High Dimensional Discrete Integration by Hashing and Optimization

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Abstract

Recently Ermon et al. (2013) pioneered a way to practically compute approximations to large scale counting or discrete integration problems by using random hashes. The hashes are used to reduce the counting problem into many separate discrete optimization problems. The optimization problems then can be solved by an NP-oracle such as commercial SAT solvers or integer linear programming (ILP) solvers. In particular, Ermon et al. showed that if the domain of integration is \{0, 1\}^n then it is possible to obtain a solution within a factor of 16 of the optimal (a 16-approximation) by this technique.

In many crucial counting tasks, such as computation of partition function of ferromagnetic Potts model, the domain of integration is naturally \{0, 1, \ldots, q - 1\}^n, q > 2. The straightforward extension of Ermon et al.’s method allows a \(q^2\)-approximation for this problem. For large values of \(q\), this is undesirable. In this paper, we show an improved technique to obtain an approximation factor of \(4 + O(1/q^2)\) to this problem. We are able to achieve this by using an idea of optimization over multiple bins of the hash functions, that can be easily implemented by inequality constraints, or even in unconstrained way. Also the burden on the NP-oracle is not increased by our method (an ILP solver can still be used). Our method extends to the case when the domain of integration is the symmetric group, and as a result we can obtain a \((4 + o(1))\)-approximation of the permanent of a matrix. All these results hold assuming the existence of an NP-oracle. We provide experimental simulation results to support the theoretical guarantees of our algorithms, including comparison to the popular Markov-Chain-Monte-Carlo (MCMC) methods.

1 Introduction

Large scale counting problems, such as computing the permanent of a matrix or computing the partition function of a graphical probabilistic generative model, come up often in variety of inference tasks. These problems can, without loss of any generality, be written as discrete integration: the summation of evaluations of a nonnegative function \(w : \Omega \to \mathbb{R}\) over all elements of \(\Omega\):

\[
S_\Omega (w) \equiv \sum_{\sigma \in \Omega} w(\sigma).
\]

These problems are computationally intractable because of the exponential (and sometime super-exponential) size of \(\Omega\). A special case is the set of problems \#P, counting problems associated with the decision problems in NP. For example, one might ask how many variable assignments a given CNF (conjunctive normal form)
where the arithmetic operations are over within a factor of \( \sigma \) where \( \delta \) is the label of vertex \( u \). Clearly, here \( S_n \) is playing the role of \( \Omega \), and \( w(\sigma) = \prod_{i=1}^n A_{i, \sigma(i)} \). Therefore computing permanent of a matrix is a canonical example of a problem defined by eq. \( (1) \).

Similar counting problems arise when one wants to compute the partition functions of the well-known probabilistic generative models of statistical physics, such as the Ising model, or more generally the Ferromagnetic Potts Model \( [17] \). Given a graph \( G(V, E) \), and a label-space \( Q \equiv \{0, 1, 2, \ldots, q-1\} \), the partition function \( Z(G) \) of the Potts model is given by,

\[
\sum_{\sigma \in Q^{|V|}} \exp \left( -\zeta J \sum_{(u,v) \in E} \delta(\sigma(u), \sigma(v)) + H \sum_{u \in V} \delta(\sigma(u), 0) \right),
\]

where \( \zeta, J \) and \( H \) are system-constants (representing the temperature, spin-coupling and external force), \( \delta(x, y) \) is the delta-function that is \( = 1 \) if and only if \( x = y \) and otherwise \( 0 \), and \( \sigma \) represents a label-vector, where \( \sigma(u) \) is the label of vertex \( u \).

It has been shown that, under the availability of an NP-oracle, every problem in \#P can be approximated within a factor of \( (1 \pm \epsilon) \), \( \epsilon > 0 \), with high probability via a randomized algorithm \( [20] \). This result says \#P can be approximated by \( \text{BPP}^{\text{NP}} \) and the power of an NP-oracle and randomization is sufficient. However, depending on the weight function \( w(\cdot) \), eq. \( (1) \) may not be in \#P. There are related approaches to count the number of models of propositional formulas based on SAT-solvers, such as \( [3, 14, 25, 16, 4, 5] \) among others.

The standard techniques to evaluate eq. \( (1) \) include the very influential fast variational methods \( [24] \), and Markov-Chain-Monte-Carlo based sampling schemes \( [12] \). In practice, except for limited number of cases, these approaches are mostly used in a heuristic manner without nonasymptotic qualitative guarantees. Recently, Ermon et al. proposed an alternative approach (that they call Weighted-Integrals-And-Sums-By-Hashing) to solve these counting problems \( [6, 8] \) by breaking them into multiple optimization problems. Namely, they use families of hash functions \( h : \Omega \to \tilde{\Omega}, |\tilde{\Omega}| < |\Omega| \), and use a (possibly NP) oracle that can return the correct solution of the optimization problem: \( \max_{\sigma : h(\sigma) = a} w(\sigma) \). We call this oracle a MAX-oracle. In particular, when \( \Omega \) can be represented as \( \{0, 1\}^n \), and \( h(\cdot) \) is a random hash function, assuming the availability of a MAX-oracle, Ermon et al. \( [6] \) propose a randomized algorithm that approximates the discrete sum within a factor of sixteen (a 16-approximation) with high probability. Ermon et al. use simple linear sketches over \( \mathbb{F}_2 \), i.e., the hash function \( h_{\mathbb{A}, b} : \mathbb{F}_2^n \to \mathbb{F}_2^m, A \in \mathbb{F}_2^{m \times n}, b \in \mathbb{F}_2^m \) is defined to be

\[
h_{\mathbb{A}, b}(x) = Ax + b,
\]

where the arithmetic operations are over \( \mathbb{F}_2 \). The matrix \( A \) and the vector \( b \) are randomly and uniformly chosen from the respective sample spaces. The MAX-oracle in this case simply provides solutions to the optimization problem: \( \max_{\sigma \in \mathbb{F}_2^n : A\sigma = b} w(\sigma) \).

The constraint space \( \{ \sigma \in \mathbb{F}_2^n : A\sigma = b \} \) is nice since it is a coset of the nullspace of \( A \), and experimental results showed them to be manageable by optimization softwares/SAT solvers. In particular it was observed that being Integer Programming constraints, real-world instances are often solved quickly. Since the implementation of the hash function heavily affects the runtime, it makes sense to keep constraints of the MAX-oracle as an affine space as above. These constraints are also called parity constraints. The idea of using such constraints to show reduction among class of problems appeared in several papers before,
The key property that the hash functions \( \{h_{A, b}\} \) satisfy is that they are pairwise independent. This property can be relaxed somewhat - and in a subsequent paper Ermon et al. show that a hash family would work even if the matrix \( A \) is sparse and random, thus effectively reducing the randomness as well as making the problem more tractable empirically [7]. Subsequently, Achlioptas and Jiang [2] have shown another way of achieving similar guarantees. Instead of arriving at the set \( \{\sigma \in \mathbb{F}_q^n : A\sigma = b\} \) as a solution of a system of linear equations (over \( \mathbb{F}_2 \)), they view the set as the image of a lower-dimensional space. This is akin to the generator matrix view of a linear error-correcting code as opposed to the parity-check matrix view. This viewpoint allows their MAX-oracle to solve just an unconstrained optimization problem.

**Drawbacks of obvious extensions of [6] to large alphabets.** Note that, some crucial counting problems, such as computing the partition function of the Ferromagnetic Potts model of Eq. (3), naturally have \( \Omega = \mathbb{F}_q^n \) for \( q > 2 \). It is worth noting that while there exists polynomial time approximation (FPRAS) for the Ising model \((q = 2)\), FPRAS for general Potts model \((q > 2)\) is significantly more challenging (and likely impossible [9]). There are a few possible obvious extensions of Ermon et al. [6] to larger alphabets.

- (The straightforward extension). The method of [6] can be used for \( q \)-ary in stead of binary. However, the drawback is that it provides a \( q^2 \)-approximation at best which is particularly bad if \( q \) is large (or growing with \( n \)).

- (Convert \( q \)-ary to binary). To use the binary-domain algorithm of [6] for any \( \Omega = \mathbb{F}_q^n \), we need to use a look-up table to map \( q \)-ary numbers to binary. In this process the number of variables (and also the number of constraints) increases by a factor of \( \log q \). This makes the MAX-oracle significantly slower, especially when \( q \) is large. Also, for the permanent problem, where \(|\Omega| = \exp(n \log n)\), this creates a computational bottleneck. It would be useful to extend the method of [6] for \( \Omega = \mathbb{F}_q^n \) without increasing the number of variables.

Furthermore, when \( q \) is not a power of \( 2 \), by converting \( q \)-ary configurations to binary, we introduce exponentially many invalid configurations. To account for these, the MAX-oracle must be adjusted accordingly. This motivates us to keep the problem in its original domain and not convert the domain to binary.

- For the binary setting, it has been noted in [6] section 5.3] that the approximation ratio can be improved to any \( \alpha > 1 \) by increasing the number of variables, which extends to this \( q \)-ary setting. However this also results in an increase in number of variables by a factor of \( \log_\alpha (q^2) \) which is undesirable.

**Our contributions.** Our first contribution in this paper is to provide a new and improved algorithm to handle counting problems over nonbinary domains. For any \( \Omega = \mathbb{F}_q^n \), \( q \) is a power of prime, our algorithm provides a \( 4(1 + \frac{1}{q-1})^2 \)-approximation, when \( q \) is odd, and \( 4(1 + \frac{2}{q-2})^2 \)-approximation, when \( q > 2 \) is even, to the optimization problem of [1] assuming availability of the MAX-oracle. Our algorithm utilizes an idea of using optimization over multiple bins of the hash function that can be easily implemented via inequality constraints. The constraint space of the MAX-oracle remains an affine space and still can be represented as a modular integer linear program (ILP). In general, for arbitrary \( \Omega \), if represented as as \( \{0, 1\}^n \), the approximation factor is at best 16 by the technique of [6]. But by having it represented as \( \{0, 1, \ldots, q-1\}^n \) the approximation factor can be improved to \( \sim 4 \) by our technique. Our multi-bin technique can also be use to extend the generator-matrix based algorithm of Achlioptas and Jiang [2]. As a result, we need the MAX-oracle to only perform unconstrained maximization, as opposed to constrained. This lead to significant speed-up in the system, while resulting in the same approximation guarantees.

Secondly, we show that by using our technique and some modifications to the MAX-oracle, it is possible to obtain close-to-4-approximation to the problem of computing permanent of nonnegative matrices. The NP-oracle still is amenable to be implemented in an ILP solver. It is to be noted that our idea of optimization
over multiple bins is crucial here, since the straightforward generalization of Ermon et al.’s result would have given an approximation factor of $\Omega(n^2)$. While there already exists a polynomial time randomized approximation scheme $(1 \pm \varepsilon$-approximation) of permanent of a nonnegative matrix $[13]$, the runtime there is $O(n^{10})$. Since we are delegating the hard task to a professional optimization solver, our method can still be of interest here.

While only of auxiliary interest here, we note that it is possible to derandomize the hash families based on parity-constraints to the optimal extent while maintaining the essential properties necessary for their performance. Namely, it can be ensured that the hash family can still be represented as $\{x \mapsto Ax + b\}$ while using information theoretically optimal memory to generate them.

Finally, we show the performance of our algorithms to compute the partition function of the ferromagnetic Potts model by running experiments on both synthetic datasets and real-worlds datasets. While in this paper we concentrate on theoretical results, the experiments serve as good ‘proof of concepts’ for applications. We also use our algorithm to compute the Total Variation (TV) distance between two joint probability distributions over a large number of variables. The algorithm to compute permanent is also validated experimentally. We propose our method as a possible alternative to the popular Markov-Chain-Monte-Carlo (MCMC) method for discrete integration and show experimental comparisons. All the experiments exhibit good performance guarantees.

**Organization.** The paper is organized as follows. In Section 2 we describe the technique by [6], and then elaborate our new ideas and main results. In Section 3 we provide an improvement of the WISH algorithm by [6] that lead to an improved approximation. We provide an algorithm with un constrained optimization oracle (similar to [2]) and its analysis in Section 4. Section 5 is devoted to computation of permanent of a matrix. In Section 6 we show how to optimally derandomize the hash function used in our algorithm. The experimental results on computation of partition functions, total variation distance, and the permanent, as well as comparisons with MCMC, are provided in Section 7.

2 Background and our techniques

In this section we describe the main ideas developed by [6] and provide an overview of the techniques that we use to arrive at our new results.

First of all, notice that from (1) we obtain: $S_0(w) = \sum_{u \geq 0} \{\sigma \in \Omega : w(\sigma) = u\} = \sum_{u \geq 0} \{\sigma \in \Omega : w(\sigma) \geq u\} = \sum_{u \geq 0} T(u)$, where $T(u) \equiv \{\sigma \in \Omega : w(\sigma) \geq u\}$ is the tail distribution of weights and a nonincreasing function of $u$. Note that, $0 \leq T(u) \leq |\Omega|$. We can split the range of $T(u)$ into geometrically growing values $1, q, q^2, \ldots, q^n$ such that $q^n \geq |\Omega|$. Let $\beta_i = u : T(u) = q^i, i = 0, 1, \ldots, n'$. Clearly $\beta_0 > \beta_1 > \cdots > \beta_{n'}$. As we have not made any assumption on the values of the weight function, $\beta_i$ and $\beta_{i+1}$ can be far from each other and they are hard to bound despite the fact that $T(u)$ is monotonic in nature. On the other hand we can try to bound the area under the curve $T(u)$ by bounding the area of the slice between $\beta_i$ and $\beta_{i+1}$. This area is at least $q^i(\beta_i - \beta_{i+1})$ and at most $q^{i+1}(\beta_i - \beta_{i+1})$. Therefore: $\sum_{i=0}^{n'-1} q^i(\beta_i - \beta_{i+1}) + q^{n'} \beta_{n'} \leq S_0(w) \leq \sum_{i=0}^{n'-1} q^{i+1}(\beta_i - \beta_{i+1}) + q^{n'} \beta_{n'}$, which implies

$$\beta_0 + (q - 1) \sum_{i=1}^{n'} q^{i-1} \beta_i \leq S_0(w) \leq \beta_0 + (q - 1) \sum_{i=1}^{n'} q^i \beta_i. \tag{5}$$

Hence $\beta_0 + (q - 1) \sum_{i=1}^{n'} q^{i-1} \beta_i$ is a $q$-factor approximation of $S_0(w)$ and if we are able to find a $k$ approximation of each value of $\beta_i$ we will be able to obtain a $kq$-factor approximation of $S_0(w)$. In [6], subsequently the main idea is to estimate the coefficients $\{\beta_i, 0 \leq i \leq n'\}$.

Now note that, $q^i = |\{\sigma \in \Omega : w(\sigma) \geq \beta_i\}|$. Suppose, using a random hash function $h : \Omega \rightarrow \{0, 1, \ldots, q^i - 1\}$ we compute hashes of all elements in $\Omega$. The pre-image of an entry in $\{0, 1, \ldots, q^i - 1\}$
is called the bin corresponding to that value, i.e., \( \{ \sigma : h(\sigma) = x \} \) is the bin corresponding to the value \( x \in \{0, 1, \ldots, q^l - 1 \} \). In every bin for the hash function, there is on average one element \( \sigma \) such that \( w(\sigma) \geq \beta_i \). So for a randomly and arbitrarily chosen bin if \( \sigma^* = \max_{\sigma : h(\sigma) = x} w(\sigma) \), then \( \sigma^* \geq \beta_i \) on expectation. However suppose one performs this random hashing \( \ell = O(\log n) \) times and then take the aggregate (in this case the median) value of \( \sigma \)'s. That is say, \( \sigma^* = \text{median}(\sigma_1^*, \ldots, \sigma_k^*) \). Then by using the independence of the hash functions, it can be shown that the aggregate is an upper bound on \( \beta_i \) with high probability. Indeed, without loss of generality, if we assume that the configurations within \( \Omega \) are ordered according to the value of the function \( w \), i.e., \( w(\sigma_1) \geq w(\sigma_2) \geq \cdots \geq w(\sigma_{|\Omega|}) \) then we can take \( \beta_i = w(\sigma_{q^l}). \) If the hash family is pairwise independent, then by using the Chebyshev inequality it can be shown that \( \sigma^* \in [\beta_{i+c}, \beta_{i-c}] \) with high probability, \( c \geq 2 \). This lead to a \( q^{2c} \)-approximation for \( S_{\Omega}(w) \). For \( c = 2 \) this leads to the 16-approximation, because \cite{6} identified \( \Omega \) with \( \mathbb{F}_q^n \) and took \( q = 2 \). The WISH algorithm proposed by \cite{6} makes use of the above analysis and provides a 16-approximation of \( S_w(\Omega) \). If we naively extend this algorithm by identifying \( S_w(\Omega) \) with \( \mathbb{F}_q^n \) then the approximation factor we achieve is \( q^{2c} \), \( q > 2, c \geq 1 \). Note that, for \( q = 2 \), it was not possible to take \( c = 1 \), but as we will see later that it is possible to take \( c = 1 \) when \( q > 2 \), and for \( q = 3 \), this observation immediately gives a 9-approximation to \( S_w(\Omega) \).

Instead of using a straight-forward analysis for the \( q \)-ary case, in this paper we use a MAX-oracle that can optimize over multiple bins of the hash function. Using this oracle we proposed a modified WISH algorithm and call it MB-WISH (Multi-Bin WISH). Just as in the case of \cite{6,7}, the MAX-oracle constraints can be integer linear programming constraints and commercial softwares such as CPLEX can be used.

The main idea of using an optimization over multiple bins is that it boosts the probability that the \( \sigma^* \) we are getting above is close to \( b_i \). However if we restrict ourselves to the binary alphabet then (as will be clear later) there is no immediate way to represent such multiple bins in a compact way in the MAX-oracle. For the non-binary case, it is possible to represent multiple bins of the hash function as simple inequality constraints. This idea lead to an improvement in the approximation factor of \( S_w(\Omega) \) to \( 4 + \epsilon \), where \( \epsilon \) decays to 0 proportional to \( q^{-1} \). Note that we need to choose \( q \) to be a power of prime so that \( \mathbb{F}_q \) is a field.

In \cite{2}, the bins (as described above) are produced as images of some function, and not as pre-images of hashes. Since we want the number of bins to be \( q^l \), this can be achieved by looking at images of \( g : \mathbb{F}_q^{n-1} \rightarrow \Omega \) where \( \{|g(\sigma) : \sigma \in \mathbb{F}_q^{n-1}\}| = q^{n-l}. \) The rest of the analysis of \cite{2} is almost same as above. The benefit of this approach is that the MAX-oracle just has to solve an unconstrained optimization here. Implementing our multi-bin idea for this perspective of \cite{2} is not straight-forward as we can no longer use inequality constraints for this. However, as we show later, we found a way to combine bins here in a succinct way generalizing the design of \( g \). As a result, we get the same approximation guarantee as in MB-WISH, with the oracle load heavily reduced (this algorithm, that we call Unconstrained MB-WISH, can be found in Section 4).

Coming back to the discussion on MB-WISH, for computing the permanent, the domain of integration is the symmetric group \( S_n \). However \( S_n \) can be embedded in \( \mathbb{F}_q^d \) for a \( q > n \). Therefore we can try to use MB-WISH algorithm and same set of hashes on elements of \( S_n \) treating them as \( q \)-ary vectors, \( q > n \). We need to be careful though since it is essential that the MAX-oracle returns a permutation and not an arbitrary vector. The modified MAX-oracle for permanents therefore must have some additional constraints. However those being affine constraints, it turns out MAX-oracle is still implementable in common optimization softwares easily.

For the analysis of \cite{6,7} to go through, we needed a family of hash functions that are pairwise independent\footnote{It is sufficient to have the hash family satisfy some weaker constraints, such as being pairwise negatively correlated.}. A hash family \( \mathcal{H} = \{ h : \Omega \rightarrow \tilde{\Omega} \} \) is called uniform and pairwise independent if the following two criteria are met for a randomly and uniformly chosen \( h \) from \( \mathcal{H} \): 1) for every \( x \in \Omega \), \( h(x) \) is uniformly distributed in \( \tilde{\Omega} \) and 2) for any two \( x, y \in \Omega \) and \( u, v \in \tilde{\Omega} \), \( \Pr(h(x) = u, h(y) = v) = \)
Theorem 1. Let \( \Omega = \mathbb{F}_q^n \) where \( q \) is a prime-power. Let us also fix an ordering among the elements of \( \mathbb{F}_q \equiv \{ a_0, a_1, \ldots, a_{q-1} \} \) and write \( a_0 < a_1 < \cdots < a_{q-1} \). In this section, the symbol ‘<’ just signifies a fixed ordering and has no real meaning over the finite field. Extending this notation, for any two vectors \( x, y \in \mathbb{F}_q^m \), we will say \( x < y \) if and only if the \( i \)th coordinates of \( x \) and \( y \), satisfy \( x_i < y_i \) for all \( i = 1, \ldots, m \). Below \( \lfloor E \rfloor \) denotes an all-one vector of a dimension that would be clear from context. Also, for any event \( E \) let \( 1[E] \) denote the indicator for the event \( E \).

The MAX-oracle for MB-WISH performs the following optimization, given \( A \in \mathbb{F}_2^{m \times n}; b, s \in \mathbb{F}_q \):

\[
\max_{\sigma \in \mathbb{F}_q^n; A\sigma + b < s} w(\sigma). 
\tag{6}
\]

The modified WISH algorithm is presented as Algorithm 1. The main result of this section is below.

**Algorithm 1** MB-WISH algorithm for \( \Omega = \mathbb{F}_q^n \)

Initialize: \( r, \gamma = \frac{q}{\sqrt{r}} \left( \frac{1}{2} - \frac{c}{q} \right)^2, \ell = \lceil \frac{1}{\ell} \ln \frac{2n}{\ell} \rceil, n' = \lceil n \log_q r \rceil \)

\( M_0 \equiv \max_{\sigma \in \mathbb{F}_q^n} w(\sigma) \)

for \( i \in \{1, 2, \ldots, n'\} \) do

for \( k \in \{1, \ldots, \ell\} \) do

Sample hash functions \( h_i \equiv h_{A_i, b_i} \) uniformly at random from \( \mathcal{H}_{i,n} \) as defined in (7)

\( w_i^{(k)} = \max_{\sigma; A_i\sigma + b_i < a_{r_i-1}} w(\sigma) \)

end for

\( M_i = \text{Median}(w_i^{(1)}, w_i^{(2)}, \ldots, w_i^{(\ell)}) \)

end for

Return \( M_0 + \left( \frac{q}{r} - 1 \right) \sum_{i=0}^{n'-1} M_{i+1} \left( \frac{q}{r} \right)^i \)

**Theorem 1.** Let \( q \) be a prime power, \( \Omega = \mathbb{F}_q^n \) and \( r = \left\lfloor \frac{2n}{\ell} \right\rfloor \). For any \( \delta > 0 \) and a positive constant \( \gamma = \frac{q}{\sqrt{r}} \left( \frac{1}{2} - \frac{c}{q} \right)^2 \), Algorithm 1 makes \( \Theta(n \log \frac{r}{\delta}) \) calls to the MAX-oracle and, with probability \( \geq 1 - \delta \) outputs a \( (\frac{q}{r})^2 \)-approximation of \( S_w(\Omega) \).

The theorem will be proved by a series of lemmas. The key trick that we are using is to ask the MAX-oracle to solve an optimization problem over not a single bin, but multiple bins of the hash function. The hash family is defined in the following way. We have \( h_{A,b} : \mathbb{F}_q^n \rightarrow \mathbb{F}_q^n : x \mapsto Ax + b \), the operations are over \( \mathbb{F}_q \). Let

\[
\mathcal{H}_{m,n} = \{ h_{A,b} : A \in \mathbb{F}_q^{m \times n}, b \in \mathbb{F}_q^m \}. 
\tag{7}
\]
The coding theoretic intuition behind our technique is following. The set of configurations $\{\sigma \in \mathbb{F}_q^n : A\sigma = 0\}$ forms a linear code of dimension $n - m$. The bins of the hash function define the cosets of this linear code. We would like to choose $q^r$ cosets of a random linear code and find the optimum value of $w$ over the configurations of these cosets as the MAX-oracle. To choose a hash function uniformly and randomly from $\mathcal{H}$, we can just choose the entries of $A$ and $b$ uniformly at random from $\mathbb{F}_q$ independently.

Note that, the hash family $\mathcal{H}_{m,n}$ as defined in (7) is uniform and pairwise independent. It follows from the following more general result.

**Lemma 1.** Let us define $Z_{\alpha}$ to be the indicator random variable denoting $A\sigma + b < \alpha_r \cdot 1$ for some $r \in \{0, \ldots, q - 1\}$ and $A, b$ randomly and uniformly sampled from $\mathcal{H}_{m,n}$. Then $\Pr(Z_{\alpha} = 1) = \left(\frac{\alpha}{q}\right)^m$ and for any two configurations $\sigma_1, \sigma_2 \in \mathbb{F}_q^n$ the random variables $Z_{\sigma_1}$ and $Z_{\sigma_2}$ are independent.

**Proof.** Let $A_i$ denote the $i$th row of $i$ and $b_i$ denote the $i$th entry of $b$. Then $\mathbb{I}[A\sigma + b < \alpha_r \cdot 1] = \bigwedge_{i=1}^m \mathbb{I}[A_i\sigma + b_i < \alpha_r]$.

For all configurations $\sigma \in \Omega, \forall i$, we must have

$$\Pr(A_i\sigma + b_i < \alpha_r) = \sum_{j=0}^{r-1} \Pr(A_i\sigma + b_j = \alpha_j) = \frac{r}{q}.$$

As $A_i, b_i$ are independent $1 \leq i \leq m$, we must have that $\Pr(A\sigma + b < \alpha_r \cdot 1) = \left(\frac{\alpha}{q}\right)^m$. Now for any two configurations $\sigma_1, \sigma_2 \in \mathbb{F}_q^n$,

$$\Pr(A_i\sigma_1 + b_i < \alpha_r \land A_i\sigma_2 + b_i < \alpha_r)$$

$$= \sum_{k=0}^{r-1} \sum_{j=0}^{r-1} \Pr(A_i\sigma_1 + b_l = \alpha_k \land A_i\sigma_2 + b_l = \alpha_j)$$

$$= \sum_{k=0}^{r-1} \sum_{j=0}^{r-1} \Pr(A_i\sigma_1 + b_l = \alpha_k) \cdot \Pr(A_i\sigma_2 + b_l = \alpha_j)$$

$$= \sum_{k=0}^{r-1} \sum_{j=0}^{r-1} \Pr(A_i\sigma_1 + b_l = \alpha_k) Pr(A_i(\sigma_2 - \sigma_1) = \alpha_j - \alpha_k)$$

$$= r^2 \frac{1}{q^2} \left(\frac{1}{q}\right)^2 = \frac{r^2}{q^2} \left(\frac{1}{q}\right)^2.$$

As all the rows are independent, $\Pr(A\sigma_1 + b < \alpha_r \cdot 1 \land A\sigma_2 + b < \alpha_r \cdot 1) = \left(\frac{\alpha}{q}\right)^{2m}$. \hfill \Box

Fix an ordering of the configurations $(\sigma_i, 1 \leq i \leq q^n)$ such that $1 \leq j \leq q^n, w(\sigma_j) \geq w(\sigma_{j+1})$. We can also interpolate the space of configuration to make it continuous by the following technique. For any positive real number $x = z + f$, where $z = \lfloor x \rfloor$ is the integer part and $f = x - z$ is the fractional part, define $w(\sigma_x) = w(\sigma_z)$. For $i \in \{0, 1, 2, \ldots, n' = \lceil n \log_q \left(\frac{1}{q}\right)\rceil\}$, define $\beta_i = w(\sigma_{i^t}) = w(\sigma_{t_{i^t}})$, where $t = \frac{q}{2}$. We take $w(\sigma_k) = 0$ for $k > q^n$. To prove Theorem 1 we need the following crucial lemma as well.

**Lemma 2.** Let $M_i = \text{Median}(w_i^{(1)}, \ldots, w_i^{(\ell)})$ be defined as in the Algorithm 1. Then for $\gamma = \frac{q}{3n} (\frac{1}{2} - \frac{r}{q})^2$, we have, $\Pr \left( M_i \in [\beta_{\min(i+1,n')}, \beta_{\max(i-1,0)}] \right) \geq 1 - 2 \exp(-\gamma \ell)$.

**Proof of Lemma 3.** Consider the set of $\lceil t^j \rceil$ heaviest configuration $\Omega_j = \{\sigma_1, \ldots, \sigma_{t^j}\}$. 


Let $S_j(h_i) = |\{\sigma \in \Omega_j : A^i \sigma + b^i < \alpha_r \cdot 1\}|$. By the uniformity property of the hash function,

$$\mathbb{E} S_j(h_i) = \mathbb{E} \sum_{\sigma \in \Omega_j} \mathbb{I}[h_i(\sigma) < \alpha_r \cdot 1] = \frac{|t^j|}{t^i}.$$  

For each configuration $\sigma$ let us denote the random variable $Z^j_\sigma = \mathbb{I}[h_i(\sigma) < \alpha_r \cdot 1] - \frac{1}{t^i}$. By our design \(\mathbb{E}Z^j_\sigma = 0\). Note that, $S_j(h_i) - \mathbb{E}S_j(h_i) = \sum_{\sigma \in \Omega_j} Z^j_\sigma$. Also, from Lemma 1 the random variables $Z^j_\sigma$s are pairwise independent. Therefore,

$$\text{var} S_j(h_i) = \text{var} \left( \sum_{\sigma \in \Omega_j} Z^j_\sigma \right) = \sum_{\sigma \in \Omega_j} \mathbb{E} Z^j_\sigma^2 = \frac{|t^j|}{t^i} \left(1 - \frac{1}{t^i}\right).$$

Now, for any $1 \leq k \leq \ell$,

$$\Pr(w^{(k)}(i) \geq \beta_j) = \Pr(\gamma w^{(i)} \geq w(\sigma_{\ell+1})) \geq \Pr(S_j(h_i) \geq 1) \geq 1 - \Pr(S_j(h_i) \leq 0).$$

Let $j = i + 1$. Then, using Chebyshev inequality,

$$\Pr(S_j(h_i) \leq 0) = \Pr \left( S_j(h_i) - \mathbb{E} S_j(h_i) \leq -\frac{|t^j|}{t^i} \right) \leq \frac{\text{var} S_j(h_i)}{\left(\frac{|t^j|}{t^i}\right)^2} \leq \frac{t^i(1 - 1/t^i)}{|t^j|} < \frac{t^i - 1}{t^i+1 - 1} \leq \frac{1}{t} = \frac{r}{q}.$$  

Therefore,

$$\Pr(w^{(k)}(i) \geq \beta_{i+1}) \geq 1 - \frac{r}{q}.$$  

Also, $\Pr(w^{(k)}(i) \leq \beta_{i-1}) = \Pr(\gamma w^{(i)} \leq w(\sigma_{\ell+1})) \geq \Pr(S_{i-1}(h_i) = 0)$. Notice that the last inequality is satisfied because $S_{i-1}(h_i) = 0$ implies $w^{(k)}(i) \leq w(\sigma_{\ell+1})$. Now, continuing the chain of inequalities, using Markov inequality,

$$\Pr(w^{(k)}(i) \leq \beta_{i-1}) \geq 1 - \Pr(S_{i-1}(h_i) \geq 1) \geq 1 - \mathbb{E} S_{i-1}(h_i) = 1 - \frac{|t^{i-1}|}{t^i} \geq 1 - \frac{1}{t} = 1 - \frac{r}{q}.$$  

Now just by using Chernoff bound\(^2\)

$$\Pr(M_i \leq \beta_{i+1}) \leq \exp \left(-\frac{\ell q}{3r} \left(\frac{1}{2} - \frac{r}{q}\right)^2\right), \quad \text{and} \quad \Pr(M_i \geq \beta_{i-1}) \leq \exp \left(-\frac{\ell q}{3r} \left(\frac{1}{2} - \frac{r}{q}\right)^2\right).$$

This proves the lemma. \(\square\)

From Lemma 2 the output of the algorithm lies in the range $[L', U']$ with probability at least $1 - \delta$ where $L' = \beta_0 + (t - 1) \sum_{i=0}^{\ell-1} \beta_{\min(i+2, n')} t^i$ and $U' = \beta_0 + (t - 1) \sum_{i=0}^{\ell-1} \beta_{i} t^i$. $L'$ and $U'$ are a factor of $t^2$ apart. Now, following an argument similar to \(6\), we can show $L' \leq S_w(\Omega) \leq U'$.

Therefore Algorithm 1 provides a $t^2$-approximation to $S_w(\Omega)$. Let us now give the full proof of Theorem 1.

**Proof of Theorem 1** From Lemma 2 we have, $\Pr \left( \bigcap_{i=1}^{\ell} M_i \in [\beta_{\min(i+1, n')}, \beta_{\max(i-1, 0)}] \right) \geq 1 - 2n \exp(-\gamma \ell) = 1 - \delta$ for $\ell = \frac{1}{\gamma} \ln \frac{2n}{\delta}$ and by definition $M_0 = \beta_0$.\(^2\)

\(^2\)We use the fact that if $X$ is a sum of iid $\{0, 1\}$ random variables then $\Pr(X \geq \mathbb{E}X(1+\delta)) \leq \exp(-\mathbb{E}X\delta^2/3)$. 

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The algorithm outputs $M_0 + (t-1) \sum_{i=0}^{n'-1} M_{i+1} t^i$ which lies in the range $[L', U']$ with probability at least $1 - \delta$ where

$$L' = \beta_0 + (t-1) \sum_{i=0}^{n'-1} \beta_{\min \{i+2, n'\}} t^i \quad \text{and} \quad U' = \beta_0 + (t-1) \sum_{i=0}^{n'-1} \beta_i t^i.$$ 

Now notice that, as $\beta_0 \geq \beta_1$, we have

$$U' = \beta_0 + (t-1) \sum_{i=0}^{n'-1} \beta_i t^i$$

$$= \beta_0 + (t-1)(\beta_0 + \beta_1 t) + \sum_{i=2}^{n'-1} \beta_i t^i$$

$$\leq t^2 \beta_0 + t^2.(t-1). \sum_{i=2}^{n'-1} \beta_i t^{i-2}$$

$$\leq t^2(\beta_0 + (t-1) \sum_{i=0}^{n'-1} \beta_{\min \{i+2, n'\}} t^i) = t^2 L'.$$

The only thing that remains to be proved is that $L' \leq S_\omega(\Omega) \leq U'$. However that is true, by just following an argument similar to [5]. Indeed,

$$\sum_{i=0}^{n'-1} \beta_{i+1}(t^{i+1} - t^i) \leq S_\omega(w) \leq \sum_{i=0}^{n'-1} \beta_i(t^{i+1} - t^i)$$

which implies $L' \leq S_\omega(\omega) \leq U'$.

Therefore Algorithm 1 provides a $t^2$-approximation to $S_\omega(w)$. The total number of calls to the MAX-oracle is $n' \ell + 1 = O(n \log(n/\delta))$. \hfill \Box

To exemplify this result, suppose $q = 3$. In this case the algorithm provides a 9-approximation. Later, in the experimental section, we have used a ferromagnetic Potts model with $q = 5$. MB-WISH provides a $2^{3} = 6.25$-approximation in that case. Note that, for a 5-ary Potts model, it is only natural to use our algorithm instead of converting it to binary in conjunction with the original algorithm of Ermon et al.

Instead of pairwise independent hash families, if we employ $k$-wise independent families, it leads to a better decay probability of error. However it does not improve the approximation factor.

**MB-WISH with unconstrained optimization oracle.** We can modify and generalize the results of Achlioptas and Jiang [2] to formulate a version of MB-WISH that can use unconstrained optimizers as the MAX-oracle. The MAX-oracle for this algorithm performs an unconstrained optimization of the form: max$_{a \in B} w(A a + b)$, given $A \in \mathbb{F}^m_q \times n$, $b \in \mathbb{F}^m_q$ and a set $B \subseteq \mathbb{F}^m_q$.

The aim is to carefully design $B$ so that all the desirable statistical properties are satisfied. This part is quite different from the hashing-based analysis and not an immediate extension of [2]. We provide the algorithm (Unconstrained MB-WISH) and its analysis in the next section.

## 4 MB-WISH with unconstrained optimization oracle

In this section, we provide an algorithm that uses unconstrained optimizations for the oracle, as in the case of Achlioptas and Jiang [2]. We call this algorithm Unconstrained MB-WISH.
Let us assume $\Omega = \mathbb{F}_q^n$ where $q$ is a prime-power. As before, let us also fix an ordering among the elements of $\mathbb{F}_q \equiv \{\alpha_0, \alpha_1, \ldots, \alpha_{q-1}\}$ and write $\alpha_0 < \alpha_1 < \cdots < \alpha_{q-1}$. Recall that, here the symbol ‘<’ just signifies a fixed ordering and has no real meaning over the finite field.

The MAX-oracle for Unconstrained MB-WISH performs an unconstrained optimization of the following form, given $A \in \mathbb{F}_q^{m \times n}, b \in \mathbb{F}_q^n$ and a set $B \subseteq \mathbb{F}_q^m$:

$$\max_{\sigma \in B} w(A\sigma + b). \quad (8)$$

The Unconstrained MB-WISH algorithm is presented as Algorithm 2. The main result of this section is the following.

Theorem 2. Let $q$ be a power of prime and $r = \lfloor \frac{q-1}{2} \rfloor$. Let $\Omega = \mathbb{F}_q^n$. For any $\delta > 0$ and a positive constant $\gamma = \frac{q}{3r} (\frac{1}{2} - \frac{\ell}{q})^2$, Algorithm 2 makes $\Theta(n \log \frac{n}{\delta})$ calls to the MAX-oracle (cf. (8)) and, with probability at least $1 - \delta$ outputs a $(\frac{q}{2})^2$-approximation of $S_w(\Omega)$.

Algorithm 2 Unconstrained MB-WISH algorithm for $\Omega = \mathbb{F}_q^n$

Initialize: $\ell \rightarrow \lfloor \frac{1}{r} \ln \frac{2}{\delta} \rfloor$, $r, n' = \lfloor n \log q/r \rfloor$

$M_0 = \max_{\sigma \in \mathbb{F}_q^n} w(\sigma)$

for $i \in \{1, 2, \ldots, n\}$ do

for $k \in \{1, \ldots, \ell\}$ do

Sample $n$ linearly independent vectors spanning $\mathbb{F}_q^n$ and construct matrices $A$ and $R$ by taking the first $n - i$ columns and the last $i$ columns respectively

$w_i^{(k)} = \max_{x \in \mathbb{F}_q^{n-i}} \min_{y \in \{a_0, a_1, \ldots, a_{r-1}\}^i} w(Ax + Ry + b)$

end for

$M_i = \text{Median}(w_i^{(1)}, w_i^{(2)}, \ldots, w_i^{(\ell)})$

end for

for $i \in \{n + 1, \ldots, n'\}$ do

for $k \in \{1, \ldots, \ell\}$ do

Sample full rank matrix $A \in \mathbb{F}_q^{m \times n}, b \in \mathbb{F}_q^n$ uniformly at random. Set $S_i$ as defined in Equation 10

$w_i^{(k)} = \max_{y \in S_i} w(Ay + b)$

end for

$M_i = \text{Median}(w_i^{(1)}, w_i^{(2)}, \ldots, w_i^{(\ell)})$

end for

Return $M_0 + (\frac{q}{r} - 1) \sum_{i=0}^{n'-1} M_{i+1} (\frac{q}{2})^i$

To prove this theorem we borrow some ideas from coding theory. We define a linear $q$-ary code $C$ of dimension $n - m$ and length $n$ as the set of vectors $\{Ax : x \in \mathbb{F}_q^{n-m}\}$ where $A$ is a full-rank matrix of size $n \times n - m$ and rank $n - m$. For a vector $a \in \mathbb{F}_q^n$, we define the set $\{a + C\}$ as a coset of $C$. It is well known that $\mathbb{F}_q^n$ is partitioned by the $q^m$ distinct cosets, each of size $q^{n-m}$. The main technique behind our algorithm is that for a random linear code $C$ of size $q^{n-m}$, we randomly sample $r^m$ distinct cosets of $C$. Subsequently, we find the maximum value $w(x)$ of an element among those $r^m$ cosets.

Let $E \equiv \{e_i\}_{i=1}^n$ be a set of $n$ linearly independent vectors in $\mathbb{F}_q^n$ chosen randomly and uniformly (one can uniformly sample the columns of $E$ and resample if it belongs to the span of the already chosen columns). Let $A$ denote the matrix formed by the first $n - m$ vectors of $E$ as columns and let $R$ be the matrix formed by the remaining $m$ vectors as column. Also let $b$ be a vector sampled randomly and uniformly from $\mathbb{F}_q^n$.
The MAX-oracle for Unconstrained MB-WISH is going to perform the following optimization when \( m \leq n \):

\[
\max_{\sigma_1 \in \mathbb{F}_q^{n-m}, \sigma_2 \in \{a_0, a_1, \ldots, a_{r-1}\}^{m}} w(A\sigma_1 + R\sigma_2 + b). \tag{9}
\]

Analogous to Theorem 1 here we are creating union of \( r^m \) distinct random bins. If we can prove that, for any element of \( \mathbb{F}_q^n \), the probability that it belongs to one of these bins is \( \left( \frac{r}{q} \right)^m \) and for any pair of different elements from \( \mathbb{F}_q^n \), whether they belong to one of these bins are independent (pairwise independence), the rest of the proof of Theorem 2 will just follow that of Theorem 1.

In particular, we just have to prove the lemma that is analogous to Lemma 1. Define a set

\[
S_{A,R,b} \equiv \{Ax + b + Ry \mid x \in \mathbb{F}_q^{n-m}, y \in \{a_0, a_1, \ldots, a_{r-1}\}^m\}.
\]

For each configuration \( \sigma \in \mathbb{F}_q^n \), associate an indicator random variable \( Z_\sigma \) denoting whether \( \sigma \in S_{A,R,b} \).

**Lemma 3.** For each configuration \( \sigma \in \mathbb{F}_q^n \), we must have \( \Pr(Z_\sigma = 1) = \left( \frac{r}{q} \right)^m \) and moreover for any two distinct configurations \( \sigma_1, \sigma_2 \in \mathbb{F}_q^n \) the random variables \( Z_{\sigma_1} \) and \( Z_{\sigma_2} \) are independent.

**Proof.** Notice that \( S_{A,R,b} \) is a union of distinct cosets and therefore,

\[
S_{A,R,0} \equiv \bigcup_{y \in \{a_0, a_1, \ldots, a_{r-1}\}^m} S_{A,0}(y),
\]

where \( S_{A,0}(y) \equiv \{Ax + Ry \mid x \in \mathbb{F}_q^{n-m}\} \) is defined as a particular coset with a fixed \( y \in \{a_0, a_1, \ldots, a_{r-1}\}^m \). Hence \( |S_{A,R,0}| = q^{n-m}r^m \) and since \( S_{A,R,b} \) is simply a random affine shift of \( S_{A,R,0} \), \( |S_{A,R,b}| = q^{n-m}r^m \) as well. Now for a vector \( \sigma \in \mathbb{F}_q^n \), we must have

\[
\Pr(Z_\sigma) = \sum_{y \in S_{A,R,b}} \Pr(\sigma = y) = \frac{|S_{A,R,b}|}{q^n} = \left( \frac{r}{q} \right)^m.
\]

Next, for two configurations \( \sigma_1, \sigma_2 \in \mathbb{F}_q^n \), we have that

\[
\Pr(Z_{\sigma_1} = 1 \land Z_{\sigma_2} = 1) = \sum_{y_1, y_2} \Pr(\sigma_1 \in S_{A,b}(y_1) \land \sigma_2 \in S_{A,b}(y_2))
\]

\[
= \sum_{y_1, y_2} \Pr(\sigma_1 \in S_{A,b}(y_1) \mid \sigma_2 \in S_{A,b}(y_2)) \Pr(\sigma_2 \in S_{A,b}(y_2))
\]

\[
= \sum_{y_1, y_2} \Pr(\sigma_1 - \sigma_2 \in S_{A,0}(y_1 - y_2)) \Pr(\sigma_2 \in S_{A,b}(y_2)).
\]

Therefore we just need to evaluate the probability of the event \( \Pr(\tau \in S_{A,0}(z)) \) for \( \tau = \sigma_1 - \sigma_2 \neq 0 \) and \( z = y_1 - y_2 \). Now, if \( z = 0 \), \( \Pr(\tau \in S_{A,0}(z)) \) is simply equal to \( \frac{1}{q^m} \) since the columns of \( A \) are independent, i.e., \( |\{Ax : x \in \mathbb{F}_q^{n-m}\}| = q^{n-m} \). Now, since the linearly independent columns of \( R \) are sampled randomly, we have

\[
\Pr(\tau \in S_{A,0}(z) \mid z \neq 0) = \frac{1}{q^m - 1}.
\]

Hence,

\[
\Pr(\tau \in \tau \in S_{A,0}(z) \mid z \neq 0) = \left( 1 - \frac{1}{q^m} \right) \frac{1}{q^m - 1} = \frac{1}{q^m}.
\]
Therefore, we have that
\[
\Pr(Z_{\sigma_1} = 1 \land Z_{\sigma_2} = 1) = \sum_{y_1, y_2} \frac{1}{q^{2m}} = \left(\frac{r}{q}\right)^{2m}
\]
and hence we have the statement of the lemma.

From Algorithm 3 it is clear that Lemma 3 allows us to obtain the values of \( M_i \) for \( i \in \{1, 2, \ldots, n\} \). Indeed, the MAX-oracle is not well defined when \( m > n \). In order to obtain the values of \( M_i \) for \( i \in \{n + 1, \ldots, n'\} \), we propose the following technique.

Recall that the elements of \( \mathbb{F}_q^n \) can be represented as \( n \) dimensional vectors where each element belongs to \( \mathbb{F}_q \). Moreover we defined an ordering over the elements of the finite field \( \mathbb{F}_q = \{\alpha_0, \alpha_1, \ldots, \alpha_{q-1}\} \) so that \( \alpha_i < \alpha_j \) for \( i < j \). Consider the lexicographic ordering of the elements (vectors) of \( \mathbb{F}_q^n \). Let \( s_m \) be the \( \left\lceil\frac{r^m}{q^{m-n}}\right\rceil \) th element in this ordering of \( \mathbb{F}_q^n \). Define the set
\[
S_m = \{x \in \mathbb{F}_q^n \mid x < s_m\} \tag{10}
\]
for all \( m > n \). Generate a random uniform full rank matrix \( A \in \mathbb{F}_q^{n \times n} \) and a uniform random vector \( b \in \mathbb{F}_q^n \). Subsequently, the MAX-Oracle for MBA-WISH solves the following optimization problem for \( m > n \):
\[
\max_{y \in S_m} w(Ay + b).
\]

In order to analyze the statistical properties of this oracle, define the random set
\[
T_{A,b,m} \equiv \{Ay + b \mid y \in S_m\}.
\]
Again, for each configuration \( \sigma \in \mathbb{F}_q^n \), associate an indicator random variable \( Z_{\sigma} \) denoting \( \sigma \in T_{A,b,m} \).

**Lemma 4.** For each configuration \( \sigma \in \mathbb{F}_q^n \), we must have \( \Pr(Z_{\sigma} = 1) \approx \left(\frac{r}{q}\right)^m \) and moreover for any two configurations \( \sigma_1, \sigma_2 \in \mathbb{F}_q^n \), \( \Pr(Z_{\sigma_1} = 1 \land Z_{\sigma_2} = 1) \leq (\Pr(Z_{\sigma_1} = 1))^2 \).

**Proof.** We have,
\[
\Pr(Z_{\sigma} = 1) = \sum_{y \in T_{A,b,m}} \Pr(\sigma = y) = \frac{|T_{A,b,m}|}{q^n} = \frac{1}{q^n} \left(\frac{r^m}{q^{m-n}}\right) \approx \left(\frac{r}{q}\right)^m.
\]

Next, for two distinct configurations \( \sigma_1, \sigma_2 \in \mathbb{F}_q^n \), we have that
\[
\Pr(Z_{\sigma_1} = 1 \land Z_{\sigma_2} = 1) = \sum_{y_1, y_2} \Pr(\sigma_1 = y_1 \land \sigma_2 = y_2)
= \sum_{y_1, y_2 \in S_m} \Pr(\sigma_1 = Ay_1 + b \land \sigma_2 = Ay_2 + b)
= \sum_{y_2 \in S_m} \Pr(\sigma_2 = Ay_2 + b) \sum_{y_1 \in S_m} \Pr(\sigma_1 = Ay_1 + b \mid \sigma_2 = Ay_2 + b)
= \sum_{y_2 \in S_m} \Pr(\sigma_2 = Ay_2 + b) \sum_{y_1 \in S_m} \Pr(\sigma_1 - \sigma_2 = A(y_1 - y_2))
\]
Since $\sigma_1 \neq \sigma_2$, we must have that $\Pr(\sigma_1 - \sigma_2 = A(y_1 - y_2) \mid y_1 = y_2) = 0$. For $y_1 \neq y_2$, every configuration $\sigma \in \mathbb{F}_q^n \backslash \{0\}$ is equally probable to be $A(y_1 - y_2)$ since $A$ is uniformly and randomly sampled full rank matrix. Hence,

$$
\Pr(Z_{\sigma_1} = 1 \wedge Z_{\sigma_2} = 1) = \frac{1}{q^n(q^n - 1)} \left\lceil \frac{r^m}{q^{m-n}} \right\rceil \left(\frac{r^m}{q^{m-n}} - 1\right) \leq (\Pr(Z_\sigma = 1))^2.
$$

\[ \square \]

The remainder of the proof of Theorem 2 follows that of Theorem 1 in a straightforward manner.

### 5 MB-WISH for computing permanent

Recall the permanent of a matrix as defined in Eq. 2: $\text{Perm}(A) \equiv \sum_{\sigma \in S_n} \prod_{i=1}^n A_{i, \sigma(i)}$. We will show that it is possible to approximate the permanent with a modification of the MB-WISH algorithm and our idea of using multiple bins for optimization in the calls to MAX-oracle. Also, recall from Section 3 that we set $\mathbb{F}_q \equiv \{a_0, a_1, \ldots, a_{q-1}\}$ where there exists a fixed ordering among the elements. We set $q \geq n$ and consider any $\sigma \in S_n$ as an $n$-length vector over $\mathbb{F}_q$ (that is by identifying $1, 2, \ldots, n$ as $a_0, a_1, \ldots, a_{n-1}$ respectively). Then we define a modified hash family $\mathcal{H}_{m,n} = \{h_{A,b} : A \in \mathbb{F}_q^{m \times n}, b \in \mathbb{F}_q^m\}$ with $h_{A,b} : S_n \rightarrow \mathbb{F}_q^m : \sigma \mapsto A\sigma + b$, the operations are over $\mathbb{F}_q$.

However, when calling the MAX-oracle, we need to make sure that we are getting a permutation as the output. Hence the modified MAX-oracle for computing permanent will be:

$$
\max_{\sigma \in \mathbb{F}_q^m} w(\sigma)
$$

s.t., $A\sigma + b < a_r \cdot 1; \sigma < a_{n-1} \cdot 1; \sigma(i) \neq \sigma(j) \forall i \neq j.$

(11)

These constraints, which are all linear, ensures that the MAX-oracle returns a permutation over $n$ elements. With this change we propose Algorithm 3 to compute permanent of a matrix and call it PERM-WISH. The full algorithm is provided as Algorithm 3.

**Algorithm 3 PERM-WISH for $\Omega = S_n$**

**Initialize:** $\ell \rightarrow \lceil \frac{1}{\ell} \ln \frac{2n}{\delta} \rceil$, $q > n$, $r, n' = \lceil n \log_q r \rceil$

$M_0 = \max_{\sigma \in S_n} w(\sigma)$

for $i \in \{1, 2, \ldots, n'\}$ do

for $k \in \{1, \ldots, \ell\}$ do

Sample hash functions $h_i \equiv h_{A^{(i)}, b^{(i)}}$ uniformly at random from $\mathcal{H}_{i,n}$ as defined in (7)

$w_i^{(k)} = \max_{\sigma \in \mathbb{F}_q^m} w(\sigma)$ such that $A^{(i)} \sigma + b^{(i)} < a_r \cdot 1; \sigma < a_{n-1} \cdot 1; \sigma(k) \neq \sigma(l) \forall k \neq l$.

end for

$M_i = \text{Median}(w_i^{(1)}, w_i^{(2)}, \ldots, w_i^{(\ell)})$

end for

Return $M_0 + (\frac{q}{r} - 1) \sum_{i=0}^{n'-1} M_{i+1} \left(\frac{q}{r}\right)^i$

The main result of this section is the following.

**Theorem 3.** Let $D$ be any $n \times n$ matrix. Let $q > n$ be a power of prime and $r = \lceil \frac{q-1}{2} \rceil$. For any $\delta > 0$ and a positive constant $\gamma = \frac{q}{3r} (\frac{1}{2} - \frac{\gamma}{2})^2$, Algorithm 3 makes $\Theta(n^2 \text{poly}(\log \frac{n}{\delta}))$ calls to the MAX-oracle and, with probability at least $1 - \delta$ outputs a $(\frac{q}{r})^2 = (4 + O(1/n))$-approximation of $\text{Perm}(D)$. 


The proof of Theorem 3 follows the same trajectory as in Theorem 1. The constraints in MAX-oracle ensures that a permutation is always returned. So in the proof of Theorem 1 the \( w_i^{(k)} \)'s can be though of as permutations instead in this setting. It should be noted that, we must take \( q > n \) for PERM-WISH to work. That is the reason we get a \( (4 + O(1/n)) \)-approximation for the permanent.

It also has to be noted that, since \( q \) is large, the straightforward extension of WISH algorithm would have provided only a \( q^2 = n^2 \)-approximation of the permanent. Therefore the idea of using optimizations with multiple bins are crucial here as it lead to a close to \( 4 \)-approximation.

**Remark 1 (Constraints).** It turns out that the constraints in the MAX-oracle in Algorithm 3 are linear/affine. Therefore they are still easy to implement in different CSP softwares.

### 6 Derandomization: structured hashes

In this section, we show that it is possible to construct pairwise independent hash family \( \{F_2^n \rightarrow F_2^m \} \) using only \( O(n) \) random bits such that any hash function from the family still has the structure \( h(x) = Ax + b \). While memory optimal pairwise independent hash functions are quite standard, we feel for completeness it would be good to show that they can be represented as the above matrix-vector product form. All of the statements of this section can be easily extended to \( q \)-ary alphabets.

**Construction 1:** Let \( f(x) \in F_2[x] \) be an irreducible polynomial of degree \( n \). We construct the finite field \( F_{2^n} \) with the \( \zeta \), root of \( f(x) \) as a generator of \( F_{2^n} \). Now, any \( x \in F_2^n \) can be written as a power of \( \zeta \) via a natural map \( \phi : F_2^n \rightarrow F_{2^n} \). Indeed, for any element \( \zeta^k \in F_{2^n} \) consider the polynomial \( \zeta^k \mod f(\zeta) \) of degree \( n - 1 \). The coefficients of this polynomial from an element of \( F_2^n \). \( \phi \) is just the inverse of this map. Also, assume that the all-zero vector is mapped to 0 under \( \phi \).

Let \( x \in F_2^n \) be the configuration to be hashed. Suppose the hash function is \( h_{\nu,b} \), indexed by \( \nu \in F_2^n \) and \( b \in F_2^m \). The hash function is defined as follows: Let \( \nu \in F_2^n \). Compute \( z = \phi^{-1}(\phi(x) \cdot \phi(\nu) \mod f(\zeta)) \in F_2^n \). Let \( y \in F_2^m \) be the first \( m \) bits of \( z \). Finally, output \( y + b \), where \( b \in F_2^m \).

**Proposition 1.** The hash function \( h_{\nu,b} \) can be written as an affine transform \( (x \mapsto Ax + b) \) over \( F_2^n \).

**Proof.** It is sufficient to show that \( z \) can be obtained as a linear transform of \( \nu \). Note that the product of \( \phi(x) \) and \( \phi(\nu) \) can be written as a convolution between \( x \) and \( \nu \equiv (v_1, v_2, \ldots, v_n) \) (as we can view this as product between two polynomials). Let \( \Gamma \) be the \((2n - 1) \times n\) matrix,

\[
\Gamma = \begin{bmatrix}
 v_1 & 0 & 0 & \ldots & 0 \\
 v_2 & v_1 & 0 & \ldots & 0 \\
 v_3 & v_2 & v_1 & \ldots & 0 \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 v_n & v_{n-1} & v_{n-2} & \ldots & v_1 \\
 0 & v_n & v_{n-1} & \ldots & v_2 \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 0 & 0 & 0 & \ldots & v_n
\end{bmatrix}.
\]

The reduction modulo \( f(\zeta) \) can also be written as a linear operation. Just consider the \( n \times (2n - 1) \) matrix \( P \) whose \( i \)th column contains the coefficients of the polynomial \( \zeta^{i-1} \mod f(\zeta) \), \( 1 \leq i \leq 2n - 1 \). Note that the first \( n \) columns of the matrix is simply the identity matrix. We can write, \( z = PTx \). \( \square \)

Note that, to chose a random and uniform hash function from \( \{h_{\nu,b} \in F_2^n, b \in F_2^m \} \), one needs \( m + n \) random bits. It follows that the hash family is pairwise independent.
Proposition 2. The hash family \( \{ h_{v,b} \in \mathbb{F}_2^n, b \in \mathbb{F}_2^m \} \) is uniform and pairwise independent.

Proof. Suppose \( v, b \) are randomly and uniformly chosen. For any \( x_1, x_2 \in \mathbb{F}_2^n \) and \( y_1, y_2 \in \mathbb{F}_2^m \), first of all

\[
\Pr(h_{v,b}(x_1) = y_1) = \frac{1}{2^m},
\]

since \( b \) is uniform. Now,

\[
\Pr(h_{v,b}(x_1) = y_1, h_{v,b}(x_2) = y_2)
\]

\[
= \frac{1}{2^m} \Pr(h_{v,b}(x_2) = y_2| h_{v,b}(x_1) = y_1)
\]

\[
= \frac{1}{2^m} \Pr(h_{v,b}(x_2) - h_{v,b}(x_1) = y_2 - y_1| h_{v,b}(x_1) = y_1)
\]

\[
= \frac{1}{2^m} \Pr(h_{v,b}(x_2) - h_{v,b}(x_1) = y_2 - y_1).
\]

Now, since \( \Pr((\phi(x_1) - \phi(x_2)) \cdot \phi(v) \mod f(ζ) = u) = \frac{1}{2^m} \) for any \( u \), we must have \( \Pr(h_{v,b}(x_2) - h_{v,b}(x_1) = y_2 - y_1) = \frac{1}{2^m} \). Therefore the claim is proved. \(\square\)

Moreover the randomness used to construct this hash function is also optimal. It can be shown that, the size of a pairwise independent hash family \( \{ h : \{0,1\}^n \rightarrow \{0,1\}^m \} \) is at least \( 2^{m+n} - 2^n + 1 \) (see, [19]). This implies that \( m + n \) random bits were essential for the construction.

Construction 2: Toeplitz matrix. In [8], a Toeplitz matrix was used as the hash function. In a Toeplitz matrix, each descending diagonal from left to right is fixed, i.e., if \( A_{i,j} \) is the \((i,j)\)th entry of a Toeplitz matrix, then \( A_{i,j} = A_{i-1,j-1} \). So to specify an \( m \times n \) Toeplitz matrix one needs to provide only \( m + n - 1 \) entries (entries of the first row and first column). Consider the random \( m \times n \) Toeplitz matrix \( A_T \) where each of the entries of the first row and first column are chosen with equal probability from \( \{0,1\} \), i.e., each entry in the first row and column is a Bernoulli(0.5) random variable. The hash function \( h_{A_T,b} : x \mapsto A_Tx + b \), is constructed by choosing a uniformly random \( b \in \mathbb{F}_2^m \).

Proposition 3. The hash family \( \{ h_{A_T,b} \} \) is uniform and pairwise independent [8].

Proof. First of all, the uniformity of the family is immediate since \( b \) is uniformly chosen. For any \( x_1, x_2 \in \mathbb{F}_2^n \) and \( y_1, y_2 \in \mathbb{F}_2^m \), \( \Pr(h_{A_T,b}(x_1) = y_1, h_{A_T,b}(x_2) = y_2) = \frac{1}{2^m} \Pr(h_{A_T,b}(x_2) = y_2| h_{A_T,b}(x_1) = y_1) = \frac{1}{2^m} \Pr(A_T(x_1 - x_2) = y_1 - y_2) \). It remains to prove that \( \Pr(A_Tx = y) = \frac{1}{2^m} \) for any fixed \( x, y \). Let the \( k \)th coordinate of \( x \) is the first to be in the support of \( x \). Now consider the inner product of the \( j \)th row of \( A_T \) with \( x \). This product will contain the entry \( A_T(j,k) \), the \((j,k)\)th entry of \( A_T \). Note that, this entry would not have appeared in any of the inner products of \( i \)th row of \( A_T \) and \( x \), for \( i < j \). Therefore the probability that this inner product is any fixed value is exactly \( \frac{1}{2} \) given inner product of all previous rows with \( x \). Therefore, \( \Pr(A_Tx = y) = \frac{1}{2^m} \). \(\square\)

Note that, the number of random bits required from this construction is \( 2m + n - 1 \). Toeplitz matrix allow for much faster computation of the hash function (matrix-vector multiplication with Toeplitz matrix takes only \( O(n \log n) \) time compared to \( \Omega(mn) \) for unstructured matrices).

We remark that sparse Toeplitz Matrices also can be used as our hash family, further reducing the randomness. In particular, we could construct a Toeplitz matrix with Bernoulli(p) entries for \( p < 0.5 \). While the pairwise independence of the hash family is lost, it is still possible to analyze the MB-WISH algorithm with this family of hashes since they form a strongly universal family [19]. The number of random bits used in this hash family is \( (m + n - 1)h(p) + m \). This construction allows us to have sparse rows in the matrix for small values of \( p \), which can lead to further speed-up.

Both the constructions of this section extend to \( q \)-ary alphabet straightforwardly.
7 Experimental results

All the experiments were performed in a shared parallel computing environment that is equipped with 50 compute nodes with 28 cores Xeon E5-2680 v4 2.40GHz processors with 128GB RAM.

**Experiments on simulated Potts model.** We implemented our algorithm to estimate the partition function of Potts Model. Recall that the partition function of the Potts model on a graph \( G = (V, E) \) is given in Eq. (3). For our simulation, we have randomly generated the graph \( G \) with number of nodes \( n \equiv |V| \) varying in \( 4, 5, 6, 7, 8, 9, 10, 11, 12 \) and corresponding regular degree \( d = 2, 4, 4, 4, 6, 6, 8 \) using a python library networkx. We took the number of states of the Potts model \( q = 5 \), the external force \( H \) and the spin-coupling \( J \) to be 0.1 and then varied the values of \( \zeta \). The partition functions for different cases are calculated using both brute force and our algorithm. We have used a python module constraint to handle the constrained optimization for MAX-oracle. The obtained approximation factors for different \( \zeta \) are listed in Table 2.

For \( n = 10, 11, d = 6 \) the approximation factor for MB-WISH is exactly 1 (up to the precision of the number system used). However the time taken by MB-WISH is much higher. For \( n = 12, d = 8 \), MB-WISH gives an approximation factor of 2.5 after running for eight hours in the above parallel computing environment.

| \( n \) | \( \zeta = 1 \) | \( \zeta = 2 \) | \( \zeta = 5 \) |
|---|---|---|---|
| 10 | 0.703 (0.685) | 0.537 (0.673) | 0.608 (1.0878) |
| 15 | 0.844 (0.715) | 0.894 (0.871) | 0.669 (1.182) |
| 20 | 1.012 (0.989) | 1.021 (1.279) | 0.819 (1.381) |
| 25 | 0.605 (0.517) | 0.968 (0.631) | 0.602 (1.253) |
| 30 | 0.726 (0.741) | 0.654 (0.687) | 1.126 (1.362) |
| 40 | 0.834 (0.869) | 0.696 (0.934) | 1.199 (1.538) |
| 50 | 0.761 (0.741) | 0.809 (0.878) | 2.191 (1.000) |

Table 1: The ratio of the partition function calculated by unconstrained MB-WISH and the approximate value calculated by belief propagation: \( \hat{\zeta} \). The values in the brackets are the corresponding ratios computed with the sparse fast unconstrained MB-WISH and belief propagation.

In Figure 1 we show how the number of bins (the variable \( r \) in MB-WISH) affects the approximation ratio for the partition function of the Potts model. For these figures, we have taken a random graph of degree 4 on \( n = 20 \) vertices, \( q = 11 \) and \( J = H = 0.5 \) with a time-out of fifteen minutes for each calls to MAX-oracle. The best approximation ratio is achieved with \( r = 3 \) for the both cases we plotted. Note that, the guarantee of Theorem 1 suggests to take \( r = 5 \) bins for these cases. In Figure 2 an example of the variation of approximation ratio with time-out for MAX-oracle is shown for Potts Model with \( n = 20, q = 5 \) and \( J = H = 0.2 \).

For graphs with larger number of vertices, it is difficult to compute the partition function of Potts Model by brute force. Therefore, we compare the partition function computed by MB-WISH \( \hat{Z} \) with the one \( Z \) computed by a belief propagation algorithm in the in the PGMPY library in python [1]. Again, for our simulation, we have randomly generated the graph \( G \) with number of nodes \( n \equiv |V| \) varying in \( 10, 15, 20, 25, 30, 40, 50 \), and with regular degree \( d = 4 \) using a python library networkx. We took the number of states of the Potts model \( q = 5 \), the external force \( H \) and the spin-coupling to be 0.1 and then varied the values of \( \zeta \). In our experiments each optimization instances are run with a timeout of 3, 5, 10, 15, 20, 20, 25 minutes for \( n = 10, 15, 20, 25, 30, 40, 50 \) respectively. The results are summarized in
Figure 1: Variation in the approximation factor with number of bins in a $n = 20$ vertex Potts model.

(a) $\xi = -1$

(b) $\xi = -2$

Figure 2: Approximation factor with time allocated per calls to MAX-oracle ($n = 20$ vertex Potts Model).
\[ n = 4, d = 2 \] 
\[ n = 5, d = 2 \] 
\[ n = 6, d = 4 \] 
\[ n = 7, d = 4 \] 
\[ n = 8, d = 4 \] 
\[ n = 9, d = 4 \] 
\begin{array}{cccccc}
\hline
\zeta & n = 4, d = 2 & n = 5, d = 2 & n = 6, d = 4 & n = 7, d = 4 & n = 8, d = 4 & n = 9, d = 4 \\
\hline
0 & 0.976 & 1.220 & 0.610 & 1.907 & 0.953 & 1.192 \\
5 & 0.580 & 0.708 & 1.639 & 0.755 & 0.630 & 0.599 \\
10 & 0.7470 & 1.191 & 3.271 & 0.989 & 1.875 & 1.25 \\
15 & 1.430 & 1.036 & 1.013 & 1.224 & 1.399 & 1.692 \\
20 & 1.032 & 1.590 & 1.141 & 1.173 & 1.365 & 1.491 \\
25 & 0.839 & 1.118 & 1.339 & 1.035 & 1.429 & 1.326 \\
30 & 0.510 & 4.0562 & 2.226 & 1.060 & 0.690 & 2.122 \\
35 & 1.073 & 5.442 & 0.489 & 2.871 & 1.639 & 1.263 \\
40 & 1.210 & 2.434 & 0.980 & 0.582 & 0.666 & 0.969 \\
45 & 1.127 & 4.640 & 2.348 & 1.336 & 0.3673 & 1.341 \\
50 & 1.152 & 1.025 & 2.511 & 3.4307 & 1.1522 & 2.636 \\
\hline
\end{array}

Table 2: The ratio of the partition function calculated by MB-WISH and the actual value calculated by brute force: \( \frac{\hat{Z}}{Z} \).

Table 1. The same experiment is repeated with a sparse random matrix for unconstrained MB-WISH, where each entry is zero with probability 0.8 and any other value of \( \mathbb{F}_5 \) with probability 0.05. For each optimization instance we give a timeout of only 1, 1.5, 10, 10, 10 minutes for \( n = 10, 15, 20, 25, 30, 40, 50 \) respectively. The results are summarized in values in the brackets in Table 1 and are comparable to the non-sparse counterparts.

**Real-world constraint satisfaction problem (CSPs).** Many instances of real-world graphical models are available in [http://www.cs.huji.ac.il/project/PASCAL/showExample.php](http://www.cs.huji.ac.il/project/PASCAL/showExample.php). Notably, some of them (e.g., image alignment, protein folding) are defined on non-Boolean domains, which justify the use of MB-WISH. We have computed the partition functions for several of them.

The dataset Network.uai is a Markov network with 120 nodes each having a binary value. A configuration here is a binary sequence of length 120. To calculate the partition function, we need to find the sum of weights for \( 2^{120} \) different configurations. In order to use Unconstrained MB-WISH, we view each configuration as a 16-ary string of length 30. Our results for the log-partition came out to be 156.00 with one hour time out for each call to the MAX-oracle. The benchmark for the log-partition function is provided to be 163.204.

\[
\begin{array}{cccc}
\hline
n & \zeta = 1 & \zeta = 2 & \zeta = 5 \\
\hline
10 & 0.054273 & 0.054390 & 0.054318 \\
15 & 0.063036 & 0.0631594 & 0.0633923 \\
20 & 0.09653491 & 0.096632 & 0.09662014 \\
25 & 0.115449 & 0.1159425 & 0.116080 \\
30 & 0.1285637 & 0.12862 & 0.128368 \\
40 & 0.09931 & 0.0995325 & 0.099551 \\
50 & 0.0998276 & 0.099575 & 0.09992 \\
\hline
\end{array}
\]

Table 3: The ratio of partition function computed with MCMC to that computed with belief propagation.

The Object detection dataset comprised of 60 nodes each having a 11-ary value and by Unconstrained MB-WISH we found the log-partition function to be \(-38.9334\). The CSP dataset is a
Markov network with 30 node having a ternary value: we found the log partition function to be \(-39.9933\). For these datasets there were no baselines.

**Permanent.** We use the PERM-WISH algorithm to find the permanent of randomly generated matrices of size \(n \times n, n = 5, 6, 7, 8, 9, 10\) and compute the ratio of the value achieved by our method (\(\hat{Z}\)) and actual permanent (\(Z\)). For the purpose of constrained optimization, we use the python modules described above. For the experiment we take \(q = 11\) and \(r = 5\). We find \(\hat{Z}/Z = 2.137, 1.103, 1.245, 2.407, 0.730, 1.527\) for \(n = 5, 6, 7, 8, 9, 10\) respectively.

**Comparison with Markov Chain Monte Carlo.** Markov Chain Monte Carlo or MCMC is a standard method for approximating a high-dimensional integration \([12]\). We employ the popular Metropolis-Hastings (MH) algorithm \([15]\) to sample random points from \(\Omega\), where we evaluate the function \(w : \Omega \to \mathbb{R}\) and take a scaled-sum to estimate the discrete integration problem. We test this on the same simulated dataset of Potts model as in Table 1 and report the result in Table 3. We have calculated the average of the partition function over 10 different sample paths of the MH algorithm, and each instance has the same time-out as we had in MB-WISH in computing the values of Table 1. It can be observed that the partition functions computed with MCMC deviate significantly from that computed with belief propagation, whereas MB-WISH gives values closer to the belief propagation results.

We compare MB-WISH with MCMC method for the nonbinary knapsack counting problem as well. In this problem, for \(a \in \mathbb{R}^n, b \in \mathbb{R}\), we are interested in estimating the size of the set \(S_{a,b} = \{x \in \{0,1,\ldots,q-1\}^n : a^T x \leq b\}\). For \(q = 5, n = 12\), we compute by the MCMC methods (average over 10 different sample paths with timeout of 3 minutes each) \(|S_{a,b}|\) for six different values of \((a, b)\)-tuples. We compare this with \(|S_{a,b}|\) computed by brute-force and by our unconstrained MB-WISH algorithm with 3 minute timeout for MAX-oracle. The approximation factors for the six trials are reported in Table 4.

| MCMC | MB-WISH | MCMC | MB-WISH |
|------|---------|------|---------|
| 0.3952 | 1.15 | 3.03718e+26 | 1.2195e+26 |
| 20.41 | 0.663 | 2.92370e+26 | 7.523e+23 |
| 3.8809 | 2.6250 | 2.92946e+25 | 7.7037e+21 |
| 314.9 | 0.008 | 2.68252e+25 | 4.7331e+19 |
| 0.6600 | 0.723 | 4.07255e+25 | 1.7800e+20 |
| 25.175 | 0.246 | 1.34819e+25 | 4.7132e+19 |

Table 4: Left: Approximate ratio of counting in the knapsack problem \((n = 12, q = 5)\) for six trials. Right: Absolute count for four trials \((n = 40, q = 5)\).

We test MCMC and MB-WISH on the knapsack counting problem for \(n = 40, q = 5\) where brute-force computation is not possible because of larger value of \(n\). For unconstrained MB-WISH, each call to MAX-oracle was given a 20 minutes timeout, and for MCMC the same amount of time was used. The counts for four trials are reported in Table 4. All these results indicate that MB-WISH is a viable alternative to MCMC for high dimensional integration/counting problems.

**Experimental results on computing Total Variation distance.** We use Unconstrained MB-WISH to compute total variation distances between two high dimensional (up to dimension 100) probability distributions, generated via an iid model and two different Markov chains (domain size up to \(5^{100}\)). There is no baseline to compare with for the Markov chain case, but for the product distributions the method shows good accuracy. The detailed results are provided below.
The total variation (TV) distance between any two discrete distributions $P$ and $Q$ with common sample space $\mathcal{P}$ is defined to be

$$\|P - Q\|_{TV} = \sup_{A \in \mathcal{P}} |P(A) - Q(A)| = \frac{1}{2} \sum_{\sigma \in \mathcal{P}} |P(\sigma) - Q(\sigma)|.$$ 

It is difficult to estimate the TV distance between two distribution over product spaces. Even if the random variables are independent, there is no easy way to analytically compute the total variation distance. Simply consider finding TV distance between joint distributions of $n$ random variables that can take value in $\{0, 1, \ldots, q - 1\}$. In that case, we seek to find,

$$\frac{1}{2} \sum_{\sigma \in \{0, 1, \ldots, q-1\}^n} |P^n(\sigma) - Q^n(\sigma)|,$$

which is in the exact form of Eq. (1). Therefore we can use MB-WISH algorithm to estimate the total variation distance. To see how good the performance is, we compare the computed value with the known upper and lower bound on TV distance based on Hellinger distance: $h(P, Q)^2 \equiv \sum_{\sigma \in \mathcal{P}} (\sqrt{P(\sigma)} - \sqrt{Q(\sigma)})^2$. It is known that\(^3\)

$$\frac{1}{2} h(P, Q)^2 \leq \|P - Q\|_{TV} \leq h(P, Q)\sqrt{1 - h(P, Q)^2}/4.$$

For the experiments, we choose two distribution over 5 points ($q = 5$): $P = [0.2, 0.2, 0.2, 0.2, 0.2]$ and $Q = [0.2, 0.2 + \epsilon, 0.2 - \epsilon, 0.2 + \epsilon, 0.2 - \epsilon]$, where $\epsilon = 10^{-2}$. The distributions are chosen very close to each other. Here the distribution $P^n$ and $Q^n$ are supported on $\{0, 1, 2, 3, 4\}^n$ where $n$ can be any natural number. It is known that,

$$h(P^n, Q^n)^2 = 2 - 2 \prod_{i=1}^{n} (1 - \frac{1}{2} h(P_i, Q_i)^2).$$

To compare our method with the upper and lower bound with Hellinger distance we choose the random variables to be independent, although that our method is capable of approximation irrespective of any such conditions. We do our experiments in a time constrained manner (10 minute for each calls to MAX-oracle). The results are summarized in Table 5 and shown in Figure 3.

| $n$ | Lower Bound | MB-WISH | Upper Bound |
|-----|-------------|---------|-------------|
| $n = 4$ | 0.001 | 0.023 | 0.0316 |
| $n = 6$ | 0.0015 | 0.025 | 0.0387 |
| $n = 8$ | 0.002 | 0.0255 | 0.0447 |
| $n = 10$ | 0.0025 | 0.045 | 0.05 |
| $n = 12$ | 0.003 | 0.0186 | 0.0547 |
| $n = 30$ | 0.007492 | 0.1097 | 0.086557 |
| $n = 40$ | 0.00998 | 0.1147 | 0.099917 |
| $n = 50$ | 0.012471 | 0.07265 | 0.1116 |
| $n = 100$ | 0.02486 | 0.1767 | 0.15768 |

Table 5: Computation of TV distance of product distribution by MB-WISH compared with upper bound (UB) and lower bound (LB) based on Hellinger distance. Here $\epsilon = 10^{-2}$.

\(^3\)See [https://stanford.edu/class/stats311/Lectures/full_notes.pdf](https://stanford.edu/class/stats311/Lectures/full_notes.pdf)
Figure 3: Computation of TV distance of two product distributions via Unconstrained MB-WISH

Table 6: Computation of TV distance for Markov case by Unconstrained MB-WISH. Each call to MAX-oracle is time limited to 40 minutes.

We also ran the experiment when the joint distributions are not of independent random variables and therefore no standard upper or lower bounds are available. We assume the random variables $X_1, X_2, \ldots, X_n$ form a Markov chain over 5 states. We consider two different first order Markov chains with initial probability distributions $P = [0.2, 0.2, 0.2, 0.2, 0.2]$ and $Q = [0.2, 0.21, 0.19, 0.19, 0.21]$ respectively and the state-transition matrices given by:

$$T = \begin{bmatrix}
0.2204 & 0.2813 & 0.2285 & 0.02819 & 0.24155 \\
0.11137 & 0.1277 & 0.04995 & 0.3949 & 0.3159 \\
0.01068 & 0.3220 & 0.2.387 & 0.11459 & 0.3139 \\
0.3714 & 0.3397 & 0.1599 & 0.02134 & 0.1074 \\
0.02691 & 0.38807 & 0.2.869 & 0.05981 & 0.2382
\end{bmatrix}$$

and $T + D$ where every row of $D$ is given by the vector $[0, 10^{-4}, -10^{-4}, -10^{-4}, 10^{-4}]$. We estimate the total variation distance between $P(X_1, X_2, \ldots, X_n)$ and $Q(X_1, X_2, \ldots, X_n)$ in Table 6 below.
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