given a ROBP M of width at most W and a small-space source D of width at most S. Then  $\mathbf{Pr}_{x\sim D}[M(x)=1]$  can be computed exactly in time O(nSW).

Claim 21 ([GKM10]). Given a (W, n)-ROBP M, the uniform distribution over M's accepting inputs,  $\{x \mid M(x) = 1\}$  is a width W small-space source.

We further require the following important result from [GKM10].

**Theorem 22** ([GKM10]). Given a monotone (W, n)-ROBP M,  $\delta > 0$ , and a small-space source D over  $\{0,1\}^n$  of width at most S, there exists an  $(O(n^2S/\delta), n)$ -monotone ROBP  $M_0$  such that for all z, it is the case that  $M(z) \leq M_0(z)$  and

$$\Pr_{z \sim D}[M(z) = 1] \le \Pr_{z \sim D}[M_0(z) = 1] \le (1 + \delta) \Pr_{z \sim D}[M(z) = 1].$$

Moreover, given an implicit description of M and a description of D,  $M_0$  can be constructed in deterministic time  $O(n^3S(S + \log W)\log(n/\delta)/\delta)$ .

The main take-away of Theorem 22 is that the number of accepting paths of  $M_0$  (under the distribution D) approximates the number of accepting paths of M (under the distribution D), and moreover  $M_0$  has small width.

#### 5.3.2 Proof of Theorem 11

We prove Theorem 11. To this end, we require Lemma 23, which is based on the Dyer's rounding scheme in the context of standard #KNAPSACK. We extend it to the setting of #MASKEDKNAPSACK.

**Lemma 23** (Rounding). Given a collection of #MASKEDKNAPSACK instances  $K_1, \ldots, K_m$ , each over n variables and with a total weight of at most W, we can deterministically in time  $O(n^3 \log W)$  construct new #MASKEDKNAPSACK instances  $K'_1, \ldots, K'_m$  each with a total weight of at most  $O(n^3)$  with the following property. Let  $S_1, \ldots, S_m$ , be the solution sets of  $K_1, \ldots, K_m$  and let  $S'_1, \ldots, S'_m$  be the solution sets of  $K'_1, \ldots, K'_m$ , respectively. Then

- 1.  $S_i \subseteq S_i'$  for all  $1 \le i \le m$  and
- 2.  $\left| \bigcap_{i=1}^{m} S_i' \right| \le n^m \left| \bigcap_{i=1}^{m} S_i \right|$ .

*Proof.* Let

$$S_i := \left\{ x \in \{0,1\}^n \mid \sum_{j=1}^n a_{i,j} (x_j \oplus u_{i,j}) \le b_i \right\},$$

whereby  $0 \le a_{i,1} \le \cdots \le a_{i,n} \le b_i$ . Let  $k_i$  be such that  $a_{i,j} \le b_i/n$  for  $j \le k_i$  and either  $k_i = n$  or  $a_{i,k_i+1} > b_i/n$ . Let  $C_i := \{z, u_{i,k_i+1}, \dots, u_{i,n} \mid z \in \{0,1\}^{k_i}\}$ . If  $x \in C_i$ , then

$$\sum_{j=1}^{n} a_j (x_j \oplus u_{i,j}) \le \sum_{j=1}^{n} a_j \le k_i b_i / n \le b_i$$

and so  $x \in S_i$ . That is,  $C_i \subseteq S_i$ . Let now  $\alpha_{i,j} := \lfloor n^2 a_{i,j}/b_i \rfloor$  and  $\delta_{i,j} := n^2 a_{i,j}/b_i - \alpha_{i,j}$ , such that  $0 \le \delta_{i,j} < 1$ . Let also

$$S_i' := \left\{ x \in \{0, 1\}^n \mid \sum_{j=1}^n \alpha_{i,j} (x_j \oplus u_{i,j}) \le n^2 \right\}$$

and  $S := \bigcap_{i=1}^m S_i$ ,  $S' := \bigcap_{i=1}^m S_i'$ . We will prove that  $|S| \le |S'| \le n^m |S|$ . Let us first prove that  $|S| \le |S'|$ . Let  $x \in S$ . Then for all i we have

$$\sum_{j=1}^{n} \alpha_{i,j} (x_j \oplus u_{i,j}) \le (n^2/b_i) \sum_{j=1}^{n} a_{i,j} (x_j \oplus u_{i,j}) \le (n^2/b_i) b_i = n^2,$$

so  $x \in S'_i$  and therefore  $x \in S'$ . Thus  $S \subseteq S'$  and so  $|S| \le |S'|$ .

Let us now show that  $|S'| \leq n^m |S|$ . To this end, let  $L_i := \{j \mid a_{i,j} \leq b_i/n\}$ . For  $x \in S' \setminus S$ , let  $I(x) := \{i \mid x \in S'_i \setminus S_i\}$ . For every  $i \in I(x)$ , there exists  $p_i(x) \notin L_i$  such that  $x_{p_i} \oplus u_{i,p_i} = 1$  and  $\alpha_{i,p_i(x)} \geq n$ . Otherwise,  $x \in C_i \subseteq S_i \subseteq S'_i$ . (If there exist more than one such integer, take  $p_i(x)$  to be the smallest.) Construct f(x) = y by  $y_{p_i(x)} = 0$  for  $i \in I(x)$  and  $y_j = x_j$  otherwise. Then for any  $x \in S' \setminus S$ , with y = f(x), we have

$$\sum_{j=1}^{n} a_{i,j} (y_{j} \oplus u_{i,j}) = \frac{b_{i}}{n^{2}} \sum_{j=1}^{n} (\alpha_{i,j} + \delta_{i,j}) (y_{j} \oplus u_{i,j})$$

$$= \frac{b_{i}}{n^{2}} \left( \sum_{j=1}^{n} \alpha_{i,j} (y_{j} \oplus u_{i,j}) + \sum_{j=1}^{n} \delta_{i,j} (y_{j} \oplus u_{i,j}) \right)$$

$$= \frac{b_{i}}{n^{2}} \left( \sum_{j=1}^{n} \alpha_{i,j} (x_{j} \oplus u_{i,j}) - \alpha_{i,p_{i}(x)} (x_{p_{i}} \oplus u_{i,p_{i}(x)}) + \sum_{j=1}^{n} \delta_{i,j} (y_{j} \oplus u_{i,j}) \right)$$

$$= \frac{b_{i}}{n^{2}} \left( \sum_{j=1}^{n} \alpha_{i,j} (x_{j} \oplus u_{i,j}) - \alpha_{i,p_{i}(x)} + \sum_{j=1}^{n} \delta_{i,j} (y_{j} \oplus u_{i,j}) \right)$$

$$\leq \frac{b_i}{n^2} \left( n^2 - n + n \right)$$
$$= b_i.$$

That is,  $f(x) \in S_i$  and so  $f(x) \in S$ . Hence f(S') = S. The inverse mapping changes some set of coordinates P with  $0 \le |P| \le m$ , so

$$\left|f^{-1}(y)\right| \le 1 + n + \binom{n}{2} + \dots + \binom{n}{m} \le n^m.$$

That is,  $|S| \le n^m |S'|$  and therefore  $|S'| \le |f^{-1}(S)| \le n^m |S|$ .

We also need the following observation that states that a #MASKEDKNAPSACK instance can be represented as a monotone ROBP.

**Observation 24.** Given a collection of #MASKEDKNAPSACK instances  $K_1, \ldots, K_m$ , each over n variables and with a total weight of at most W, there is a monotone  $(W^m, n)$ -ROBP M so that  $\bigcap_{i=1}^m S_i = \{x \mid M(x) = 1\}$ , where  $S_i$  is the solution set of  $K_i$ .

We may now prove Theorem 11 by using Lemma 23.

Proof of Theorem 11. First, we will apply Lemma 23 to obtain #MASKEDKNAPSACK instances  $K'_1, \ldots, K'_m$ , each with a total weight of at most  $O(n^3)$ , and with solution sets  $S'_1, \ldots, S'_m$ , respectively.

Let D be the uniform distribution over the set  $S' := \bigcap_{i=1}^m S_i'$  and observe that by Claim 21 D can be generated by an explicit  $O(n^{3m})$  space source. For  $1 \le i \le m$ , let  $M^i$  be a monotone, (W, n)-ROBP exactly computing the indicator function for  $S_i$ . Let  $\delta = O(\varepsilon/(m(n+1)^m))$  to be chosen later. For every  $1 \le i \le m$ , by Theorem 22 we can explicitly in time  $n^{O(m)}(\log W)/\delta$  construct a  $(n^{O(m)}/\delta, n)$ -ROBP  $M_r^i$  such that

$$\Pr[M_r^i(x) \neq M^i(x)] \leq \delta.$$

Define M such that  $M(x) := \bigwedge_{i=1}^m M_r^i(x)$  for any x. Then M is a  $\left(n^{O(m^2)}/\delta^m, n\right)$ -ROBP. By a union bound,

$$\Pr_{x \sim D} \left[ M(x) \neq \bigwedge_{i=1}^{m} M^{i}(x) \right] \leq m\delta.$$

On the other hand, by Lemma 23,

$$\Pr_{x \sim D} \left[ \bigwedge_{i=1}^{m} M^{i}(x) = 1 \right] \ge 1/(n+1)^{m}.$$

Therefore, by setting  $\delta := \varepsilon / (2m(n+1)^m)$ , we get

$$\Pr_{x \sim D}[M(x) = 1] \le \Pr_{x \sim D} \left[ \bigwedge_{i=1}^{m} M^{i}(x) = 1 \right] (1 + \varepsilon) \Pr_{x \sim D}[M(x) = 1].$$

Thus,  $p := \mathbf{Pr}_{x \sim \{0,1\}^n}[x \in S'] \mathbf{Pr}_{x \sim D}[M(x) = 1]$  is a  $(1 + \varepsilon)$ -multiplicative approximation to the fraction of solutions to all constraints

$$\Pr_{x \sim \{0,1\}^n} \left[ \bigwedge_{i=1}^m M^i(x) = 1 \right] = \Pr_{x \sim \{0,1\}^n} \left[ x \in S' \right] \cdot \Pr_{x \sim D} \left[ \bigwedge_{i=1}^m M^i(x) = 1 \right].$$

The result now follows since we can compute p in time  $(n/\delta)^{O(m^2)}$  using Claim 20, as D is a small-space source of width  $O(n^{3m})$  and M has width  $(n/\delta)^{O(m^2)}$ .

#### 5.4 Estimating Statistical Similarity

We now prove Theorem 8.

Proof of Theorem 8. By Proposition 13, the  $(1 + \delta)$ -multiplicative approximation of  $S_{\text{stat}}(P,Q)$  reduces to the  $(1 + \varepsilon)$ -multiplicative approximation of polynomially-many #MINPMFATLEAST instances over P,Q, namely  $t_1,\ldots,t_k$ , for  $\varepsilon=\Omega(\delta/2)$  and  $k=\text{poly}(\ell,n)$ . By Proposition 14, the instances  $t_1,\ldots,t_k$  can be reduced to multidimensional #MASKEDKNAPSACK for m=2. Using Theorem 11, we can estimate each  $t_j$  up to a  $(1+\varepsilon)$ -multiplicative approximation in polynomial time.

The running time of this algorithm is polynomial in  $\ell, n, 1/\delta$  because we ran a polynomial-time approximation algorithm for multidimensional #MASKEDKNAPSACK polynomially many times. In particular, the running time is  $\operatorname{poly}(\ell, n, 1/\varepsilon) \cdot O\left((n/\delta)^{O(1)}\right) \log W = O\left((\ell \cdot n/\delta)^{O(1)}\right)$  (since it is the case that  $W = \operatorname{poly}(n)$ , by Lemma 23).

### 6 NP-hardness of Estimating Statistical Similarity

We show that it is NP-hard to efficiently multiplicatively estimate  $S_{\text{stat}}(P,Q)$  for arbitrary Bayes net distributions P,Q. That is, we prove Theorem 10. We first formally define Bayes nets.

#### 6.1 Bayes Nets

For a directed acyclic graph (DAG) G and a node v in G, let  $\Pi(v)$  denote the set of parents of v.

**Definition 25** (Bayes nets). A Bayes net is specified by a DAG over a vertex set [n] and a collection of probability distributions over symbols in  $[\ell]$ , as follows. Each vertex i is associated with a random variable  $X_i$  whose range is  $[\ell]$ . Each node i of G has a Conditional Probability Table (CPT) that describes the following: For every  $x \in [\ell]$  and every  $y \in [\ell]^k$ , where k is the size of  $\Pi(i)$ , the CPT has the value of  $\mathbf{Pr}[X_i = x | X_{\Pi(i)} = y]$  stored. Given such a Bayes net, its associated probability distribution P is given by the following: For all  $x \in [\ell]^n$ , P(x) is equal to

$$\Pr_{P}[X = x] = \prod_{i=1}^{n} \Pr_{P}[X_i = x_i | X_{\Pi(i)} = x_{\Pi(i)}].$$

Here, X is the joint distribution  $(X_1, \ldots, X_n)$  and  $x_{\Pi(i)}$  is the projection of x to the indices in  $\Pi(i)$ .

Note that P(x) can be computed in linear time by using the CPTs of P to retrieve each  $\mathbf{Pr}_P[X_i = x_i | X_{\Pi(i)} = x_{\Pi(i)}]$ . One may also use  $P_{i|\Pi(i)}(x_i | x_{\Pi(i)})$  to denote this probability.

#### 6.2 Proof of Theorem 10

The proof is similar to the proof of hardness of approximating TV distance between Bayes net distributions presented in [BGM<sup>+</sup>23]. However, the present proof gives more tight relationship between the number satisfying assignments of a CNF formula and statistical similarity of Bayes net distributions.

The reduction takes a CNF formula  $\phi$  on n variables and produces two Bayes net distributions P and Q (with in-degree at most 2) so that

$$S_{\text{stat}}(P,Q) = \frac{|\text{Sol}(\phi)|}{2^n},$$

where  $Sol(\phi)$  is the set of satisfying assignments for  $\phi$ .

Let  $\phi$  be a CNF formula. Without loss of generality, view  $\phi$  as a Boolean circuit (with AND, OR, NOT gates) of fan-in at most two with n input variables  $\mathcal{X} = \{X_1, \ldots, X_n\}$  and m internal gates  $\mathcal{Y} = \{Y_1, \ldots, Y_m\}$ . Let  $G_{\phi}$  be the DAG representing this circuit with vertex set  $\mathcal{X} \cup \mathcal{Y}$ . So in total there are n+m nodes in  $G_{\phi}$ . Assume  $\mathcal{X} \cup \mathcal{Y}$  is topologically sorted in the order  $X_1, \ldots, X_n, Y_1, \ldots, Y_m$ , whereby  $Y_m$  is the output gate. For every internal gate node  $Y_i$ , there is directed edge from node  $Y_i$  to node  $Y_j$  if the gate/variable corresponding to  $Y_i$  is an input to  $Y_j$ .

We will define two Bayes net distributions P and Q on the same DAG  $G_{\phi}$ . Let  $X_i$  be a binary random variable corresponding to the input variable node  $X_i$  for  $1 \le i \le n$  and  $Y_j$  be a binary random variable corresponding to the internal gate  $Y_j$  for  $1 \le j \le m$ . The distributions P and Q on G are given by Conditional Probability Tables (CPTs) defined as follows. The CPTs of P and Q will only differ in  $Y_m$ .

For both P and Q, each  $X_i$   $(1 \le i \le n)$  is a uniform random bit. For each  $Y_i$   $(1 \le i \le m-1)$ , its CPT is the deterministic function defined by its associated gate. For example, if  $Y_i$  is an OR gate in  $G_{\phi}$ , then  $Y_i = 1$  with probability 1 except when the inputs are 00, in which case  $Y_i = 0$  with probability 1. The CPTs for AND and NOT nodes are similar.

For P, the value of  $Y_m$  is given by the deterministic function of the output gate  $Y_m$  in  $G_{\phi}$ . For Q, the value of  $Y_m$  is 1 (independently of the input).

Note that even though the sample space is  $\{0,1\}^{n+m}$ , there are only  $2^n$  strings in the support of P and Q. In particular, a point z in the sample space  $\{0,1\}^{n+m}$  can be written as xy where x is the first n bits and y is the last m bits. By construction, it is clear that for every x, there is only one y (which are the gate values for the input assignment x) for which xy has positive probability in both the distributions, and this probability is exactly  $\frac{1}{2^n}$ . For any x, let  $f_P(x)$  (respectively,  $f_Q(x)$ ) denote this unique y in P (respectively, in Q). The crucial observation is that  $f_P(x)$  and  $f_Q(x)$  are the same if and only if x is in  $Sol(\phi)$ . In this case, denote  $f_P(x) = f_Q(x) = f(x)$ .

Consider  $z = xy \in \{0,1\}^{n+m}$ . If xy is not in the support of both P and Q, then the minimum of P(z) and Q(z) is 0, so assume that xy is in the support of at least one.

Case 1: Assume that x is a not a satisfying assignment of  $\phi$ . Then  $z = xf_P(x)$  is in the support of P however it is not in the support of Q as the last bit of z = 0. Similarly  $xf_Q(x)$  is in the support of Q but not in P. Hence,  $\min(P(z), Q(z)) = 0$ .

Case 2: Assume that x is a satisfying assignment of  $\phi$ . In this case the last bit of  $z = xf_P(x)$  is 1 and hence is in the support on both P and Q and has a probability of  $\frac{1}{2^n}$ . Thus  $\min(P(z),Q(z))=\frac{1}{2^n}$ . Hence we have

$$\begin{split} S_{\text{stat}}(P,Q) &= \sum_{z \in \{0,1\}^{n+m}} \min\left(P(z),Q(z)\right) \\ &= \sum_{x \in \text{Sol}(\phi)} \min(P(xf(x),Q(xf(x)) + \sum_{x \notin \text{Sol}(\phi)} \min(P(xf_P(x),Q(xf_P(x))) \\ &+ \sum_{x \notin \text{Sol}(\phi)} \min(P(xf_Q(x)),Q(xf_Q(x))) \\ &= \frac{|\text{Sol}(\phi)|}{2^n} + 0 + 0 \\ &= \frac{|\text{Sol}(\phi)|}{2^n}. \end{split}$$

This concludes the proof.

### 7 Conclusion

Statistical Similarity ( $S_{\text{stat}}$ ) between distributions is a fundamental quantity. In this work, we initiated a computational study of  $S_{\text{stat}}$ . Prior results on statistical distance computation imply that the exact computation of  $S_{\text{stat}}$  for high-dimensional distributions is computationally intractable.

Our primary contribution is a fully polynomial-time deterministic approximation scheme (FPTAS) for estimating statistical similarity between two product distributions. Notably, the existing FPTAS for statistical distance [FLL24] does not directly yield an FPTAS for  $S_{\rm stat}$ . Our algorithm is based on a reduction to a new knapsack counting problem called (multidimensional) #MASKEDKNAPSACK which might be of independent interest. We also establish a complementary hardness result: Approximating  $S_{\rm stat}$  for Bayes net distributions is NP-hard. Extending our results beyond product distributions to more structured settings, such as tree distributions, remains a significant and promising research direction.

We believe  $S_{\rm stat}$  computation is a compelling problem from a complexity theory perspective. Interestingly, for product distributions, both  $S_{\rm stat}$  and its complement  $(1-S_{\rm stat})$  admit FPTAS, making it one of the rare problems with this property. A deeper complexity-theoretic study of functions f in #P with range in [0,1], where approximation schemes for both f and 1-f have approximation schemes, is an intriguing direction for future research. Finally, this work is on the algorithmic foundational aspects of  $S_{\rm stat}$  computation. We leave the experimental evaluation of the algorithm for future work.

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### References

- [BGM+23] Arnab Bhattacharyya, Sutanu Gayen, Kuldeep S. Meel, Dimitrios Myrisiotis, A. Pavan, and N. V. Vinodchandran. On approximating total variation distance. In Proceedings of IJCAI, 2023.
- [BGMV20] Arnab Bhattacharyya, Sutanu Gayen, Kuldeep S. Meel, and N. V. Vinodchandran. Efficient distance approximation for structured high-dimensional distributions via learning. In *Proc. of NeurIPS*, 2020.

- [BK15] Daniel Berend and Aryeh Kontorovich. A finite sample analysis of the naive Bayes classifier. J. Mach. Learn. Res., 16:1519–1545, 2015.
- [Dev85] Pierre A. Devijver. A multiclass, k-NN approach to Bayes risk estimation. Pattern Recognition Letters, 3(1):1-6, 1985.
- [Doe38] Wolfang Doeblin. Exposé de la théorie des chaines simples constantes de markova un nombre fini d'états. *Mathématique de l'Union Interbalkanique*, 2(77-105):78–80, 1938.
- [Dye03] Martin E. Dyer. Approximate counting by dynamic programming. In *Proc. of STOC*, June 9-11, 2003, San Diego, CA, USA, pages 693–699. ACM, 2003.
- [FGJW23] Weiming Feng, Heng Guo, Mark Jerrum, and Jiaheng Wang. A simple polynomial-time approximation algorithm for the total variation distance between two product distributions. *TheoretiCS*, 2, 2023.
- [FH75] Keinosuke Fukunaga and Larry D. Hostetler. k-nearest-neighbor Bayes-risk estimation. *IEEE Transactions on Information Theory*, 21(3):285–293, 1975.
- [FLL24] Weiming Feng, Liqiang Liu, and Tianren Liu. On deterministically approximating total variation distance. In *Proceedings of SODA*, 2024.
- [GKM10] Parikshit Gopalan, Adam R. Klivans, and Raghu Meka. Polynomial-time approximation schemes for Knapsack and related counting problems using branching programs. *Electron. Colloquium Comput. Complex.*, page 133, 2010.
- [IYC<sup>+</sup>23] Takashi Ishida, Ikko Yamane, Nontawat Charoenphakdee, Gang Niu, and Masashi Sugiyama. Is the performance of my deep network too good to be true? A direct approach to estimating the Bayes error in binary classification. In *The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023.* OpenReview.net, 2023.
- [KA24] Aryeh Kontorovich and Ariel Avital. Sharp bounds on aggregate expert error, 2024.
- [KLM89] Richard M. Karp, Michael Luby, and Neal Madras. Monte-Carlo approximation algorithms for enumeration problems. *J. Algorithms*, 10(3):429–448, 1989.
- [KRVZ11] Jesse Kamp, Anup Rao, Salil P. Vadhan, and David Zuckerman. Deterministic extractors for small-space sources. *J. Comput. Syst. Sci.*, 77(1):191–220, 2011.
- [Lin02] Torgny Lindvall. Lectures on the coupling method. Courier Corporation, 2002.
- [LPW06] David A. Levin, Yuval Peres, and Elizabeth L. Wilmer. *Markov chains and mixing times*. American Mathematical Society, 2006.
- [LR08] Erich Leo Lehmann and Joseph P. Romano. Testing Statistical Hypotheses, Third Edition. Springer texts in statistics. Springer, 2008.
- [MT12] Sean P Meyn and Richard L Tweedie. *Markov chains and stochastic stability*. Springer Science & Business Media, 2012.
- [Nie14] Frank Nielsen. Generalized Bhattacharyya and Chernoff upper bounds on Bayes error using quasi-arithmetic means. *Pattern Recognit. Lett.*, 42:25–34, 2014.

- [NXH19] Morteza Noshad, Li Xu, and Alfred Hero. Learning to benchmark: Determining best achievable misclassification error from training data. arXiv preprint arXiv:1909.07192, 2019.
- [PSNK14] Fabio Parisi, Francesco Strino, Boaz Nadler, and Yuval Kluger. Ranking and combining multiple predictors without labeled data. *Proceedings of the National Academy of Sciences*, 111(4):1253–1258, 2014.
- [SV03] Amit Sahai and Salil P. Vadhan. A complete problem for statistical zero knowledge. J. ACM, 50(2):196–249, 2003.
- [Tsy09] Alexandre B. Tsybakov. *Introduction to Nonparametric Estimation*. Springer series in statistics. Springer, 2009.
- [TWV<sup>+</sup>21] Ryan Theisen, Huan Wang, Lav R. Varshney, Caiming Xiong, and Richard Socher. Evaluating state-of-the-art classification models against bayes optimality. In *Advances in Neural Information Processing Systems*, volume 34, pages 29808–29820, 2021.

### A Bayes Error and Statistical Similarity

A binary prediction problem is a distribution P of  $X \times \{0,1\}$  where X is a (finite) feature space. A classifier is a deterministic function  $g: X \to \{0,1\}$ . The 0-1 error of the predictor g is  $\mathbf{Pr}_{(x,y)\sim P}[g(x)\neq y]$ .

The Bayes optimal classifier is the classifier that outputs 1 if and only if  $P(x|1) \ge P(x|0)$ . The error of Bayes optimal classifier denoted as  $R^*$  is called the Bayes error. Bayes error is the minimum error possible in the sense that the error of any classifier is at least Bayes error. It is known that for a prediction problem P, its Bayes error  $R^*$  is given by the following marginal expectation:

$$R^* = \mathbf{E}[\min(P(0|X), P(1|X))].$$

Let the prior probabilities P(0) and P(1) be denoted by  $\alpha_0$  and  $\alpha_1$  respectively. Note that  $\alpha_0$  and  $\alpha_1$  are constants that sum up to 1. We call P balanced if P(0) = P(1) = 1/2. For simplifying notation, we will also denote the likelihood distributions P(X|0) and P(X|1) as  $P_0$  and  $P_1$  respectively.

**Theorem 26.** For a prediction problem P, its Bayes error is given by

$$R^* = S_{\text{stat}}(\alpha_0 P_0, \alpha_1 P_1).$$

In particular, for a balanced prediction problem P, its Bayes error is given by  $R^* = \frac{S_{\text{stat}}(P_0, P_1)}{2}$ .

*Proof.* The proof is a simple application of the Bayes theorem. That is,

$$\begin{split} R^* &= \mathop{\mathbf{E}}_{X}[\min(P(0|X), P(1|X)] \\ &= \sum_{x \in X} P(x) \cdot \min(P(0|x), P(1|x)) \\ &= \sum_{x} P(x) \cdot \min\left(\frac{P(x|0)P(0)}{P(x)}, \frac{P(x|1)P(1)}{P(x)}\right) \\ &= \sum_{x} \min(P(x|0)P(0), P(x|1)P(1)) \end{split}$$

$$= S_{\text{stat}}(\alpha_0 P_0, \alpha_1 P_1).$$

The balanced case follows from the fact that  $\alpha_0 = \alpha_1 = \frac{1}{2}$ .

#### В Pseudocode

16:  $p_D \leftarrow \mathbf{Pr}_{x \sim D}[M(x) = 1]$ 

17:  $p_{S'} \leftarrow |S'|/2^n$ 

18:  $p \leftarrow p_D \cdot p_{S'}$ 19: return p

We present the pseudocode of our algorithms, in reverse order. We present the pseudocode for Theorem 11 in Algorithm 1.

#### **Algorithm 1** The pseudocode for Theorem 11.

Require: m instances of MaskedKnapsack, specified by weights  $\{a_i\}_{i=1}^m$ , whereby  $a_i =$  $a_{i,1},\ldots,a_{i,n}$ , mask vectors  $\{u_i\}_{i=1}^m$ , whereby  $u_i=u_{i,1},\ldots,u_{i,n}$ , capacities  $b_1,\ldots,b_m$ , and an accuracy error parameter  $\varepsilon$ .

**Ensure:** The output p is an  $(1 + \varepsilon)$ -estimate to multidimensional #MASKEDKNAPSACK.

```
1: {By parsing the input, we can compute m and n.}
 2: for i \leftarrow 1, \ldots, m do
        for j \leftarrow 1, \ldots, n do
            \alpha_{i,j} \leftarrow \lfloor n^2 a_{i,j}/b_i \rfloor
 5:
 6: end for
 7: S' \leftarrow \{0,1\}^n
 8: for i \leftarrow 1, \ldots, m do
        {It is the case that S_i := \left\{ x \in \{0,1\}^n \mid \sum_{j=1}^n a_{i,j} (x_j \oplus u_{i,j}) \le b_i \right\}.}
        Compute a description of M^i {M^i is a (W, n)-ROBP exactly computing the indicator
10:
         function for S_i.
        Compute a description of M_r^i {M_r^i is a (n^{O(m)}/\delta, n)-ROBP that is a rounding of M^i, as
11:
        given by Theorem 22.}
        S'_{i} \leftarrow \left\{x \in \{0,1\}^{n} \mid \sum_{j=1}^{n} \alpha_{i,j} (x_{j} \oplus u_{i,j}) \leq n^{2}\right\} {The set S'_{i} can be computed by dynamic programming in time polynomial in n.}
12:
         S' \leftarrow S' \cap S'_i
13:
14: end for
15: M \leftarrow \bigwedge_{i=1}^{m} M_r^i
```

{The probability  $p_D$  can be computed by Claim 20.}

{Note that  $p_{S'} = \mathbf{Pr}_{x \sim \{0,1\}^n}[x \in S'].$ }

We present the pseudocode for Proposition 14 in Algorithm 2.

We present the pseudocode for Proposition 13 in Algorithm 3.

#### **Algorithm 2** The pseudocode for Proposition 14.

**Require:** Product distributions P, Q through their Bernoulli parameters  $p_1, \ldots, p_n, q_1, \ldots, q_n$ , and a parameter C.

**Ensure:** The output I is an instance of the multidimensional #MaskedKnapsack problem for m=2.

```
1: {By parsing the input, we can compute n.}
  2: \Pi_a \leftarrow 1
 3: \Pi_b \leftarrow 1
  4: \Pi_c \leftarrow 1
  5: \Pi_d \leftarrow 1
 6: for i \leftarrow 1, \ldots, n do
          a_i \leftarrow \max\left(\frac{p_i}{1-p_i}, \frac{1-p_i}{p_i}\right)
b_i \leftarrow \min(p_i, 1-p_i)
c_i \leftarrow \max\left(\frac{q_i}{1-q_i}, \frac{1-q_i}{q_i}\right)
           d_i \leftarrow \min(q_i, 1 - q_i)
           \Pi_a \leftarrow \Pi_a \cdot a_i
11:
           \Pi_b \leftarrow \Pi_b \cdot b_i
12:
           \Pi_c \leftarrow \Pi_c \cdot c_i
13:
           \Pi_d \leftarrow \Pi_d \cdot d_i
14:
           if p_i \geq 1/2 then
15:
               u_{P,i} \leftarrow 1
16:
           else
17:
18:
               u_{P,i} \leftarrow 0
           end if
19:
           if q_i \geq 1/2 then
20:
               u_{Q,i} \leftarrow 1
21:
           else
22:
23:
               u_{Q,i} \leftarrow 0
           end if
24:
25: end for
26: C_P \leftarrow \log(\Pi_a \Pi_b / C)
27: C_Q \leftarrow \log(\Pi_c \Pi_d / C)
28: I_P \leftarrow ((\log a_i)_{i=1}^n, u_P, C_P)
29: I_Q \leftarrow ((\log c_i)_{i=1}^{n-1}, u_Q, C_Q)
30: I \leftarrow (I_P, I_Q)
31: return I
```

```
Algorithm 3 The pseudocode for Proposition 13.
```

**Require:** Product distributions P, Q through their Bernoulli parameters  $p_1, \ldots, p_n, q_1, \ldots, q_n$ and an accuracy error parameter  $\delta$ .

**Ensure:** The output d is an  $(1 + \delta)$ -estimate of  $S_{\text{stat}}(P, Q)$ .

```
1: {By parsing the input, we can compute n.}
```

2: {We define  $\langle \cdot \rangle$  to be a function that maps any number x to its (standard) binary representation in  $\{0,1\}^*$ .

```
3: \ell \leftarrow 0
```

4: for 
$$i \leftarrow 1, \ldots, n$$
 do

5: 
$$\ell \leftarrow \max(\ell, |\langle p_i \rangle|, |\langle q_i \rangle|)$$

7: 
$$m_0 \leftarrow 2^{-\ell n}$$

8: 
$$V \leftarrow 2^{\ell n}$$

9: 
$$u \leftarrow \log_{1+\varepsilon} V$$
  
10:  $n_u \leftarrow 2^n$ 

{Note that  $u \leq \text{poly}(\ell, n, 1/\epsilon)$ .}

10: 
$$n_u \leftarrow 2^n$$

11: 
$$d \leftarrow (1+\varepsilon) n_u$$

12: for 
$$k \leftarrow 2, \dots, u$$
 do

13: 
$$t_k \leftarrow \text{Algorithm } 1\left(\text{Algorithm } 2\left(P, Q, (1+\varepsilon)^k m_0\right), \delta/2\right)$$
14:  $d \leftarrow d + \left((1+\varepsilon)^k - (1+\varepsilon)^{k-1}\right)t_k$ 

14: 
$$d \leftarrow d + \left( (1+\varepsilon)^k - (1+\varepsilon)^{k-1} \right) t_k$$

- 15: end for
- 16:  $\mathbf{return}$  d