Kolmogorov Approximation

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1 Introduction

Many different approaches to approximation of probability distributions are studied in the literature [4, 6, 7]. The papers vary in the types random variables involved, how they are represented, and in the criteria used for evaluation of the quality of the approximations. This paper is on approximating discrete distributions represented as explicit probability mass functions with ones that are simpler to store and to manipulate. This is needed, for example, when a discrete distribution is given as a large data-set, obtained, e.g., by sampling, and we want to represent it approximately with a small table.

The main contribution of this paper is an efficient algorithm for computing the best possible approximation of a given random variable with a random variable whose complexity is not above a prescribed threshold, where the measures of the quality of the approximation and the complexity of the random variable are as specified in the following two paragraphs.

We measure the quality of an approximation by the distance between the original variable and the approximate one. Specifically, we use the Kolmogorov distance which is one of the most used in statistical practice and literature. Given two random variables X and X' whose cumulative distribution functions (cdfs) are F_X and $F_{X'}$, respectively, the Kolmogorov distance between X and X' is $d_K(X, X') = \sup_t |F_X(t) - F_{X'}(t)|$ (see, e.g., [3]). We say taht X' is a good approximation of X if $d_K(X, X')$ is small.

The complexity of a random variable is measured by the size of its support, the number of values that it can take, $|\operatorname{support}(X)| = |\{x\colon Pr(X = x) \neq 0\}|$. When distributions are maintained as explicit tables, as done in many implementations of statistical software, the size of the support of a variable is proportional to the amount of memory needed to store it and to the complexity of the computations around it.

In summary, the exact notion of optimality of the approximation targeted in this paper is:

Definition 1. *A random variable X' is an optimal m-approximation of a random variable X if $|\operatorname{support}(X')| \leq m$ and there is no random variable X'' such that $|\operatorname{support}(X'')| \leq m$ and $d_k(X, X'') < d_k(X, X')$.*

The main contribution of the paper is a constructive proof of:

Theorem 2. *Given a random variable X and a number m, there is an algorithm with memory and time complexity $O(|\operatorname{support}(X)|^2 \cdot m)$ that computes an optimal m-approximation of X.*

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The rest of the paper is organized as follows. In Section 2 we describe how our work relates to other algorithms and problems studied in the literature. In Section **??** we detail the proposed algorithm, analyze its properties, and prove Theorem **??**. In Section **??** we demonstrate how the proposed approach performs on the problem of estimating the probability of hitting deadlines is plans and compare it to alternatives approximation approaches from the literature. We also demonstrate the performance of our approximation algorithm on some randomly generated random variables. The paper is concluded with a discussion in Section **??**.

2 Related Work

The problem studied in this paper is related to the theory of Sparse Approximation (aka Sparse Representation) that deals with sparse solutions for systems of linear equations, as follows.

Given a matrix $D \in \mathbb{R}^{n \times p}$ and a vector $x \in \mathbb{R}^n$, the most studied sparse representation problem is finding the sparsest possible representation $\alpha \in \mathbb{R}^p$ satisfying $x = D\alpha$:

$$\min_{\alpha \in \mathbb{R}^p} \|\alpha\|_0 \text{ subject to } x = D\alpha.$$

where $\|\alpha\|_0 = |\{i : \alpha_i \neq 0,\ i = 1, \ldots, p\}|$ is the ℓ_0 pseudo-norm, counting the number of non-zero coordinates of α. This problem is known to be NP-Hard with a reduction to NP-complete subset selection problems.

In these terms, using also the ℓ_∞ norm that represents the maximal coordinate and the ℓ_1 norm that represents the sum of the coordinates, our problem can be phrased as:

$$\min_{\alpha \in [0,\infty)^p} \|x - D\alpha\|_\infty \text{ subject to } \|\alpha\|_0 = m \text{ and } \|\alpha\|_1 = 1.$$

where D is the all-ones triangular matrix (the entry at row i and column j is one if $i \leq j$ and zero otherwise), x is related to X such that the ith coordinate of x is $F_X(x_i)$ where $\text{support}(X) = \{x_1 < x_2 < \cdots < x_n\}$ and α is related to X' such that the ith coordinate of α is $f_{X'}(x_i)$. The functions F_X and $f_{X'}$ represent, respectively, the cumulative distribution function of X and the mass distribution function of X'. This, of course, means that the coordinates of x are assumed to be positive and monotonically increasing and that the last coordinate of x must be one. We demonstrate an application for this specific sparse representation problem and show that it can be solve in $O(n^2 m)$ time and memory.

3 An Algorithm for Optimal Approximation

[[DF: move somewhere to intro: Obviously every random variable with support of size of at most m serves as some approximation, the challenge is how to find an m-*optimal* approximation for X.]] [[DF: move to intro: we call the distance between X and the m-optimal-approximation random variable of X, the *m-optimal distance* from X.]]

We next describe in details the proof of theorem **??**.

In the following we set X as a random variable with a finite support of size n, and we set $0 < m \leq n$. We need to find an m-optimal approximation random variable X'.

Our first step is to show that it is enough to limit our search to X's such that $\text{support}(X') \subseteq \text{support}(X)$.

Lemma 3. *There is an m-optimal-approximation X' of X such that* $\text{support}(X') \subseteq \text{support}(X)$.

[DF: This proof is unclear to me, please clean.] Assume for contradiction is a random variable X'' with support size m such that $d_K(X, X'')$ is minimal but $\text{support}(X'') \not\subseteq \text{support}(X)$. We will show how to transform X'' support such that it will be contained in $\text{support}(X)$. Let v' be the first $v' \in \text{support}(X'')$ and $v' \notin \text{support}(X)$. Let $v = \max\{i : i < v' \wedge i \in \text{support}(X)\}$. Every v' we will replace with v and name the new random variable X', we will show that $d_K(X, X'') = d_K(X, X')$. First, note that: $F_{X''}(v') = F_{X'}(v)$, $F_X(v') = F_X(v)$. Second, $F_{X'}(v') - F_X(v') = F_{X'}(v) - F_X(v)$. Therefore, $d_K(X, X'') = d_K(X, X')$ and X' is also an optimal approximation of X. □

Next, note that every random variable X'' with support of size at most m that is contained in $\text{support}(X)$ be described by first setting the (at most m) elements of the support of X''; then for every such option, determine X'' by setting probability values for the elements in the chosen support of X', and setting 0 for rest of the elements.

Since from Lemma 3 we can assume wlog that if X' is an m-optimal approximation variable for X then $\text{support}(X') \subseteq \text{support}(X)$, our search to find such X' takes two steps. Denote the set of random variables with support S by $\mathbb{X}_S$. In step 1, we find the m-optimal approximation random variable among all random variables in $\mathbb{X}_S$, and denote the m-optimal distance for $\mathbb{X}_S$ by $\varepsilon(X, S)$. Next, in Step 2, among all the possible supports we find the support setting S of size $\leq m$ for which $\varepsilon(X, S)$ is minimal: We describe an efficient way to do so.

3.1 Step 1

We first fix a set $S \subseteq \text{support}(X)$ of size at most m, and among all the random variables in $\mathbb{X}_S$ find one with a minimal distance from X. To that, set $S = \{x_1 < \cdots < x_m\} \subseteq \text{support}(X)$. To simplify the proofs set $x_0 = -\infty$, and $x_{m+1} = \infty$. Then $x_0 < x_1$ and $x_m < x_{m+1}$. In addition recall that for every random variable X'' $F_{X''}(-\infty) = 0$ and $F_{X''}(\infty) = 1$. For the rest of this section we assume S is fixed and therefore is not necessarily included in the notation.

Next, as the elements of S are also elements of $\text{support}(X)$, we can define the following weight function that we use to find the m-optimal distance $\varepsilon(X, S)$.

Definition 4. *For* $0 \leq i < m$ *let*

$$w(x_i, x_{i+1}) = \begin{cases} P(x_i < X < x_{i+1}) & \text{if } i = 0 \text{ or } i = m; \\ P(x_i < X < x_{i+1})/2 & \text{otherwise.} \end{cases}$$

Note that when $i = 0$ (resp. $i = m + 1$) then $x_i = -\infty$ (resp. $x_i = \infty$).

Finally define:

$$\varepsilon(X, S) = \max_{i=0,\ldots,m} w(x_i, x_{i+1}) \tag{1}$$

We first show that $\varepsilon(X, S)$ is a lower bound. That is, every random variable in $\mathbb{X}_S$ has a distance at least $\varepsilon(X, S)$. Then, we present a random variable $X' \in \mathbb{X}_S$ with distance $\varepsilon(X, S)$. It then follows that such X' is an m-optimal approximation random variable among all random variables in $\mathbb{X}_S$.

The intuition behind choosing these specific weights and $\varepsilon(X, S)$ being a lower bound is as follows. For every $1 \leq i \leq m$ let $\hat{x}_i$ be the maximal element of $\text{support}(X)$ that is smaller than x_i. Then since for every $X' \in \mathbb{X}_S$ the probability values of X' for the elements not in S are set to 0, we

have that $F_{X'}(\hat{x}_{i+1}) = F_{X'}(x_i)$. Therefore the distance between X' and X at points x_i and $\hat{x}_{i+1}$ is increased by $F_X(\hat{x}_{i+1}) - F_X(x_i) = P(x_i < X < x_{i+1})$.

Formally we have the following.

Proposition 5. *For every random variable X' with* $\text{support}(X') = S$ *we have* $d_k(X, X') \geq \varepsilon(X, S)$.

Proof. Let X' be a random variable with support S. Then by definition, for every $0 \leq i \leq m$, $d_k(X, X') \geq \max\{|F_X(x_i) - F_{X'}(x_i)|, |F_X(\hat{x}_{i+1}) - F_{X'}(\hat{x}_{i+1})|\}$. Note that $F_{X'}(x_i) = F_{X'}(\hat{x}_{i+1})$ since the probability value for all the elements not in S is set to 0.

If $i = 0$, that is $x_i = -\infty$, we have that $F_X(x_i) = F_{X'}(x_i) = F_{X'}(\hat{x}_{i+1}) = 0$ and therefore $d_k(X, X') \geq ||F_X(\hat{x}_{i+1}| = |F_X(\hat{x}_{i+1}) - F_X(x_i)| = P(x_i < X < x_{i+1}) == w(x_i, x_{i+1})$.

If $i = m$, that is $x_{i+1} = \infty$, note that $F_X(\hat{x}_{i+1}) = F_{X'}(\hat{x}_{i+1}) = 1$. Therefore $F_{X'}(x_i) = 1$ as well. Therefore $d_k(X, X') \geq ||F_X(\hat{x}_i| = |F_X(\hat{x}_{i+1}) - F_X(x_i)| = P(x_i < X < x_{i+1}) = w(x_i, x_{i+1})$. [[DF: fix]]

Otherwise for every $1 \leq i < m$, we use the fact that $max\{|a|, |b|\} \geq |a - b|/2$ for every $a, b \in \Re$, to have $d_k(X, X') \geq \max\{|F_X(x_i) - F_{X'}(x_i)|, |F_X(\hat{x}_{i+1}) - F_{X'}(\hat{x}_{i+1})|\}$, and therefore $d_k(X, X') \geq 1/2|F_X(x_i) - F_X(\hat{x}_{i+1}) + F_{X'}(\hat{x}_{i+1}) - F_{X'}(x_i)|$. Since it is given that $F_{X'}(\hat{x}_{i+1}) - F_{X'}(x_i) = P(x_i < X' < x_{i+1}) = 0$, we have that $d_k(X, X') \geq 1/2|F_X(x_i) - F_X(\hat{x}_{i+1})| = P(x_1 < X < x_2)/2 == w(x_i, x_{i+1})$.

We saw that $d_k(X, X') \geq w(x_i, x_{i+1})$ for every $0 \leq i \leq m$. Therefore by definition of $\varepsilon(X, S)$, proof follows. □

[[DF: here I stopped]]

Definition 6. *Let X' to by $f_{X'}(x_i) = w(x_{i-1}, x_i) + w(x_i, x_{i+1}) + f_X(x_i)$ for $i = 1, \ldots, m$ and $f_{X'}(x) = 0$ for $x \notin S$.*

Lemma 7. *For $i > 1$, if $F_{X'}(x_i) - F_X(x_i) = w(x_i, x_{i+1})$ then $F_{X'}(x_{i+1}) - F_X(x_{i+1}) = w(x_{i+1}, x_{i+2})$.*

Proof.

$$
\begin{aligned}
&F_{X'}(x_{i+1}) - F_X(x_{i+1}) = && (2)\\
&= f_{X'}(x_{i+1}) - f_X(x_{i+1}) - P(X < x_{i+1}) + P(X' < x_{i+1})\\
&= f_{X'}(x_{i+1}) - f_X(x_{i+1}) - F_X(x_i) - P(x_i < X < x_{i+1}) + F_{X'}(x_i)\\
&= f_{X'}(x_{i+1}) - f_X(x_{i+1}) - F_X(x_i) - 2w(x_i, x_{i+1}) + F_{X'}(x_i) && (3)\\
&= f_{X'}(x_{i+1}) - f_X(x_{i+1}) - 2w(x_i, x_{i+1}) + w(x_i, x_{i+1}) && (4)\\
&= w(x_i, x_{i+1}) + w(x_{i+1}, x_{i+2}) - 2w(x_i, x_{i+1}) + w(x_i, x_{i+1}) && (5)\\
&= w(x_{i+1}, x_{i+2})
\end{aligned}
$$

By Definition 4 the probability $P(x_{i-1} < X < x_i) = 2w(x_{i-1}, x_i)$ as in Equation (3). Equation (4) is deduced by the induction hypothesis and Equation (5) where $f_{X'}(x_i) - f_X(x_i) = w(x_{i-1}, x_i) + w(x_i, x_{i+1})$ is true by construction, see Definition6. □

Lemma 8. *Base case: $i = 1, F_{X'}(x_1) - F_X(x_1) = w(x_1, x_2)$.*

Proof.

$$\begin{aligned} F_{X'}(x_1) - F_X(x_1) = & \\ &= f_{X'}(x_1) - f_X(x_1) - w(x_0, x_1) \\ &= w(x_0, x_1) + w(x_1, x_2) - w(x_0, x_1) \\ &= w(x_1, x_2) \end{aligned}$$

□

Proposition 9. *There exists X' such that* $\mathrm{support}(X') = S$ *and* $d_k(X, X') = \varepsilon(X, S)$.

Chakravarty, Orlin, and Rothblum [1] proposed a polynomial-time method that, given certain objective functions (additive), finds an optimal consecutive partition. Their method involves the construction of a graph such that the (consecutive) set partitioning problem is reduced to the problem of finding the shortest path in that graph.

The $\mathrm{KolmogorovApprox}$ algorithm (Algorithm 1) starts by constructing a directed weighted graph G similar to the method of Chakravarty, Orlin, and Rothblum [1]. The nodes V consist of the support of X together with an extra two nodes, $-\infty$ and ∞ for technical reasons, whereas the edges E connect every pair of nodes in one direction (lines 1-2). The weight w of each edge $e = (i, j) \in E$ is determined by one of two cases as in Definition 4. The first is where i or j are the source or target nodes respectively. In this case the weight is the probability of X to get a value between i and j, non inclusive, i.e., $w(e) = Pr(i < X < j)$ (lines 4-5). The second case is where i or j are not a source or target nodes, here the weight is the probability of X to get a value between i and j, non inclusive, divided by two i.e., $w(e) = Pr(i < X < j)/2$ (lines 6-7). The values taken are non inclusive, since we are interested only in the error value. The source node of the shortest path problem at hand corresponds to the $-\infty$ node added to G in the construction phase, and the target node is the extra node ∞. The set of all solution paths in G, i.e., those starting at $-\infty$ and ending in ∞ with at most m edges, is called $paths(G, -\infty, \infty)$. The goal is to find the path l in $paths(G, -\infty, \infty)$ with the lightest bottleneck (lines 8-9). This can be achieved by using the $Bellman - Ford$ algorithm with two tweaks. The first is to iterate the graph G in order to find only paths with length of at most m edges. The second is to find the lightest bottleneck as opposed to the traditional objective of finding the shortest path. This is performed by modifying the manner of "relaxation" to $bottleneck(x) = min[max(bottleneck(v), w(e))]$, done also in [8]. Consequently, we find the lightest maximal edge in a path of length $\leq m$, which represents the minimal error, $\varepsilon(X, S)$, defined in Definition **??** where the nodes in path l represent the elements in set S. The approximated random variable X' is then derived from the resulting path l (lines 10-17). Every node $n \in l$ represent a value in the new calculated random variable X', we than iterate the path l to fine the probability of the event $f_{X'}(n)$ as described in Definition 6. For every edge $(i, j) \in l$ we determine: if (i, j) is the first edge in the path l (i.e. $i = -\infty$), then node j gets the full weight $w(i, j)$ and it's own weight in X such that $f_{X'}(j) = f_X(j) + w(i, j)$ (lines 11-12). If (i, j) in not the first nor the last edge in path l then we divide it's weight between nodes i and j in addition to their own original weight in X and the probability that already accumulated (lines 16-17). If (i, j) is the last edge in the path l (i.e. $i == \infty$) then node i gets the full weight $w(i, j)$ in addition to what was already accumulated such that $f_{X'}(j) = f_{X'}(j) + w(i, j)$ (lines 13-14).

Theorem 10. $\mathrm{KolmogorovApprox}(X, m) = X'$ *where X' is an m-optimal-approximation.*

Theorem 11. *The* $\mathrm{KolmogorovApprox}(X, m)$ *algorithm runs in time $O(mn^2)$, using $O(n^2)$ memory where* $n = |\mathrm{support}(X)|$.

Algorithm 1: $\mathrm{KolmogorovApprox}(X, m)$

$S = \mathrm{support}(X) \cup \{\infty, -\infty\}$
$G = (V, E) = (S, \{(x, y) \colon x < y\})$
$(x_0, \ldots, x_{m+1}) = l = \mathrm{argmin}_{l \in paths(G, -\infty, \infty), |l| \leq m} \max\{w(e) \colon e \in l\}$
for $0 < i < m + 1$ **do**
  $f_{X'}(x_i) = w(x_{i-1}, x_i) + w(x_i, x_{i+1}) + f_X(x_i)$
return X'

Proof. Constructing the graph G takes $O(n^2)$. The number of edges is $O(E) \approx O(n^2)$ and for every edge the weight is at most the sum of all probabilities between the source node $-\infty$ and the target node ∞, which can be done efficiently by aggregating the weights of already calculated edges. The construction is also the only stage that requires memory allocation, specifically $O(E + V) = O(n^2)$. Finding the shortest path takes $O(m(E + V)) \approx O(mn^2)$. Since G is DAG (directed acyclic graph) finding shortest path takes $O(E + V)$. We only need to find paths of length $\leq m$, which takes $O(m(E + V))$. Deriving the new random variable X' from the computed path l takes $O(mn)$. For every node in l (at most m nodes), calculating the probability $P(s < X < \infty)$ takes at most n. To conclude, the worst case run-time complexity is $O(n^2 + mn^2 + mn) = O(mn^2)$ and memory complexity is $O(E + V) = O(n^2)$. □

4 A case study and experimental results

In the first experiment we focus on the problem of task trees with deadlines, and consider three types of task trees. The first type includes logistic problems of transporting packages by trucks and airplanes (from IPC2 http://ipc.icaps-conference.org/). Hierarchical plans of those logistic problems were generated by the JSHOP2 planner [5] (see example problem, Figure 1). The second type consists of task trees used as execution plans for the ROBIL team entry in the DARPA robotics challenge (DRC simulation phase), and the third type is of linear plans (sequential task trees). The primitive tasks in all the trees are modeled as discrete random variables with support of size M obtained by discretization of uniform distributions over various intervals. The number of tasks in a tree is denoted by N.

We implemented the approximation algorithm for solving the deadline problem with four different methods of approximation. The first two are for achieving a one-sided Kolmogorov approximation – the $\mathrm{OptTrim}$ [**?**] and the Trim [2] operators, and the third is a simple sampling scheme. We used those methods as a comparison to the Kolmogorov approximation with the suggested $\mathrm{KolmogorovApprox}$ algorithm. The parameter m of $\mathrm{OptTrim}$ and $\mathrm{KolmogorovApprox}$ corresponds to the inverse of ε given to the Trim operator. Note that in order to obtain some error ε, one must take into consideration the size of the task tree N, therefore, $m/N = 1/(\varepsilon \cdot N)$. We ran also an exact computation as a reference to the approximated one in order to calculate the error. The experiments conducted with the following operators and their parameters: $\mathrm{KolmogorovApprox}$ operator with $m = 10 \cdot N$, the $\mathrm{OptTrim}$ operator with $m = 10 \cdot N$, the Trim as operator with $\varepsilon = 0.1/N$, and two simple simulations, with a different samples number $s = 10^4$ and $s = 10^6$.

Table 1 shows the results of the main experiment. The quality of the solutions provided by using the $\mathrm{OptTrim}$ operator are better (lower errors) than those provided by the Trim operator, following the optimality guarantees, but is interesting to see that the quality gaps happen in practice in each of the examined task trees. However, in some of the task trees the sampling method produced better results than the approximation algorithm with $\mathrm{OptTrim}$. Nevertheless, the approximation algorithm comes

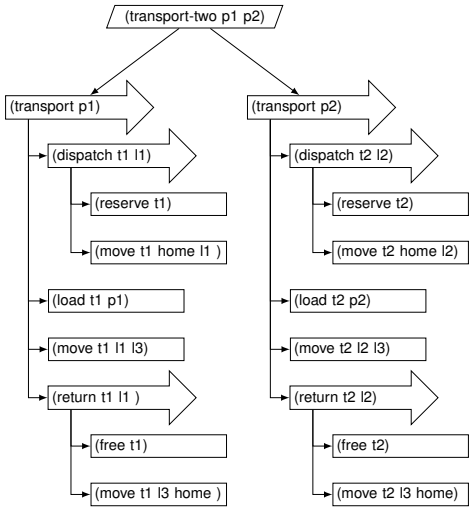

Figure 1: A plan generated by the JSHOP2 algorithm. Arrow shapes represent sequence nodes, parallelograms represent parallel nodes, and rectangles represent primitive nodes.

Task Tree	M	$\mathrm{KolmogorovApprox}$	$\mathrm{OptTrim}$	Trim	Sampling	
		$m/N{=}10$	$m/N{=}10$	$\varepsilon \cdot N{=}0.1$	$s{=}10^4$	$s{=}10^6$
Logistics ($N = 34$)	2	0	0	0.0019	0.007	0.0009
	4	0	0.0046	0.0068	0.0057	0.0005
Logistics ($N{=}45$)	2	0.0002	0.0005	0.002	0.015	0.001
	4	0	0.003	0.004	0.008	0.0006
DRC-Drive ($N{=}47$)	2	0	0.004	0.009	0.0072	0.0009
	4	0	0.008	0.019	0.0075	0.0011
Sequential ($N{=}10$)	2	0.009	0.015	0.024	0	0
	4	0.001	0.024	0.04	0.008	0.0016
	10	0	0.028	0.06	0.0117	0.001

Table 1: Comparison of estimated errors with respect to the reference exact computation on various task trees.

with an inherent advantage of providing an exact quality guarantees, as opposed to the probabilistic guarantees provided by sampling.

In order to better understand the quality gaps in practice between $\mathrm{KolmogorovApprox}$, $\mathrm{OptTrim}$, and Trim, we investigate their relative errors when applied on single random variables with support size $n = 100$, and different support sizes of the resulting random variable approximation (m). In each instance of this experiment, a random variable is randomly generated by choosing the probabilities of each element in the support from a uniform distribution and then normalizing these probabilities so that they sum to one.

Figure 2 present the error produced by the above methods. The depicted results are averages over several instances (50 instances) of random variables. The curves in the figure show the average error of $\mathrm{OptTrim}$ and Trim operators with comparison to the average error of the optimal approximation provided by $\mathrm{KolmogorovApprox}$ as a function of m.

According to the depicted results it is evident that increasing the support size of the approximation m reduces the error, as expected, in all three methods. However, errors produced by the $\mathrm{KolmogorovApprox}$ are significantly smaller, safe to say, a half of the error produced by $\mathrm{OptTrim}$ and Trim, it is clear both in the table (the relative error is mostly above 1) and in the graph.

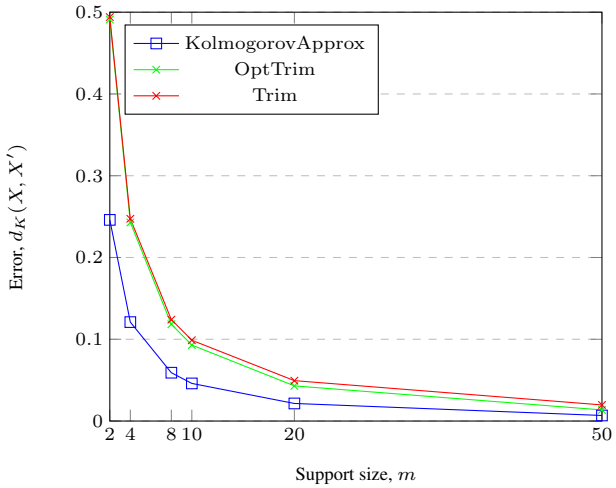

Figure 2: Error comparison between KolmogorovApprox, OptTrim, and Trim, on randomly generated random variables as function of m.

We also examined how our algorithm compares to linear programing as described and discussed, for example, in [6]. We ran an experiment to compare the run-time between the KolmogorovApprox algorithm with the run-time of a state-of-art implementation of linear programing. We used the "Minimize" function of Wolfram Mathematica and fed it with the equations $\min_{\alpha \in \mathbb{R}^n} \|x - \alpha\|_\infty$ subject to $\|\alpha\|_0 \leq m$ and $\|\alpha\|_1 = 1$. The run-time comparison results were clear and persuasive, for a random variable with support size $n = 10$ and $m = 5$, the LP algorithm run-time was 850 seconds, where the KolmogorovApprox algorithm run-time was less than a tenth of a second. For $n = 100$ and $m = 5$, the KolmogorovApprox algorithm run-time was 0.14 seconds and the LP algorithm took more than a day. Due to these timing results of the LP algorithm we did not proceed to examine it any further. Since it is not trivial to formally analyze the run-time of the LP algorithm, we conclude by the reported experiment that in this case the LP algorithm might not be as efficient as KolmogorovApprox algorithm whose complexity is proven to be polynomial in Theorem 11.

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