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# Adaptive Monte-Carlo Optimization

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## Abstract

The celebrated Monte Carlo method estimates a quantity that is expensive to compute by random sampling. We propose *adaptive Monte Carlo optimization*: a general framework for discrete optimization of an expensive-to-compute function by adaptive random sampling. Applications of this framework have already appeared in machine learning but are tied to their specific contexts and developed in isolation. We take a unified view and show that the framework has broad applicability by applying it on several common machine learning problems:  $k$ -nearest neighbors, hierarchical clustering and maximum mutual information feature selection. On real data we show that this framework allows us to develop algorithms that confer a gain of a magnitude or two over exact computation. We also characterize the performance gain theoretically under regularity assumptions on the data that we verify in real world data. The code is available at [https://github.com/govinda-kamath/combinatorial\\_MAB](https://github.com/govinda-kamath/combinatorial_MAB).

## 1 Introduction

The use of random sampling to efficiently estimate a deterministic quantity dates back to the Buffon’s needle experiment of Mario Lazzarini in 1901, and was later developed into the celebrated *Monte-Carlo method* by Stanislaw Ulam. In computer science, this idea has been applied to develop techniques such as locality-sensitive hashing (Gionis et al., 1999) and sketching (Alon et al., 1999). More recently it has been used for fast approximations of matrix operations like matrix multiplication, low rank approximation and matrix decomposition (Drineas et al., 2006a,b,c), to approximate Hessians for convex optimization (Pilanci and Wainwright, 2016, 2017). These techniques find wide applications in machine learning.

In this paper, we consider the use of random sampling to solve discrete optimization problems of the form:

$$\min_{i \in \mathcal{I}} f(i) \tag{1}$$

where  $\mathcal{I}$  is a large but finite set and  $f$  is an expensive-to-compute function. A direct application of the Monte-Carlo method to this problem is to generate enough samples to estimate each value  $f(i)$  accurately and then compute the minimum of the estimates. However, this is computationally inefficient since the values  $f(i)$ ’s which are much larger than the minimum need not be estimated as accurately as the values  $f(i)$ ’s which are closer to the minimum. Instead, a more efficient procedure is to first estimate all the  $f(i)$ ’s crudely using few samples and then *adaptively* focus the sampling on the more promising candidates. We term this general approach *adaptive Monte-Carlo optimization*.

Instances of this general approach have already been appeared in machine learning:

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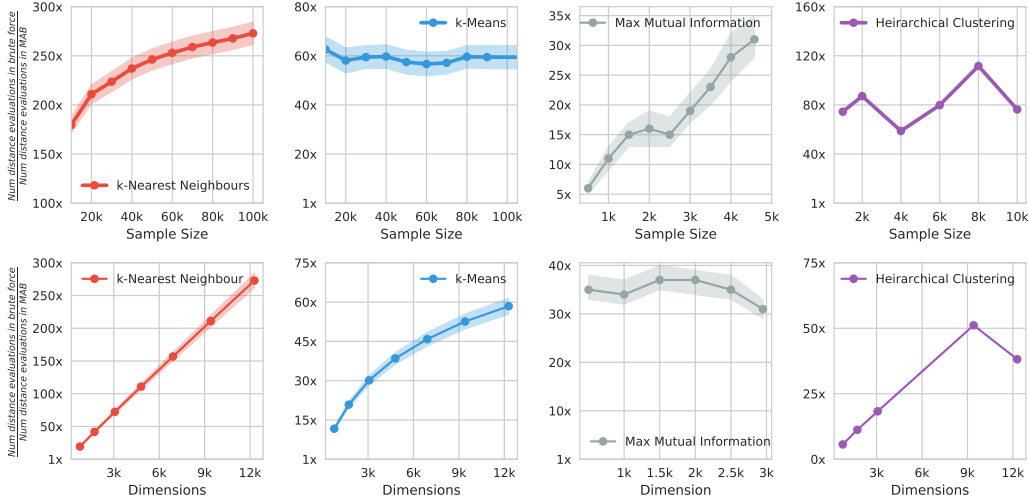


Figure 1: Performance gain of adaptive Monte Carlo optimization algorithms over the brute force algorithm in terms of number of computations in four applications: (a)  $k$ -nearest neighbors graph construction, (b)  $k$ -means, (c) hierarchical clustering (d) minimum mutual information feature selection as a function of number of points and the dimensions. We see a gain roughly linear in dimensions in the first three and linear in sample size in the last, consistent with the theoretical results in Table 1. For  $k$ -nearest neighbors,  $k$ -means and hierarchical clustering we use the tiny-imagenet dataset. For Maximum Mutual information we use the UCI Green-house Gas dataset. More details are in Appendix B.

Table 1: Scaling of naive algorithms and those designed using the adaptive Monte Carlo framework with regularity assumptions on the data.  $n$ : number of points,  $d$ : dimensions/feature size. In each application we obtain a gain in one of  $n$  or  $d$  as indicated in the fourth column. This is also reflected empirically in Fig 1.

Application	Brute time	Our running time	Appx. Gain
$k$ -nearest neighbors	$O(n^2 d)$	$O(n^2 \log^2(nd) + knd \log(n))$	$O(d)$
$k$ -means (an assignment step)	$O(nkd)$	$O(nk \log(dn) \log(k))$	$O(d)$
Hierarchical clustering	$O(n^2 d)$	$O(n^2 \log^2(nd))$	$O(d)$
Max mutual information	$O(nd)$	$O(d \log(nd) + n)$	$O(n)$

- The Monte-Carlo tree search method (Chang et al., 2005; Kocsis and Szepesvári, 2006) to solve large-scale Markov decision problems. Here, the set  $\mathcal{I}$  is the set of all possible actions at a state  $s$  and  $f(i) = Q(i, s)$ , the expected value of the total reward by taking action  $i$  at state  $s$  and then following the optimal policy. The problem of interest is estimating the action that maximizes reward, i.e. solving (1) (but with minimization replaced by maximization) at some state. The Monte-Carlo tree search method is an improvement over the non-adaptive Monte-Carlo planning method of Kearns et al. (2002), and is a central component of modern reinforcement learning systems such as AlphaZero (Silver et al., 2017).
- Adaptive hyper-parameter tuning for deep neural networks (Jamieson and Talwalkar, 2016; Li et al., 2016). Here, the set  $\mathcal{I}$  consists of the possible hyper-parameter configurations and  $f(i)$  is the validation performance of the neural network under the  $i$ th hyper-parameter configuration. The problem is to find the best hyper-parameter configuration using the validation data.
- Computing the medoid (exemplar) of a large number  $n$  of points in high-dimensional space (Bagaria et al., 2018). Here, the set  $\mathcal{I}$  consists of all the points in the dataset and  $f(i)$  is the average of the distances  $d_{ij}$ 's of point  $i$  to all the other points, i.e.

$$f(i) = \frac{1}{n-1} \sum_j d_{ij}.$$

The medoid is the point in the dataset that minimizes the average distance to the other points.

Each of these three problems is solved by a reformulation into a *multi-armed bandit* problem, where each arm corresponds to each element in the set  $\mathcal{I}$ , each arm's reward corresponds to  $f(i)$ , and each pull of arm  $i$  corresponds to generating a sample to update the estimate of  $f(i)$ . For example, in the medoid problem, each pull of the arm  $i$  corresponds to the random sampling of another point  $j$  and obtaining a distance  $d_{ij}$  from the point  $i$ , and then using it to update the estimate of the average distance of point  $i$  to the other points. Well-known algorithms developed for multi-arm bandits like the upper confidence bound (UCB) algorithm (Lai and Robbins, 1985) can be used to derive good adaptive sampling strategies. Computation savings of one or more orders-of-magnitude can sometimes be obtained by using such an algorithm. For example, under some mild conditions on the the distances, the computation cost of the medoid of  $n$  points can be reduced from a naive exact computation cost of  $O(n^2)$  to a cost of  $O(n \log n)$  using the UCB algorithm with a high probability correctness guarantee (Bagaria et al., 2018). To achieve within an accuracy of  $1 + \epsilon$  times the minimum, such an algorithm only needs  $O(1/\epsilon)$  distance computations in contrast to  $O(1/\epsilon^2)$  computations needed by a non-adaptive sampling method (Eppstein and Wang, 2006).

Curiously, although the solution approaches for these three problems are similar, their individual development is very tied to their specific context and is done in isolation of each other. The goal of the present paper is to advocate a broader and more unified view of adaptive Monte-Carlo optimization as a general framework which can be applied to a wide range of other problems in machine learning and beyond. Such opportunities are enhanced particularly by the fact that modern datasets often consist of not only large number of samples but also a large number of features, or dimensions. Thus, both computation across all features for a sample as well as a computation across all samples for a feature can be expensive, and their costs can be significantly ameliorated by adaptive Monte-Carlo optimization.

We support our thesis by applying the framework to develop new methods for several problems and evaluate their performance empirically on large datasets (Figure 1) as well as theoretically (Table 1).

- *Nearest neighbor* : The basic problem of computing the nearest neighbor of a point among  $n$  points in  $d$  dimensional space is expensive if both  $n$  and  $d$  are large. For many common distance measures which are additive, i.e. the distance between two points  $x$  and  $y$  can be written as:

$$\rho(x, y) = \sum_{j=1}^d \rho_j(x_j, y_j),$$

where  $x_j, y_j$  is the  $j$ th component of the point  $x$  and  $y$  respective, the adaptive Monte-Carlo optimization framework can be applied. The set  $\mathcal{I}$  is the set of all contending points,  $f(i)$  is the distance of point  $i$  to the point of interest, and each sample for  $f(i)$  is an evaluation of the distance from point  $i$  to the point of interest on a randomly selected coordinate. We apply this accelerated nearest neighbor subroutine to improve  $k$ -nearest neighbors graph construction as well as the assignment step of Lloyd iteration in the  $k$ -means algorithm.

- *Hierarchical clustering* : Hierarchical clustering algorithms takes  $n$  points in  $d$ -dimensional space and then deriving a binary tree representing the closeness among points. Agglomerative algorithms start off with  $n$  singleton clusters each corresponding to point and in every step the two closest clusters are merged to form a new cluster, until there is one cluster left. Finding the two closest clusters to merge at each step can be put into the adaptive Monte-Carlo optimization framework. At step  $t$  of the algorithm,  $\mathcal{I}$  is the set of all pairs of remaining clusters at that step,  $f(i)$  is the average distance between points in the  $i$ th pair of clusters. Between two clusters  $C_1$  and  $C_2$ :

$$f(i) = \frac{1}{|C_1||C_2|} \sum_{x \in C_1, y \in C_2} \rho(x, y) = \frac{1}{|C_1||C_2|} \sum_{x \in C_1, y \in C_2} \sum_j \rho_j(x_j, y_j),$$

assuming that the distance measure is additive. Each sample for  $f(i)$  can be obtained by randomly sampling along *both* points and co-ordinates. This application is an example of a dynamic algorithm in which each step is an adaptive Monte-Carlo optimization but the estimates are carried forward from one step to the next.

- *Maximum mutual information feature selection* : Consider a supervised learning problem with  $n$  training samples and  $d$  features plus one target variable. The features and the target variables are both continuous-valued. The goal is to select the feature with the maximum mutual information to the target. We pose this as an adaptive Monte-Carlo optimization, with  $\mathcal{I}$  as the set of  $d$  features.

Here  $f(i)$  is an empirical estimate of the mutual information between the feature  $i$  and the target, calculated from all the sample points. Because the features are continuous-valued, this estimate is not in an additive form across the sample points. Nevertheless we can randomly sample and efficiently update estimates of  $f(i)$ . This example shows that even complicated non-additive  $f(i)$ 's can be put into the adaptive Monte-Carlo optimization framework. Moreover, unlike the previous two examples where the set  $\mathcal{I}$  represents the sample points and the computation of  $f(i)$  is along the features (dimensions), here  $\mathcal{I}$  represents the features and the computation of  $f(i)$  is along the sample points. It shows the broad applicability of the framework.

In Sections 2-4, we pose the applications discussed above in the adaptive Monte Carlo optimization framework and derive algorithms to solve them. In Section 5 we discuss leveraging sparsity of the dataset in the adaptive Monte Carlo optimization framework. We then conclude with some discussion in Section 6.

## 2 $k$ -nearest neighbors graph construction and $k$ -means

### 2.1 $k$ -nearest neighbor graph construction

*k*-nearest neighbor graph construction is the problem of constructing  $k$ -nearest neighbor graphs from  $n$  unlabelled data points with respect to some distance metric (Hastie et al., 2009, Chapter 13). This is used as a subroutine in many unsupervised learning algorithms such as Iso-map (Tenenbaum et al., 2000), Local linear Embedding (Roweis and Saul, 2000), Hessian Eigenmaps (Donoho and Grimes, 2003), some algorithms in spectral clustering (Linderman et al., 2017) among others. In recent years there has been a lot of work in construction of  $k$ -nearest neighbor graphs on high dimensional data such as that on the YFCC100M dataset in Johnson et al. (2017). While dimensionality reduction is often helpful in applications like embedding graphs (Wang et al., 2016) and videos (Ramanathan et al., 2015), the dimensions of the space embedded in is also in a few thousand, which makes constructing  $k$  nearest neighbor graphs a problem of interest in high dimensions.

For low dimensions there are some heuristics that are known to perform well such as  $k$ - $d$  trees (Bentley, 1975) and ball-trees (Omohundro, 1989). One popular algorithm there is the KGraph (Dong, 2014) which is a heuristic algorithm improving over Dong et al. (2011).

In this section we consider the  $k$ -nearest neighbor graph construction problem, pose it in the adaptive Monte Carlo optimization framework, and then evaluate performance of the algorithm we obtain.

Let us assume that we have an  $(n \times d)$  data matrix  $X$  corresponding to  $n$  points:  $x_1, \dots, x_n \in \mathbb{R}^d$ . Our goal is to find the nearest neighbor graph in  $\ell_p$  distance. As a subroutine, let us consider finding the  $k$  nearest neighbors of point 1. Without loss of generality let us consider  $\ell_2$  distances

We consider each of the points  $\{2, \dots, n\}$  as arms. As the  $k$ -nearest neighbors with  $\ell_2$  distances is the same as finding  $k$ -nearest neighbors with squared euclidean distances, we consider  $f(i)$  as

$$f(i) = \frac{1}{d} \sum_{t=1}^d (x_{1,t} - x_{i,t})^2,$$

and the objective is to find  $k$  points with the smallest  $\ell_p$  distances to point 1.

Here and in applications to follow, we design a sequence of estimators for  $f(i)$  with increasing accuracy:  $\{\hat{f}_\ell(i)\}$ , such that: 1) we can use evaluations of  $\hat{f}_\ell(i)$  to construct confidence intervals on  $f(i)$  (which often involves making some regularity assumptions about the data), and 2) updating  $\hat{f}_\ell(i)$  to  $\hat{f}_{\ell+1}(i)$  is computationally cheap.

An estimator after  $\ell$  pulls of arm  $i$  (for squared euclidean distances) would be

$$\hat{f}_\ell(i) = \frac{1}{\ell} \sum_{k=1}^{\ell} (x_{1,t_k} - x_{i,t_k})^2, \quad (2)$$

where  $t_1, \dots, t_\ell$  are uniformly sampled from  $[d]$  with replacement.

The update of the estimator at step  $\ell + 1$  is

$$\hat{f}_{\ell+1}(i) = \frac{\ell}{\ell+1} \hat{f}_\ell(i) + \frac{1}{\ell+1} (x_{1,t_{\ell+1}} - x_{i,t_{\ell+1}})^2, \quad (3)$$

which takes  $O(1)$  time, where  $j_{\ell+1}$  is sampled from  $[d]$ , uniformly at random. We further assume that the estimator of Eq. (2) has  $\sigma$ -sub-Gaussian tails<sup>2</sup> which allows us to construct confidence intervals. Figure 2 (b) shows that such an assumption is reasonable<sup>3</sup>. Thus we have reformulated the  $k$ -nearest neighbor as a multi-armed bandit problem using the adaptive Monte Carlo optimization framework.

Throughout this manuscript, we restrict ourselves to using a slightly modified version of the standard Upper-Confidence Bound algorithm of Lai and Robbins (1985) to solve the bandit problem. We note that in reformulations obtained from the adaptive Monte Carlo optimization framework, there exists an integer MAX\_PULLS such that the total computation required to compute  $\hat{f}_{\text{MAX\_PULLS}}(i)$  (over all updates) is equal to the computation required to compute  $f(i)$  exactly. We thus evaluate  $f(i)$  exactly if arm  $i$  is pulled MAX\_PULLS times and set the confidence intervals to be of zero width giving us the only modification we make to the algorithm of Lai and Robbins (1985). Given a set of  $n$  arms  $\mathcal{A}$ , the MAX-PULLS, the number of arms to be returned  $k$  and a procedure to update them to construct confidence intervals we present this Algorithm 2 of Appendix A and call it UCB.

We find  $k$ -nearest neighbors using the algorithm defined in Algorithm 1. This leverages the UCB sub-routine of Appendix A.

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**Algorithm 1**  $k$ -nearest-neighbors UCB

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- 1:  $n$  points in  $\mathbb{R}^d$ :  $x_1, \dots, x_n$  are input to the algorithm.
  - 2: **for**  $i \in [n]$  **do**
  - 3:   Consider arms  $\mathcal{A}_\ell, 1 \leq \ell \neq i \leq n$  with estimators defined as in Eq. (2) and confidence intervals constructed using  $\sigma$ -sub-gaussianity.
  - 4:   neighbors of  $x_i$  are given by  $\text{UCB}(\{\mathcal{A}_\ell, 1 \leq \ell \neq i \leq n\}, d, k)$   $\triangleright$  MAX\_PULLS =  $d$
  - 5: **end for**
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Let  $\mu_k^*$  be the distance of the  $k$ -th nearest neighbor to point 1. Let  $\mu_i$  be the distance of point  $i$  from point 1. Define,  $\Delta_i = \max(0, \mu_i - \mu_k^*)$ .  $\Delta_i$  is 0 for the  $k$  nearest neighbours of point 1 and for the other points it measures how much larger than  $\mu_k^*$  their distance to point 1 is. In the

**Theorem 2.1.** *With probability  $1 - \frac{1}{n^2}$ , Algorithm 1 returns the  $k$ -nearest neighbors of point 1 in  $O\left(\sum_{i=2}^n \log(n) \left(\left(\frac{\sigma^2 \log(nd)}{\Delta_i^2}\right) \wedge d\right)\right)$  time.*

**Theorem 2.2.** *We can modify Algorithm 1 to obtain an algorithm, which with probability  $1 - \frac{1}{n^2}$  finds the  $k$ -nearest neighbor of point 1 upto a  $(1 + \epsilon)$ -approximation is  $O\left(\sum_{i=2}^n \log(n) \left(\frac{\sigma^2 \log(nd)}{(\max(\Delta_i, \epsilon \mu_k^*))^2}\right)\right)$*

**Remark 1.** *The running time of the above algorithm for finding  $k$ -nearest neighbors of all  $n$  points is  $O(nk \log(dn) \log(k))$  under some natural assumptions on distribution of  $\Delta_i$  which is again better than the running time of the naive algorithm which is  $O(n^2 d)$ . Detailed analysis is in Appendix E.*

**Empirical Performance :** Since the bandit based algorithms do not compute exact distances between any two points, we measure the performance of algorithms in terms of *effective number of distance evaluations*. We define effective number of distance evaluations between two points as the fraction of co-ordinates involved in estimating the distance between these two points. The effective number of distance evaluations of an algorithm is the sum of effective number of distance evaluations between every pair of points in the algorithm. For example, note that the effective number of distance evaluations to find the distance between two vectors exactly is 1 as all the co-ordinates are used.

In Figure 1 (a), we show the gain of the bandit based algorithm over the brute-force algorithm in terms of the effective number of distance evaluations on the tiny-imagenet training data. We vary the number of images from  $10k$  to  $100k$  and their dimensions from 700 to  $12k$ . We obtain a gain of more than  $100\times$  over the naive algorithm. We also notice that the gain over the naive algorithm increases almost linearly with dimensions, giving us that this algorithm behaves in an almost dimension free manner. We hasten to add that the gain in absolute running time in our proof-of-concept implementation

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<sup>2</sup> $\sigma$  being independent of  $n$

<sup>3</sup>In practice we estimate sigma from some random samples at the beginning of the run and update it as the algorithm progresses. Details in Appendix B.

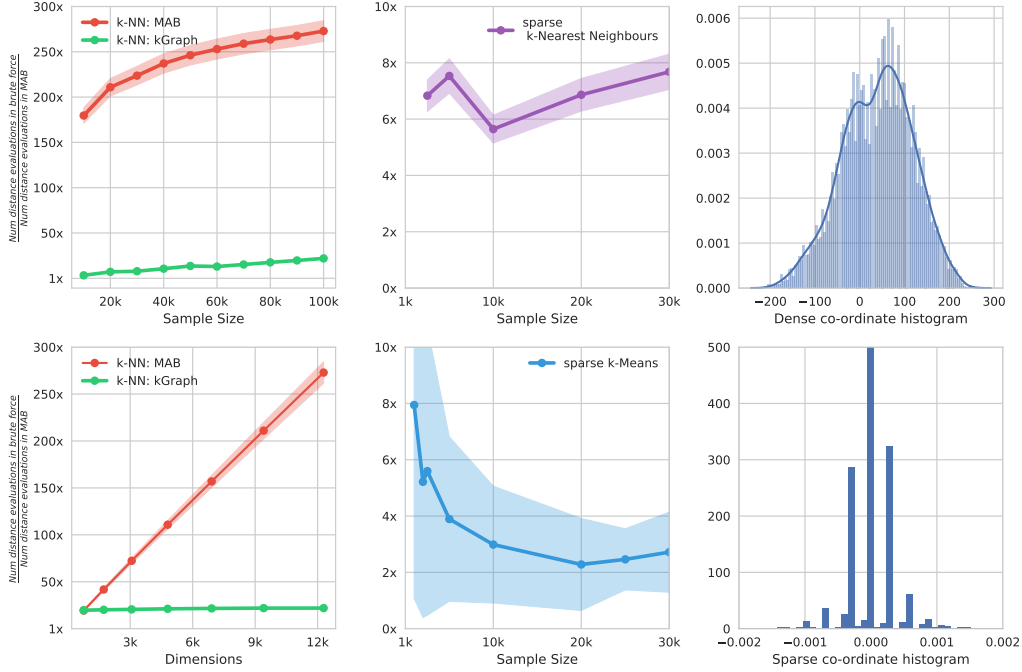


Figure 2: (a) This shows the gain of our algorithm 1 and that obtained by KGraph on the tiny-imagenet dataset, (b) shows the gain obtained by our algorithm 1 on sparse gene dataset of 10x-genomics. (c) Histogram of co-ordinate wise distances for randomly chosen pair of points in the dense dataset (imagenet) and sparse dataset (10x genomics).

(which does not have systems level optimization) was around 2x, but there is scope of significant improvement with more careful cache management and parallelization.

A state of the art algorithm for computing the  $k$ -nearest neighbor graph is KGraph (Dong, 2014). We compare our performance with KGraph on the tiny-imagenet dataset in Figure 2 (a). KGraph and the bandit based algorithm operate in two fundamentally different ways. While KGraph improves its effective number of distance evaluations by computing the distances between fewer pairs of points using the fact that neighborhoods of neighboring points have large intersections (giving it good scaling with the  $n$ ), our algorithm improves its effective number of distance evaluations by computing distances between all pairs of points approximately (giving it good scaling with  $d$ ). Combining the two approaches to improve scaling with both  $n$  and  $d$  is an avenue for further research.

**Remark 2.** Another natural algorithm for computing  $k$ -nearest neighbors would be to first project the data into lower dimensional space using Johnson-Lindenstrauss and then computing  $k$ -nearest neighbors in the lower dimensional space. We discuss connections to this in Appendix I

## 2.2 $k$ -Means

The canonical algorithm for computing  $k$ -means: Lloyd’s algorithm (Lloyd, 1982), starts with  $k$  initial centroids and then iteratively alternates between two steps: *the assignment step* : where each of the  $n$  points is assigned to the centroid closest to it, and *the update step* : where the centroids are updated. For a standard implementation every iteration of  $k$ -means, the assignment step takes  $O(kd)$  time per point and the update step is much cheaper and takes  $O(d)$  time per point, where  $d$  is the ambient dimension of the  $n$  points.

We note that one can view the assignment step of  $k$  means as finding the nearest neighbor of each of the  $n$  points among the  $k$  centroids. For each point, this can thus be posed as a nearest neighbor problem with  $k$  arms. Under mild assumptions, this algorithm has a running time of  $O((k \log(dn)) \log(k))$  per point. We analyse this formally in Appendix F. As shown in Figure 1 (b), we note that we get an improvement of 30-50x in terms of effective number of distance evaluations compared to the naive algorithm on the tiny-imagenet dataset, with  $k = 100$ .

### 3 Agglomerative Algorithms for Hierarchical clustering

We next illustrate incorporating the adaptive monte carlo optimization framework into sequential algorithms to obtain computational savings. We use hierarchical clustering as an example.

Hierarchical clustering is an algorithm that is widely used in data analysis (Leskovec et al., 2014, Chapter 7). This is especially popular if the number of clusters is not known apriori, or the data has hierarchical structure. Given a set of  $n$  points and a distance measure hierarchical clustering finds a binary tree with  $n$  leaves to represent the data with each leaf corresponding to a point, and the distance between two points along the tree showing the dis-similarity between them.

A class of algorithms for hierarchical clustering are *agglomerative algorithms* which combine points in a bottom up manner. Such algorithms start off with the  $n$  clusters, each corresponding to a point. At every step, the algorithm merges the two “closest” clusters to form a single cluster until there is only one cluster remaining. This naturally sets up a binary tree representation where the each leaf is a cluster with 1 point, the root is the cluster of all points, and all intermediate vertices are clusters formed at intermediate steps. The two children of any vertex in the tree are the clusters that were merged to form that cluster.

For two clusters which consist of only one point, the notion of closeness is unambiguously defined by the distance metric. For clusters with more than one point, one way to define the distance between clusters is the *average linkage* which is the average distance between points in the cluster.

Each step of this algorithm computes the pair of clusters with smallest distance between them. Each step can be posed as a bandit problem with the arms being each pair of clusters in the system at that step. If we consider squared euclidean distances as our distance metric (other distances can be handled using the trick discussed in Appendix D), then pulling an arm corresponds to evaluating the square of difference of two co-ordinates in two points, randomly chosen each from one of the two clusters corresponding to the arm. More detailed analysis is presented in Appendix G.

On running this on the tiny-imagenet validation dataset of  $10k \ 64 \times 64$  RGB images, we obtain a gain of more than 30x over the naive algorithm in terms of the effective number of distance computations as shown in Figure 1.

**Remark 3.** *The algorithm reduces the running time of the algorithm from  $O(n^2(d + \log(n)))$  to  $O(n^2 \log^2(nd))$  under some regularity assumptions discussed in Appendix G.*

### 4 Maximum Mutual Information Feature Selection

In all applications we considered so far,  $f(i)$  was a simple function and constructing confidence intervals for estimates of  $f(i)$  was easy. Here we consider the case where  $f(i)$  is itself a sophisticated estimator of an underlying statistical quantity: mutual information, in the context of maximum mutual information feature selection.

A reasonably popular feature selection procedure is Maximum Mutual Information Criterion (Yang and Moody, 2000; Peng et al., 2005). In this scheme, given a set of features and a target, one picks feature that has the highest estimated mutual information with the target as the most relevant feature. Approaches to pick multiple features include Max-Relevance Min-Redundancy (Peng et al., 2005), Joint Mutual Information (Yang and Moody, 2000) or Chow-Liu trees (Chow and Liu, 1968) etc. Here, we will focus on applying the adaptive Monte Carlo optimization framework to the problem of picking a single most informative feature. The framework can also be applied accelerate the approaches which pick multiple features on a sequential basis, such as building Chow-Liu trees.

As before, we have an  $(n \times d)$  data matrix  $X$  corresponding to  $n$  points each with  $d$  features. Let us also assume we have an  $n$ -vector  $Y$  corresponding to the target. Here we focus on picking the single most relevant feature to the target.<sup>4</sup> If both the features and the target are continuous, a clever non-parametric function of Kozachenko and Leonenko (1987) is often used to empirically estimate mutual information.

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<sup>4</sup>If both the features and the target are discrete, then one can use the plug-in estimators and put the problem into our framework as well.

On putting it into the framework (with min replaced by max), every feature is an arm.  $f(i)$  is an empirical mutual information of the feature  $i$  with  $Y$ . We next describe the  $f(i)$  used in this application.

We then rely on the estimator of differential entropy by Kozachenko and Leonenko (1987) to obtain  $f(i)$ . Let  $Z_1, \dots, Z_k$  be  $k$  iid samples of a random variable. Define  $R_i = \min_{j \in [k] - \{i\}} \|Z_j - Z_i\|_2$ . Then the Kozachenko-Leonenko estimator is given by  $\hat{h}_k(\{Z_1, \dots, Z_k\}) = \frac{1}{k} \sum_{i=1}^k \log R_i + c_d$ , for an absolute constant  $c_d$  depending only on dimension of the random variable. Given an iid sequence of  $k$  pairs of random variables  $\{(W_1, Z_1), \dots, (W_k, Z_k)\}$ , we estimate the mutual information between the two as

$$\hat{I}_k(\{W_i\}_1^k; \{Z_i\}_1^k) = \hat{h}_k(\{W_i\}_1^k) + \hat{h}_k(\{Z_i\}_1^k) - \hat{h}_k(\{(W_i, Z_i)\}_1^k)$$

$f(i)$  and its estimators  $\hat{f}_\ell(i)$  are given by:

$$\begin{aligned} f(i) &= \hat{I}_n(\{X_{t,i}\}_{t=1}^n, \{Y_t\}_{t=1}^n), \\ \hat{f}_\ell(i) &= \hat{I}_\ell(\{X_{t_k,i}\}_{k=1}^\ell, \{Y_{t_k}\}_{k=1}^\ell) \end{aligned}$$

We obtain the confidence intervals using a central limit theorem derived for this estimator (Delattre and Fournier, 2017; Bickel and Breiman, 1983).

While updating the estimators cheaply is not as trivial as in previous applications, it can be done cheaply as explained in Appendix H. We consider the Greenhouse gas sensor dataset of Lucas et al. (2015) obtained from the UCI repository (Dheeru and Taniskidou, 2017). This consists of greenhouse gas (GHG) concentrations measured on 2921 sensors. We consider one of the sensors as the target and empirically find that we get a saving of around 20x in the effective number of computations (which is the total number of points used in estimating the mutual information) to compute maximum mutual information as shown in Figure 1(c).

## 5 Improved Estimators for Sparse Datasets

In this section we illustrate that the performance of algorithms from our framework can be improved significantly by designing better estimators that exploit structure in the data using sparsity as an example.

Algorithms based on the adaptive Monte Carlo optimization framework adaptively sample a fraction of data to obtain estimates of  $f(i)$  to solve the minimization problem. Often we have to deal with sparse datasets. Ideally we would want to design estimators  $\hat{f}_\ell(i)$  to leverage the sparsity and only sample the non-zero entries of the data. For example in the single cell gene dataset of 10xGenomics (2017), only 7% of the entries are non-zero, even though the points live in  $28k$  dimensions.

Consider estimating the squared euclidean distance between sparse points  $x_0$  and  $x_1$  lying in  $d$  dimensional space with  $n_0$  and  $n_1$  non-zero co-ordinates respectively. Rather than sampling over all co-ordinates, we would like to sample co-ordinates which are non-zero in either one of the two points. However computing the the set union of the non-zero co-ordinates of  $x_0$  and  $x_1$ , which would take  $O(n_0 + n_1)$  time neutralizing any gain obtained using our framework. We circumvent this expensive computation by using the following estimator which does not use the set union.

$$\hat{d}_\ell(x_0, x_1) = \frac{1}{\ell} \sum_{k=1}^\ell \tilde{d}(x_0, x_1, k),$$

where the  $\tilde{d}(x_0, x_1, k)$  is obtained by first sampling  $t_k^{(0)}, t_k^{(1)}$  from the non-zero co-ordinates of  $x_0$  and  $x_1$  and

$$\tilde{d}(x_0, x_1, k) = \frac{n_0}{2d} (x_{0,t_k^{(0)}} - x_{1,t_k^{(0)}})^2 (1 + \mathbb{I}(x_{1,t_k^{(0)}} = 0)) + \frac{n_1}{2d} (x_{0,t_k^{(1)}} - x_{1,t_k^{(1)}})^2 (1 + \mathbb{I}(x_{1,t_k^{(1)}} = 0))$$

A more elaborate way of thinking about this estimator, is that at each step we follow the following procedure:

1. Sample a non-zero co-ordinate of  $x_0$  and  $x_1$ . Let the co ordinates obtained be  $t_k^{(0)}$  and  $t_k^{(1)}$  respectively.



2. Check if  $t_k^{(0)}$  is a non-zero co-ordinate of  $x_1$ . Based on this compute

$$\tilde{d}^{(0)}(x_0, x_1, k) = \begin{cases} \frac{n_0}{2d} (x_{0,t_k^{(0)}} - x_{1,t_k^{(0)}})^2 & \text{if } x_{1,t_k^{(0)}} \neq 0, \\ \frac{n_0}{d} x_{0,t_k^{(0)}}^2 & \text{if } x_{1,t_k^{(0)}} = 0. \end{cases}$$

$\tilde{d}^{(1)}(x_0, x_1, k)$  is similarly computed and depends upon if  $t_k^{(1)}$  is a non-zero co-ordinate of  $x_0$ .

3. We thus have that,

$$\tilde{d}(x_0, x_1, k) = \tilde{d}^{(0)}(x_0, x_1, k) + \tilde{d}^{(1)}(x_0, x_1, k).$$

We next claim that the estimator is unbiased. Let the set non-zero co-ordinates of  $x_0$  and  $x_1$  be  $S_0 \subseteq [d]$  and  $S_1 \subseteq [d]$ , with  $|S_0| = n_0$  and  $|S_1| = n_1$ . To see this note that, as  $t_k^{(0)}$  is sampled uniformly from the  $S_0$ , every element of  $S_0$  is picked with probability  $\frac{1}{n_0}$ . Thus, we have that

$$\mathbb{E}[\tilde{d}^{(0)}(x_0, x_1, k)] = \frac{1}{d} \sum_{j \in S_0 - S_1} (x_{0,j})^2 + \frac{1}{2d} \sum_{j \in S_0 \cap S_1} (x_{0,j} - x_{1,j})^2.$$

With an analogous evaluation of  $x_1$ , we have that,

$$\begin{aligned} \mathbb{E}[\tilde{d}(x_0, x_1, k)] &= \frac{1}{d} \sum_{j \in S_0 - S_1} (x_{0,j})^2 + \frac{1}{d} \sum_{j \in S_0 \cap S_1} (x_{0,j} - x_{1,j})^2 + \frac{1}{d} \sum_{j \in S_1 - S_0} (x_{1,j})^2, \\ &\stackrel{(a)}{=} \frac{1}{d} \sum_{j \in S_0 \cup S_1} (x_{0,j} - x_{1,j})^2, \\ &= \frac{1}{d} \sum_{j \in [d]} (x_{0,j} - x_{1,j})^2, \end{aligned}$$

which is the distance between the two points. We note that (a) follows from the definition of  $S_0$  and  $S_1$ .

We note that this estimator thus needs only two non-trivial operations: 1) sampling from the non-zero co-ordinates of a sparse vector, and 2) checking if a co-ordinate is non-zero in a sparse vector. To see that these can be done in  $O(1)$  time, we elaborate on how sparse vectors are usually stored in standard implementations.

Sparse vectors consist of a data structure a data-structure with two object: a vector  $v_{\text{data}}$  storing the non-zero entries and a dictionary (or unordered map) with maps the co-ordinate in the original vector to the co-ordinate in the  $v_{\text{data}}$ . We have that we can check membership of key in a dictionary as well find the value of the key if it is present in the dictionary in  $O(1)$  amortised time. Further we can generate a random key in the dictionary also in  $O(1)$  time. This gives us that  $\tilde{d}$  can be computed in  $O(1)$  time.

As shown in Figure 2(c), (d), we obtain 3x gain over brute force in the effective number of distance evaluations for  $k$ -nearest neighbours and  $k$ -means on the dataset of 10xGenomics (2017). The baseline considered here takes sparsity into account. We also observe if we had used the estimator of Section 2 we would not improve over the brute force algorithm.

## 6 Discussions

We show in our empirical and theoretical results that adaptive Monte-Carlo optimization is a powerful and broad framework that can provide significant computational savings in many basic machine learning problems. Some generalizations of the framework are discussed in Appendix D.

Modern datasets are often large in both sample size and dimensions. Our algorithm provides gains in one of the two. In applications such as  $k$ -nearest neighbors as KGraph (Dong, 2014), Lanczos bisection based methods (Chen et al., 2009), Locality sensitive hashing based methods (Andoni and Indyk, 2008; Andoni et al., 2015) which provides savings in the sample size, whereas our algorithm provides savings in the dimensions. Integrating both these approaches to obtain savings in both sample size and dimension is an open question.

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## A The modified UCB Algorithm

Let  $\mathcal{A}_\ell, \ell \in [n]$  is a set of arms defined by the routine (say  $k$ -nearest neighbors) that calls the function UCB. The routine calling function UCB also defines the methods to pull arms, update the estimates of their mean, and construct confidence intervals around these estimates. Further, it also provides a method to evaluate the means of the arm exactly.

Let  $\mu_i$  be the true value of the mean of arm  $i$ . Let  $\hat{\mu}_i(t)$  be the estimate of the mean of arm  $i$  at the  $t$ -th iteration of the algorithm. Let  $[\hat{\mu}_i(t) - C_i(t), \hat{\mu}_i(t) + C_i(t)]$  be the  $(1 - \delta)$ -confidence interval for  $\mu_i$  maintained at the  $t$ -th iteration of the algorithm.

The UCB algorithm defined below is essentially the UCB of Lai and Robbins (1985) with an extra condition of evaluating the mean of the arm exactly and setting the widths of the confidence interval to 0 if it is pulled more than MAX\_PULLS times.  $k$  is the number of best arms returned by the algorithm.

---

**Algorithm 2** UCB ( $\{\mathcal{A}_\ell : \ell \in [n]\}, \text{MAX\_PULLS}, k$ )

---

```

1: For each arm  $\{\mathcal{A}_\ell : \ell \in [n]\}$ , compute a  $(1 - \delta)$  confidence intervals by  $\log(n)$  steps of the
   estimator to obtain:  $[\hat{\mu}_j(1) - C_j(1), \hat{\mu}_j(1) + C_j(1)]$ 
2:  $\mathcal{B} = \{\}$  ▷ Set of  $k$  best arms
3:  $\mathcal{S} = \{\mathcal{A}_\ell : \ell \in [n]\}$  ▷ Set of arms under consideration
4: while TRUE do
5:   At iteration  $t$ , pick arm  $\mathcal{A}_t$  that minimises  $\hat{\mu}_j(t-1) - C_j(t-1)$  among arms in  $\mathcal{S}$ .
6:   if arm  $\mathcal{A}_t$  is evaluated less than MAX_PULLS times then
7:     improve the confidence interval and mean estimate of the arm  $\mathcal{A}_t$  by updating the the
       estimator by one more step.
8:   else
9:     Set  $\hat{\mu}_{\mathcal{A}_t}(t)$  to be brute force evaluation of the mean of the arm and set  $C_{\mathcal{A}_t}(t) = 0$ .
10:  end if
11:  if Arm  $\mathcal{A}_t$  is such that  $\forall \mathcal{A}_i \neq \mathcal{A}_t, \hat{\mu}_{\mathcal{A}_t}(t) + C_{\mathcal{A}_t}(t) < \hat{\mu}_{\mathcal{A}_i}(t) - C_{\mathcal{A}_i}(t)$  then
12:    Add  $\mathcal{A}_t$  to  $\mathcal{B}$ 
13:    Remove  $\mathcal{A}_t$  from the set of arms under consideration, that is  $\mathcal{S} = \mathcal{S} - \{\mathcal{A}_t\}$ .
14:    if  $|\mathcal{B}| = k$  then return  $\mathcal{B}$ 
15:  end if
16:  end if
17: end while

```

---

## B Details of experiments

### B.1 Datasets

For  $k$ -nearest neighbours,  $k$ -means and hierarchical clustering, we empirically evaluate the performance of MAB-based algorithms on two real world high-dimensional datasets: tiny-imagenet (Russakovsky et al., 2015), and 10x single cell RNA-Seq dataset (10xGenomics, 2017).

Tiny-imagenet consists of 100k images of size  $64 \times 64$  with 3 channels thus living in 12288 dimensional space. We downsize these images to evaluate our method on smaller dimensions. We chose imagenet because it is one of the most popular benchmark dataset in the field of computer vision – where many applications use nearest neighbours, clustering in their pipelines.

To further exhibit the robustness of our approach across applications, our second dataset is a single cell RNA-Seq dataset of 10xGenomics (2017) from the field of computational biology. The scale of this dataset is also large both in sample size and dimension and additionally it is a very sparse (7%). For our empirical evaluations we randomly sub-sample 100k points from this dataset. We note that each row lies in 28k dimensional space.

For Maximum Mutual information feature selection we evaluated the performance of MAB-based algorithm on smaller sized Greenhouse gas sensor dataset of Lucas et al. (2015). This was the largest dataset we could find with continuous features and continuous response. We restricted ourselves to such datasets, because we wanted to exhibit the applicability of our approach with sophisticated

estimators (like the Kozachenko-Leonenko based estimator for mutual information). This dataset consist of 4,578 rows of 2,950 dimensions i.e, it has readings from 2950 sensors for at 4578 time points. For a fixed sensor, say  $s_1$ , our goal is to find the sensor (among the other 2949 sensors) with maximum mutual information.

## B.2 Implementation and evaluation

We implemented the code in C++. The results and figures of the paper can be reproduced from our github repository.

A schematic showing the structure of implementation is shown in Figure 3.

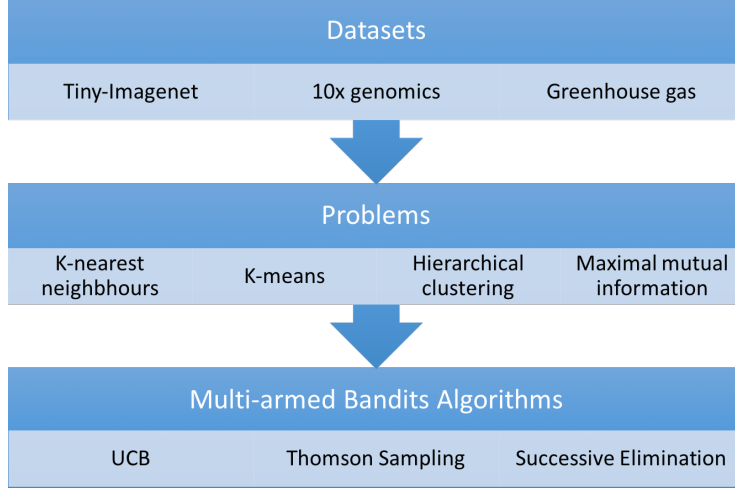


Figure 3: The implementation consists of three modules. The first module loads the data, cleans it and puts it in a form that it can be processed. The second module uses the data and designs the arms corresponding to the problem at hand and then uses a multi-armed bandit algorithm from the third module.

UCB has only one tuning parameter, For all the experiments we set  $\delta = 0.01$  in the UCB algorithm. We evaluate the accuracy of the algorithms and control it as follows:

1.  **$k$ -nearest neighbors:** For  $n$  points, let the true  $k$  nearest neighbors of point  $i$  be the set  $NN_i^*$  (evaluated using the naive algorithm) and let the answer given by bandit-based algorithm be the set  $NN_i^{MAB}$ . We define the accuracy by  $\frac{1}{n} \sum_{i=0}^n \mathbb{E} \left[ \mathbf{1} \{ NN_i^* = NN_i^{MAB} \} \right]$ . For all of the  $k$ -nearest neighbour experiments, we obtain an accuracy of  $> 99\%$  for the bandits based algorithm using  $\delta = 0.01$ .
2.  **$k$  means:** For  $n$  points and  $k$  cluster centres, let for point  $i$  let the nearest cluster be  $c_i^*$  and the answer returned by bandit-based method be  $c_i^{MAB}$ . We define the accuracy by  $\frac{1}{n} \sum_{i=0}^n \mathbb{E} \left[ \mathbf{1} \{ c_i^* = c_i^{MAB} \} \right]$ . For all of the  $k$ -means experiments, we obtain an accuracy of  $> 99\%$  for the bandits based algorithm using  $\delta = 0.01$ .
3. **Maximal Mutual Information:** For dataset with  $d$  features, let the feature with maximal mutual information with the label be  $f^*$  and let the answer given by MAB-based algorithm be  $f^{MAB}$ . We define the accuracy be  $\mathbb{E} \left[ \mathbf{1} \{ f^* = f^{MAB} \} \right]$ . For all of the Maximal Mutual Information experiments, we obtain an accuracy of  $> 99\%$  for the bandits based algorithm using  $\delta = 0.01$ .
4. **Hierarchical clustering:** For  $n$  points let the  $T^*$  be the tree graph given by the the brute hierarchical method, let  $T^{MAB}$  be the tree graph given by MAB-based algorithm and let

$T^{\text{random}}$  be a random tree graph with  $n$  leaves. We measure the accuracy of  $T^{\text{MAB}}$  as

$$1 - \frac{\sum_{i=0}^n \sum_{j=0}^{i-1} \mathbb{E} \left[ \left| \text{dist}^*(i, j) - \text{dist}^{\text{MAB}}(i, j) \right| \right]}{\sum_{i=0}^n \sum_{j=0}^{i-1} \mathbb{E} \left[ \left| \text{dist}^*(i, j) - \text{dist}^{\text{random}}(i, j) \right| \right]},$$

where  $\text{dist}^*$ ,  $\text{dist}^{\text{MAB}}$ ,  $\text{dist}^{\text{random}}$  is the distance between point  $i$  and  $j$  in tree graph  $T^*$ ,  $T^{\text{MAB}}$  and  $T^{\text{random}}$  respectively. For all hierarchical clustering experiments, our accuracy  $> 90\%$  and adjusted random score is  $> 0.7$ .

In the above expressions, the expectation is taken over the randomness in the sampling to obtain the estimators.

We evaluate the algorithms based on the effective number of dimensions or points used by estimators in the algorithm. For  $k$ -nearest neighbors,  $k$ -means, hierarchical clustering this is the *effective number of distance evaluations*.

The effective number of distance computations between two points (which are non-sparse) is the fraction of dimensions used by the algorithm to estimate distance between two points. The effective number of distance computations in an algorithm is the sum of the effective number of distance computations between all pair points in the algorithm. This is a reasonable metric as the amount of work done between distance computations is at most  $O(\log n)$ .

For the sparse case we define the effective number of distance computations between two points is the fraction of the non-zero co-ordinates used by the algorithm to estimate distance between two points. The effective number of distance computations in an algorithm is the sum of the effective number of distance computations between all pair points in the algorithm.

For the Maximum Mutual information estimation problem we use the *effective number of samples* as the metric to measure performance. This sum of the number of samples used in the all the estimators.

### B.3 Exploration vs Exploitation

The bandit based algorithm for  $k$  nearest neighbors algorithm evaluates true distance only for a handful of contenders. For the rest, it only computes an approximation of their distances. For point  $x_1$  (in  $d = 12k$ ) from imagenet, Figure 4 shows that the UCB achieves a 'good' trade-off between exploration and exploitation for  $k$  nearest neighbour problem - it evaluates distance along all the co-ordinates (measures the exact distance) to the close points whereas for far off points it calculates distances only along very few co-ordinates (to obtain a coarse estimate of the distance). These observations generalise to the other three applications.

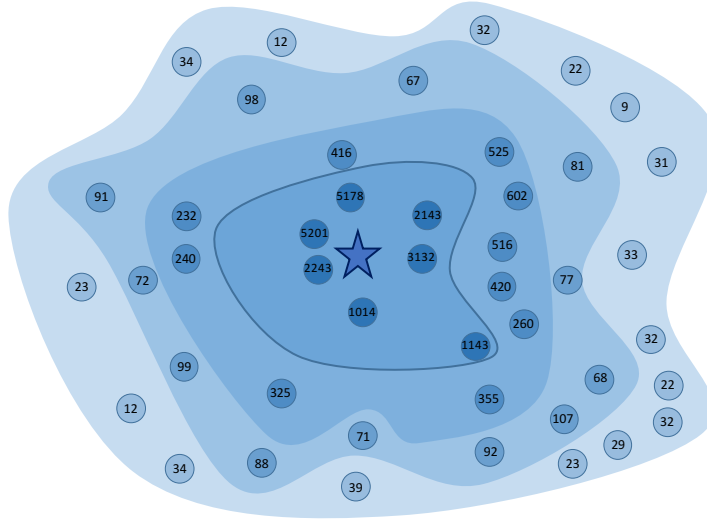


Figure 4: The number of distance evaluations for  $k$ -nearest neighbor of a point with other points in its neighborhood.

## B.4 Practice

**Speed-accuracy tradeoff:** By setting  $\delta$  to large values (say 0.1), UCB will maintain small confidence intervals around the mean estimates of each arm and this will reduce the total arm pulls by UCB. Therefore, one can trade off accuracy for faster running time. Further a deterministic running time can be achieved if one fixes the number of arm pulls for UCB. This might be desirable in certain applications.

**Confidence intervals:** UCB heavily relies on the accuracy of its confidence intervals, whose estimation depends on the value of  $\sigma$ . Overestimating the value of  $\sigma$  (likewise confidence intervals) increases running time whereas underestimating  $\sigma$  decreases the accuracy. Hence having a good estimate of  $\sigma$  is crucial for the bandit based algorithm to perform well. We do it by maintaining a (running) estimate of the mean and the second moment for every arm. For instance which are application/dataset specific, if one can obtain tighter confidence intervals, it will vastly improve the running time.

Estimating confidence intervals using other techniques could potentially improve the performance.

### Others miscellaneous observations

1. All the arms are maintained in a priority queue sorted by the lower confidence bounds of the arms. This gives us  $\log n$  overhead in the running time over the number of arm pulls.
2. In our current implementation we sample the arms without replacement for the sake of simplicity. However, we note that sampling without replacement would improve both the accuracy and the running time of UCB.
3. We have not taken cache management into consideration in our implementation. Thus the gains in complexity are not directly reflected in the gain in running times.

## C More examples in adaptive Monte Carlo optimization framework

**The medoid finding problem of Bagaria et al. (2018) :** The problem they considered was finding medoids. Given a set of  $n$  points in  $\mathbb{R}^d$ ,  $x_1, x_2, \dots, x_n$  the medoid is defined as the point with the smallest average distance from all other points in the ensemble (with respect to some distance). For simplicity of exposition we only present this in the context of  $\ell_1$  distance.<sup>5</sup>

$$\min_{i \in [n]} f(i) = \min_{i \in [n]} \frac{1}{n} \sum_{j=1}^n \sum_{k=1}^d |x_{i,k} - x_{j,k}|$$

Bagaria et al. (2018) assume that for any point  $i$ , the distances to all other points is  $\sigma$  sub-gaussian (where  $\sigma$  is an absolute constant) which allows them to get the estimator,

$$\hat{f}_\ell(i) = \frac{1}{\ell} \sum_{j=1}^{\ell} \sum_{k=1}^d |x_{i,k} - x_{t_j,k}|,$$

where  $t_j$  is uniformly sampled from  $[n] - \{i\}$  for  $j \in [\ell]$ . The sub-Gaussianity assumption gives that this estimators  $\hat{f}_\ell(i) \sim \mathcal{N}(f(i), \frac{\sigma^2}{\ell})$ . They pose the problem as a multi-armed bandit problem with each point  $i$  being an arm, and pulling an arm corresponding to updating the estimator, which can be done in constant time. They then run the UCB algorithm of Appendix A and report that this gives considerable computational savings.

**Monte-carlo tree search of Kocsis and Szepesvári (2006):** Here the authors aim to to carry out planning to decide the best possible policy at a state with respect to a finite horizon. The classical monte-carlo planning algorithms sample actions in each state and run the simulations for some fixed time and pick the action with best rewards. The authors propose treating each action as an arm and running a bandit at each state to decide on the best action.

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<sup>5</sup>We discuss how other distances fall in our framework in Appendix D.



**Hyper-parameter tuning of Jamieson and Talwalkar (2016) and Li et al. (2016) :** We note that the hyperparameter tuning example of Jamieson and Talwalkar (2016) and Li et al. (2016) can also be put into this framework with a twist. As discussed before, the authors are trying to find the hyperparameters with minimum validation error for a deep neural network. Each configuration of hyperparameters is an arm, and pulling an arm corresponds to running training for an epoch and measuring change in validation error. However, unlike our other examples, we it is not easy to come up with confidence intervals around the estimate, which makes the UCB algorithm untenable. However a successive elimination based algorithm like that of Even-Dar et al. (2006) can provide computational savings here, and Li et al. (2016) present an algorithm similar in flavour.

**Non-convex optimization :** We note that non-convex optimization algorithms, especially in alternating minimization based algorithms where one starts with different starting points and picks the one with the best objective can in general be put in such a framework, and one can use successive elimination to obtain computational savings. This falls into the framework of (Jamieson and Talwalkar, 2016; Li et al., 2016).

**Others:** Quickhull is a divide and conquer based method to compute convex hull of  $n$  points. The divide step of this algorithm involves first finds farthest points on each side of a hyperplane. One could improve the running time of this step by posing it in the framework of adaptive Monte Carlo optimization. Graph centrality measures such as betweenness centrality, closeness centrality can also be modeled in the adaptive Monte Carlo framework.

## D An extension: When we have a nice function of a good estimator

Consider a smooth function  $g : \mathbb{R} \rightarrow \mathbb{R}$ . We can generalise the adaptive Monte Carlo optimization framework of Eq. (1) to solve

$$\min_{i \in \mathcal{I}} g(f(i))$$

Let  $\hat{f}_l(i)$  be an estimator of  $f(i)$ . We use the delta method to approximate

$$\sqrt{n} \left( g(f(i)) - g(\hat{f}_l(i)) \right) \approx \sqrt{n} g'(\hat{f}_l(i)) (\hat{f}_l(i) - f(i)) \quad (4)$$

which gives us that,

$$\sqrt{n} \left( g(f(i)) - g(\hat{f}_l(i)) \right) \rightarrow \mathcal{N}(0, n g'(\hat{f}_l(i))^2 \text{Var}(\hat{f}_l(i))) \quad (5)$$

This allows us to construct confidence intervals around  $g$  using estimators of  $f$ . This allows us to extend the objective to additive functions composed with smooth functions.

If  $g$  is assumed to be uniformly continuous in the closure of the range of  $f$ , we have that  $|g'| \leq M$  for some known constant  $M$  (independent of  $n$ ). We further assume that  $|g''| \leq \kappa$  for some known constant  $\kappa$  (independent of  $n$ ).

For  $g(i)$ ,  $i \in \mathcal{I}$ , we define the sequence of estimators  $\{\hat{g}_l(i) | l \in \mathbb{N}\}$  where  $\hat{g}_l(i) := g(\hat{f}_l(i))$  and whose confidence intervals can be obtained using equation (5). We then use this in the adaptive Monte Carlo optimization framework to solve (4). We note that the estimators  $\hat{g}_l(i)$  are not necessarily unbiased and can have a bias of approximately  $\kappa \text{Var}(\hat{f}_n(x))$ . An example here would be to compute medoids on some distance like the  $\ell_2$  distance.

## E Details on $k$ -nearest neighbors

To recap the setting we note that for posing  $k$ -nearest neighbour graph construction in our framework, we run a multi-armed bandit with each arm being one of the remaining  $n - 1$  points.

We begin by noting that we measure the performance of algorithms in *effective number of distance evaluations*. We define effective number of distance evaluations between two points as the fraction of

co-ordinates involved in estimating the distance between these two points. The effective number of distance evaluations of an algorithm is the sum of effective number of distance evaluations between every pair of points in the algorithm. We define the number of *coordinate-wise distance evaluations* of an algorithm to be  $d$  times the effective number of distance evaluations of the algorithm.

Without loss of generality, we assume that we are finding the  $k$  nearest neighbors of point 1. In this case we have  $n - 1$  arms, one corresponding to each of points  $2, \dots, n$ . Further the mean of each arm can be evaluated exactly in a maximum of  $d$  pulls.

Let  $f(i)$  be used to denote the distance between point 1 and point  $i$ .

The expectation of each pull of arm  $i$  is the distance between point  $i$  and point 1. The estimator after  $\ell$  pulls of arm  $i$  is given by

$$\hat{f}_\ell(i) = \frac{1}{\ell} \sum_{j=1}^{\ell} (x_{1,t_j} - x_{i,t_j})^2, \quad (6)$$

where  $t_j$  are sampled from  $[d]$  with replacement for  $j \in [\ell]$ . The update of the estimator at step  $\ell + 1$  is

$$\hat{f}_{\ell+1}(i) = \frac{1}{\ell+1} \left( \ell \hat{f}_\ell(i) + (x_{1,t_{\ell+1}} - x_{i,t_{\ell+1}})^2 \right), \quad (7)$$

We assume that the estimators are  $\sigma$ -subgaussian, for some  $\sigma$  independent of  $n$ . In practice, we estimate  $\sigma$  from few initial samples and update it after every pull. We construct the  $1 - \delta$  confidence intervals of  $\hat{f}_\ell(i)$  as,

$$C(\ell) = \begin{cases} \sqrt{\frac{2\sigma^2 \log \frac{2}{\delta}}{\ell}} & \text{if } \ell \leq d, \\ 0 & \text{if } \ell > d, \end{cases} \quad (8)$$

$$f(i) \in \left[ \hat{f}_\ell(i) - C(\ell), \hat{f}_\ell(i) + C(\ell) \right], \text{ w.p. } 1 - \delta. \quad (9)$$

We assume that the estimate of  $\sigma$  is the true value. Further we set  $\delta = \frac{2}{n^3 d}$ . Then we have that,

**Lemma E.1.** *With probability  $1 - \frac{1}{n^2}$ , each one of our true values lies in their confidence intervals during the run of the algorithm.*

Let  $i_k^*$  be the  $k$ -th nearest neighbors of point 1, and define

$$\Delta_i = \max(0, f(i) - f(i_k^*))$$

Using this lemma, we now state the following theorem,

**Theorem E.2** (Restating Theorem 2.1). *With probability  $1 - \frac{1}{n^2}$ , Algorithm 1 returns the  $k$ -nearest neighbors of point 1 with at most*

$$M \leq \sum_{i=2}^n \left( \left( \frac{24\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2d \right) \quad (10)$$

*distance evaluations. This takes*

$$O \left( \sum_{i=2}^n \log(n) \left( \left( \frac{\sigma^2 \log(nd)}{\Delta_i^2} \right) \wedge d \right) \right) \quad (11)$$

*time.*

*Proof.* Let  $\ell_i(t)$ , be the number of times, arm  $i$  is pulled till iteration  $t$ .

Let  $i_1^*, i_2^*, \dots, i_k^*$  be the  $k$  one nearest neighbors of point 1 in order. For simplicity of notation, let us define

$$\begin{aligned} \hat{\mu}_i(t) &= \hat{f}_{\ell_i(t)}(i), \\ C_i(t) &= C(\ell_i(t)), \\ \Delta_i^{(w)} &= \max(0, f(i) - f(i_w^*)) \end{aligned}$$

In words,  $\hat{\mu}_i(t)$  is simply the estimate of the mean of arm  $i$  at the  $t$ -th iteration of the algorithm, and  $2C_i(t)$  is the width of the  $(1 - \delta)$  confidence interval of arm  $i$  at iteration  $t$  of the algorithm. For any point  $i$  which is not the  $k$  nearest neighbors,  $\Delta_i^{(w)}$  is the difference in distance of point  $i$  to point 1 and the  $w$ -th nearest neighbour. Also clearly from this definition,  $\Delta_i^{(1)} \geq \Delta_i^{(2)} \geq \dots \geq \Delta_i^{(k)}$ . Further  $\Delta_i^{(k)} = \Delta_i$  defined above.

Let us first analyse the running of the algorithm till it found the first nearest neighbour of point 1 to start with.

We observe that if we choose to update arm  $i \neq i_1^*$  at time  $t$ , then we have

$$\hat{\mu}_i(t) - C_i(t) \leq \hat{\mu}_{i_1^*}(t) - C_{i_1^*}(t).$$

For this to occur, at least one of the following three events must occur:

$$\begin{aligned} \mathcal{E}_1 &= \{\hat{\mu}_{i_1^*}(t) \geq \mu_{i_1^*}(t) + C_{i_1^*}(t)\}, \\ \mathcal{E}_2 &= \{\hat{\mu}_i(t) \leq \mu_i(t) - C_i(t)\}, \\ \mathcal{E}_3 &= \{\Delta_i^{(1)} = \mu_i - \mu_{i_1^*} \leq 2C_i(t)\}. \end{aligned}$$

To see this, note that if none of  $\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3$  occur, we have

$$\hat{\mu}_i(t) - C_i(t) \stackrel{(a)}{>} \mu_i - 2C_i(t) \stackrel{(b)}{>} \mu_{i_1^*} \stackrel{(c)}{>} \hat{\mu}_{i_1^*} - C_{i_1^*}(t),$$

where (a), (b), and (c) follow because  $\mathcal{E}_2, \mathcal{E}_3$ , and  $\mathcal{E}_1$  do not hold respectively.

We note that as we compute  $(1 - \frac{2}{n^{3d}})$ -confidence intervals at most  $d$  times for each point. Thus we have at most  $n^2 d$  computations of  $(1 - \frac{2}{n^{3d}})$ -confidence intervals in total.

Thus  $\mathcal{E}_1$  and  $\mathcal{E}_2$  do not occur during any iteration with probability  $1 - \frac{2}{n^2}$ , because

$$\text{w.p.} \left(1 - \frac{2}{n^2}\right) : |f(i) - \hat{\mu}_i(t)| \leq C_i(t), \forall i \in [n], \forall t. \quad (12)$$

This also implies that with probability  $1 - \Theta(\frac{1}{n^2})$  the algorithm does not stop unless the event  $\mathcal{E}_3$ , a deterministic condition, stops occurring.

Let  $\zeta_i^{(1)}$  be the iteration of the algorithm when it evaluates a distance to point  $i$  for the last time before declaring the 1-nearest neighbour. From the previous discussion, we have that the algorithm stops evaluating distances to points  $i$  when the following holds.

$$\begin{aligned} C_i(\zeta_i^{(1)}) \leq \frac{\Delta_i^{(1)}}{2} &\implies \frac{\Delta_i^{(1)}}{2} \geq \sqrt{\frac{2\sigma^2 \log n^3 d}{T_i(\zeta_i^{(1)})}} \text{ or } C_i(\zeta_i^{(1)}) = 0, \\ \implies T_i(\zeta_i^{(1)}) &\geq \frac{8\sigma^2}{(\Delta_i^{(1)})^2} \log(n^3 d) \text{ or } T_i(\zeta_i^{(1)}) \geq 2d. \end{aligned}$$

We note that the above is true for  $i_1^*$  as well as we have at most  $2d$  distance evaluations there.

As the bandit algorithm progresses, let us similarly define,  $\zeta_i^{(w)}$  be the iteration of the algorithm when it evaluates a distance to point  $i$  for the last time before declaring the  $w$ -th-nearest neighbour. By the same computation as above, we have that,

$$T_i(\zeta_i^{(w)}) \geq \frac{8\sigma^2}{(\Delta_i^{(w)})^2} \log(n^3 d) \text{ or } T_i(\zeta_i^{(w)}) \geq 2d.$$

We further note that the total number of distance computations is

$$\begin{aligned}
M &= \sum_{i=2}^n T_i(\zeta_i^{(k)}), \\
&\leq \sum_{i=2}^n \left( \left( \frac{8\sigma^2}{(\Delta_i^{(k)})^2} \log(n^3 d) \right) \wedge 2d \right), \\
&\stackrel{(d)}{=} \sum_{i=2}^n \left( \left( \frac{8\sigma^2}{\Delta_i^2} \log(n^3 d) \right) \wedge 2d \right), \\
&\leq \sum_{i=2}^n \left( \left( \frac{24\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2d \right),
\end{aligned}$$

where (d) follows from the definition of  $\Delta_i$ .

Thus with probability  $(1 - \Theta(\frac{1}{n^2}))$ , the algorithm returns  $i^*$  as the medoid with at most  $M$  distance evaluations, where

$$M \leq \sum_{i=2}^n T_i(\zeta_i) \leq \sum_{i=2}^n \left( \left( \frac{24\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2d \right).$$

giving us the claim in Eq. (10).

We note that each step of the multi-armed bandit can be implemented in  $O(\log n)$  time using a priority queue giving us the result of (17)  $\square$

**Theorem E.3.** *If we further assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , for some  $\gamma$ , and  $d = cn$ , for  $c \in [0, 1]$ , then we have that the expected number of co-ordinate wise distance evaluations (over randomness in  $\Delta_i$ ),*

$$\mathbb{E}[M] \leq O(n \log(nd) + kd).$$

*with probability  $1 - \Theta(\frac{1}{n^2})$  over randomness in the algorithm.*

*This gives us that the entire  $k$ -nearest neighbors takes  $O(n^2 \log(nd) + nkd)$  in expectation over randomness in the  $\Delta_i$  co-ordinate wise distance evaluations with probability  $1 - \Theta(\frac{1}{n^2})$  over randomness in the algorithm.*

*Proof.* This follows directly from the Appendix A of Bagaria, Kamath, Ntranos, Zhang, and Tse (2018)  $\square$

If instead one is just interested in approximating the  $k$  nearest neighbors of a point, then one can use a slightly modified version of the UCB algorithm of Algorithm 2. By approximating  $k$  nearest neighbors, we mean picking points that are within a distance  $\epsilon$  additively of the  $k$ -nearest neighbors of point  $i$ . We can do this by modifying line 10 of Algorithm 2 to stop if the width of the confidence interval of the best arm is of width less than  $\epsilon$  times its UCB.

As before let  $i_1^*, \dots, i_k^*$  be the  $k$  nearest neighbors of point 1, and let their distances be  $f(i_w^*) = \mu_{i_w^*}$  for  $w \in \{1, \dots, k\}$ . Also let  $\Delta_i$  be as before.

In this case with the assumptions as above, we have the following result

**Theorem E.4** (Restatement of Theorem 2.2). *With probability  $1 - \frac{1}{n^2}$  finds the  $k$ -nearest neighbor of point 1 upto a  $(1 + \epsilon)$ -approximation with at most*

$$M \leq \sum_{i=2}^n \left( \frac{24\sigma^2}{(\max(\Delta_i, \epsilon\mu_{i_k^*}))^2} \log(nd) \right) = \sum_{i=2}^n \left( \left( \frac{\sigma}{\mu_{i_k^*}} \right)^2 \frac{24}{\max\left(\left(\frac{\Delta_i}{\mu_{i_k^*}}\right)^2, \epsilon^2\right)} \log(nd) \right) \quad (13)$$

*co-ordinate wise distance computations with a running time of*

$$O\left(\sum_{i=2}^n \log(n) \left( \frac{\sigma^2 \log(nd)}{(\max(\Delta_i, \epsilon\mu_{i_k^*}))^2} \right)\right) \quad (14)$$

*Proof.* Let  $\ell_i(t)$ , be the number of times, arm  $i$  is pulled till iteration  $i$ .

Let  $i_1^*, i_2^*, \dots, i_k^*$  be the  $k$  one nearest neighbors of point 1 in order. For simplicity of notation, let us define

$$\begin{aligned}\hat{\mu}_i(t) &= \hat{f}_{\ell_i(t)}(i), \\ C_i(t) &= C(\ell_i(t)), \\ \Delta_i^{(w)} &= \max(0, f(i) - f(i_w^*))\end{aligned}$$

In words,  $\hat{\mu}_i(t)$  is simply the estimate of the mean of arm  $i$  at the  $t$ -th iteration of the algorithm, and  $2C_i(t)$  is the width of the  $(1 - \delta)$  confidence interval of arm  $i$  at iteration  $t$  of the algorithm. For any point  $i$  which is not the  $k$  nearest neighbors,  $\Delta_i^{(w)}$  is the difference in distance of point  $i$  to point 1 and the  $w$ -th nearest neighbour. Also clearly from this definition,  $\Delta_i^{(1)} \geq \Delta_i^{(2)} \geq \dots \geq \Delta_i^{(k)}$ . Further  $\Delta_i^{(k)} = \Delta_i$  defined above.

Let us first analyse the running of the algorithm till it found the first nearest neighbour of point 1 to start with.

Define

$$\begin{aligned}J_\epsilon^{(1)} &= \{i \in \{2, \dots, n\} \mid \Delta_i^{(1)} \leq f(i_1^*)\epsilon\}, \\ K_\epsilon^{(1)} &= \{2, \dots, n\} - J_\epsilon^{(1)},\end{aligned}$$

In words, we have that  $J_\epsilon^{(1)}$  are the points whose distance from point 1 is less than  $(1 + \epsilon)$  times the distance of the nearest neighbour. Thus returning any one of these points satisfies our approximation requirements.  $K_\epsilon^{(1)}$  is other points.

We observe that if we choose to update arm  $i \in K_\epsilon^{(1)}$  at time  $t$ , then we have

$$\hat{\mu}_i(t) - C_i(t) \leq \hat{\mu}_{i_1^*}(t) - C_{i_1^*}(t).$$

For this to occur, at least one of the following three events must occur:

$$\begin{aligned}\mathcal{E}_1 &= \{\hat{\mu}_{i_1^*}(t) \geq \mu_{i_1^*}(t) + C_{i_1^*}(t)\}, \\ \mathcal{E}_2 &= \{\hat{\mu}_i(t) \leq \mu_i(t) - C_i(t)\}, \\ \mathcal{E}_3 &= \{\Delta_i^{(1)} = \mu_i - \mu_{i_1^*} \leq 2C_i(t)\}.\end{aligned}$$

To see this, note that if none of  $\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3$  occur, we have

$$\hat{\mu}_i(t) - C_i(t) \stackrel{(a)}{>} \mu_i - 2C_i(t) \stackrel{(b)}{>} \mu_{i_1^*} \stackrel{(c)}{>} \hat{\mu}_{i_1^*} - C_{i_1^*}(t),$$

where (a), (b), and (c) follow because  $\mathcal{E}_2, \mathcal{E}_3$ , and  $\mathcal{E}_1$  do not hold respectively.

We note that as we compute  $(1 - \frac{2}{n^{3d}})$ -confidence intervals at most  $d$  times for each point. Thus we have at most  $n^2 d$  computations of  $(1 - \frac{2}{n^{3d}})$ -confidence intervals in total.

Thus  $\mathcal{E}_1$  and  $\mathcal{E}_2$  do not occur during any iteration with probability  $1 - \frac{2}{n^2}$ , because

$$\text{w.p. } \left(1 - \frac{2}{n^2}\right) : |f(i) - \hat{\mu}_i(t)| \leq C_i(t), \forall i \in [n], \forall t. \quad (15)$$

This also implies that with probability  $1 - \Theta(\frac{1}{n^2})$  the algorithm does not stop unless the event  $\mathcal{E}_3$ , a deterministic condition stops occurring.

Let  $\zeta_i^{(1)}$  be the iteration of the algorithm when it evaluates a distance to point  $i$  for the last time before declaring the 1-nearest neighbour. From the previous discussion, for arms in  $J_\epsilon^{(1)}$  we have that the

algorithm stops evaluating distances to points  $i$  when the following holds.

$$\begin{aligned} C_i(\zeta_i^{(1)}) &\leq \frac{\Delta_i^{(1)}}{2} \\ \implies \frac{\Delta_i^{(1)}}{2} &\geq \sqrt{\frac{2\sigma^2 \log n^3}{T_i(\zeta_i^{(1)})}} \\ \implies T_i(\zeta_i^{(1)}) &\geq \frac{8\sigma^2}{(\Delta_i^{(1)})^2} \log(n^3 d), \end{aligned}$$

where we use the fact that  $\Delta_i^{(1)} \geq \epsilon f(i_1^*)$ .

Further note that if none of  $\mathcal{E}_1, \mathcal{E}_2, \mathcal{E}_3$ , occur than no arm in  $K_\epsilon^{(1)}$  would be pulled when the width of their confidence interval is less than  $\epsilon f(i_1^*)$ . To see this, note that,

$$\epsilon(\mu_i + C_i(t)) > \epsilon f(i_1^*) \stackrel{(d)}{>} \Delta_i^{(1)} \stackrel{(e)}{>} 2C_i(t) = \text{Width of confidence interval},$$

where (d) follows from the fact that  $i \in K_\epsilon^{(1)}$  and (e) follows from the fact that  $\mathcal{E}_3$  does not occur.

Thus we exit only when one of the arms in  $K_\epsilon^{(1)}$  is pulled and each of them is pulled. Thus for each of the arms in  $K_\epsilon^{(1)}$  the following holds:

$$\begin{aligned} C_i(\zeta_i^{(1)}) &\leq \frac{\epsilon \mu_{i_1^*}}{2} \\ \implies \frac{\epsilon \mu_{i_1^*}}{2} &\geq \sqrt{\frac{2\sigma^2 \log n^3}{T_i(\zeta_i^{(1)})}} \\ \implies T_i(\zeta_i^{(1)}) &\geq \frac{8\sigma^2}{(\epsilon \mu_{i_1^*})^2} \log(n^3 d). \end{aligned}$$

Thus we can using the definition of  $K_\epsilon^{(1)}$  and  $K_\epsilon^{(1)}$ , we can write this more succinctly as

$$T_i(\zeta_i^{(1)}) \geq \frac{8\sigma^2}{\left(\max(\Delta_i^{(1)}, \epsilon \mu_{i_1^*})\right)^2} \log(n^3 d).$$

As the bandit algorithm progresses, let us similarly define,  $\zeta_i^{(w)}$  be the iteration of the algorithm when it evaluates a distance to point  $i$  for the last time before declaring the  $w$ -th-nearest neighbour. By the same computation as above, we have that,

$$T_i(\zeta_i^{(w)}) \geq \frac{8\sigma^2}{\left(\max(\Delta_i^{(w)}, \epsilon \mu_{i_w^*})\right)^2} \log(n^3 d).$$

We further note using the fact that  $T_i(\zeta_i^{(w)})$  are increasing as function of  $w$ , that the total number of distance computations is

$$\begin{aligned} M &= \sum_{i=2}^n T_i(\zeta_i^{(k)}), \\ &\leq \sum_{i=2}^n \left( \frac{8\sigma^2}{\left(\max(\Delta_i^{(k)}, \epsilon \mu_{i_k^*})\right)^2} \log(n^3 d) \right), \\ &\stackrel{(d)}{=} \sum_{i=2}^n \left( \frac{8\sigma^2}{\left(\max(\Delta_i, \epsilon \mu_{i_k^*})\right)^2} \log(n^3 d) \right), \\ &\leq \sum_{i=2}^n \left( \frac{24\sigma^2}{\left(\max(\Delta_i, \epsilon \mu_{i_k^*})\right)^2} \log(nd) \right), \end{aligned}$$

where (d) follows from the definition of  $\Delta_i$ .

We note that each step of the multi-armed bandit can be implemented in  $O(\log n)$  time using a priority queue giving us the result of (14).  $\square$

**Theorem E.5.** *If we assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , then the expected number of distance evaluations (over randomness in  $\Delta_i$ ) is*

$$\mathbb{E}[M] \leq O\left(\frac{n \log nd}{\epsilon}\right)$$

with probability  $1 - \Theta(\frac{1}{n^2})$  over randomness in the algorithm.

This gives us that the entire  $k$ -nearest neighbors takes  $O(\frac{n^2 \log(nd)}{\epsilon})$  in expectation over randomness in the  $\Delta_i$  co-ordinate wise distance evaluations with probability  $1 - \Theta(\frac{1}{n})$  over randomness in the algorithm.

*Sketch of proof.* For Gaussian  $\Delta_i$ , the

$$\min_i \gamma - \Delta_i \rightarrow \sqrt{2 \log n}.$$

Thus the fraction of points in within  $(1 + \epsilon)$  of the minimum is at most  $e^{-1-\epsilon}$ . Thus the work done for these points is  $O(\frac{1}{\epsilon})$ . Similarly, one can handle the rest of the points as well.  $\square$

*Proof of Lemma E.1.* Let  $\ell_i(t)$ , be the number of times, arm  $i$  is pulled till iteration  $i$ .

We first show that  $[\hat{f}_i(\ell_i(t)) - C(\ell_i(t)), \hat{f}_i(\ell_i(t)) + C(\ell_i(t))]$  are true  $(1 - \frac{2}{n^3 d})$ -confidence intervals of  $f(i)$  at every iteration  $t$ .

We observe that if point  $i$  is picked by less than  $d$  times at time  $t$ , then  $\ell_i(t)$  is equal to the number of times the point is picked. Further  $C_i(t)$  is the true  $(1 - \delta)$ -confidence interval from the assumption of  $\sigma$ -sub-gaussianity on the estimators.

However, if point  $i$  is picked for the  $n$ -th time at iteration  $t$  ( line 8 of Algorithm 2) then the empirical mean is computed by evaluating the distance exactly with  $d$  co-ordinate wise distance computations. As we know the mean distance of point  $i$  exactly,  $C_i(t) = 0$  is still the true confidence interval.

As throughout the algorithm we can compute at most  $n^2 d$  confidence intervals of length  $1 - \frac{1}{n^3 d}$ , with probability  $1 - \frac{1}{n^2}$ , the true value is always in the computed confidence intervals.  $\square$

## F Details on $k$ -means

Here we have  $k$  centroids. We consider the number of co-ordinate wise distance evaluated to compute the nearest of the  $k$  centroids to the first of  $n$  points of a data-set. Let  $i^*$  be the centroid closet to point 1 and for  $i \in \{1, 2, \dots, k\}$ , let  $\Delta_i$  be the difference between the distance between centroid  $i$  and the centroid  $i^*$ . However, we use  $\delta = 1 - \frac{1}{n^3 d}$  here.

Theorem 2.1 directly gives us that:

**Corollary F.1.** *With probability  $1 - \Theta(\frac{1}{n^2})$ , this algorithm find the closests of  $k$  centroids of point 1 is with at most*

$$M \leq \sum_{i=1; i \neq i^*}^k \left( \left( \frac{48\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2d \right)$$

co-ordinate wise distance evaluations. The running time is

$$\log(k) \sum_{i=1; i \neq i^*}^k \left( \left( \frac{48\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2d \right)$$

If we again assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , then we have from a direct consequence of Theorem E.3

**Corollary F.2.** *If we assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , for some  $\gamma$ ,  $d = O(n)$  and  $k$  is a constant, then we have that the expected number of co-ordinate wise distance evaluations (over randomness in  $\Delta_i$ ) over all points,*

$$\mathbb{E}[M] \leq O(nk \log(nd)).$$

*with high probability over randomness in the algorithm.*

The proof is trivial since  $\delta_i$ 's are  $O(1)$  quantities. We now consider the  $(1 + \epsilon)$  approximation algorithm as before. The definition of the approximation is the same of before, with  $\mu^*$  is the distance between point 1 and it's nearest centroid.

**Corollary F.3.** *The number of co-ordinate wise distance evaluations to find the nearest centroid of point 1 upto a  $(1 + \epsilon)$ -approximation is at most*

$$M \leq \sum_{i=1}^k \left( \frac{24\sigma^2}{(\max(\Delta_i, \epsilon\mu^*))^2} \log(nd) \right) = \sum_{i=1}^k \left( \left( \frac{\sigma}{\mu^*} \right)^2 \frac{24}{\max \left( \left( \frac{\Delta_i}{\mu^*} \right)^2, \epsilon^2 \right)} \log(nd) \right)$$

If we again assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , then we have from a direct consequence of Theorem E.5

**Corollary F.4.** *If we assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , then the expected number of distance evaluations (over randomness in  $\Delta_i$ ) is*

$$\mathbb{E}[M] \leq O \left( \frac{k \log kd}{\epsilon} \right)$$

*with probability  $1 - \Theta(\frac{1}{k^2})$  over randomness in the algorithm.*

## G Details of Hierarchical Clustering

In the main text, we have explained hierarchical clustering briefly. Here we elaborate on it. Hierarchical clustering is an algorithm that is widely used in data analysis (Leskovec et al., 2014, Chapter 7; Hastie et al., 2009, Chapter 14). This is especially popular if the number of clusters is not known apriori. In general one assumes a set of  $n$  points and a distance/similarity measure to be the input to an algorithm doing hierarchical clustering. The output of the algorithm is usually a dendrogram (or a binary tree) with  $n$  leaves.

One approach to do this are *agglomerative algorithms* which combines points in a bottom up manner. Such algorithms start of with the  $n$  points each being a cluster of one point. At every step, the algorithm merges the two “closest” clusters to form one cluster. It keeps doing this till there is only one cluster left. This has a natural binary tree representation where the leaves are the  $n$  points, the root is the cluster of all points, and all intermediate vertices are clusters formed at intermediate steps. The two children of any vertex in the tree are the clusters that were merged to form the that cluster.

For two clusters which consist of only one point, the notion of closeness is unambiguously defined by the distance metric. For clusters with more than one point, the distance between clusters can be defined in a variety of ways. Three popular ways (Murtagh and Contreras, 2012; Moseley and Wang, 2017) are

1. Average linkage: which is the average distance between points in the two clusters.
2. Single linkage: where the distance between two clusters is the minimum of the pairwise distances between points in the two clusters.
3. Complete linkage: where the distance between two clusters is defined as the pairwise distances between points in the two clusters.

We mention that there is another class of algorithms to do hierarchical clustering called divisive algorithms which take a top down approach of starting from one cluster and dividing it up to get better clusters.

In the sequel we will be considering an average linkage based agglomerate algorithm to do hierarchical clustering. At every step, instead of computing pairwise distances between every pair of clusters



(present in that step) and picking the pair with the smallest pairwise distance, we pose it in the framework of adaptive Monte Carlo optimization problem. In this formulation, pairs of clusters are considered as arms, and an arm pull being one randomly picked co-ordinate-wise evaluation of distances between two randomly picked points one in each cluster.

We now introduce some notation. Let  $x_1, x_2, \dots, x_n$  be  $n$  points in  $\mathbb{R}^d$  that we want to cluster. We define a *cluster* to be a set of points that have been merged by the algorithm. At the start of the algorithm, each cluster is a singleton point and is indexed by a singleton set corresponding to the point in the cluster. Let  $\mathcal{C}_t$  be the set of clusters in the system at time  $t$ . At the  $t$ -th step of the algorithm, we have done  $t - 1$  merges and thus have  $n - t + 1$  clusters in the system. Hence  $|\mathcal{C}_t| = n - t + 1$ . Further, note that at any step  $t$  in the algorithm, the union of the clusters  $\mathcal{C}_t$  gives us  $[n]$  because each of the points is contained in exactly one of the cluster.

We denote each arm in the system by an unordered pair of clusters. We denote  $A(C, C')$  to be the arm of clusters  $C$  and  $C'$ . Let  $\mathcal{A}_t$  be the set of arms in the system at time  $t$ . Thus,  $\mathcal{A}_t = \{A(C, C') \mid C, C' \in \mathcal{C}_t, C \neq C'\}$ . Clearly we have that  $|\mathcal{A}_t| = \binom{|\mathcal{C}_t|}{2}$ . The algorithm used is shown in 3 (We overload notation in UCB to allow MAX\_PULLS to be different for each arm and is equal to the dimension multiplied with the product of the cluster size of each arm).

---

**Algorithm 3** Dynamic-UCB

---

- 1: Points  $x_1, \dots, x_n$  are input to the algorithm. Each point is a cluster.
  - 2: Create arms for every pair of points. Let the arms in the system now be  $\mathcal{A}_1$
  - 3: Initialise estimates for points
  - 4: **for**  $t$  in  $1 : n - 2$  **do**
  - 5:     Run UCB( $\mathcal{A}_t, d_t, 1$ ). Pick the winning Arm  $A^*(C_t, C'_t)$ .  $\triangleright d_t$  is the total set of co-ordinates.
  - 6:     Delete arms contain at least one of  $C_t$  and  $C'_t$  from the the system.
  - 7:     Merge the  $C_t, C'_t$  to form a new cluster.
  - 8:     Add arms corresponding to the newly formed  $C_t \cup C'_t$  and the other clusters in the system.
  - 9:     Initialise these new arms.
  - 10:     $\mathcal{A}_{t+1}$  are the new arms in the system.
  - 11: **end for**
- 

In this notation, we have that at the beginning of the algorithm,

$$\mathcal{C}_1 = \{\{1\}, \{2\}, \dots, \{n\}\},$$

$$\mathcal{A}_1 = \{A(\{i\}, \{j\}) \mid 1 \leq i < j \leq n\}.$$

Let  $A^*(C_t, C'_t)$  be the arm that wins the MAB contest at time  $t$ . Thus the clusters that are removed from the system at time  $t$  are  $C_t$  and  $C'_t$  and the new cluster added is  $\tilde{C}_{t+1} = C_t \cup C'_t$ . In other words,

$$\mathcal{C}_{t+1} = (\mathcal{C}_t - \{C_t, C'_t\}) \cup \{\tilde{C}_{t+1}\}.$$

Thus at time  $t + 1$  the system contains arms for all unordered pairs of clusters in  $\mathcal{C}_{t+1}$ . However we note that  $\mathcal{C}_{t+1}$  contains all but two clusters in  $\mathcal{C}_t$  and contains only one cluster not in  $\mathcal{C}_t$ . Thus most of the arms in the system at time  $t$  are also in the system at time  $t + 1$  and hence a lot of computation is carried over from time  $t$ .

The arms deleted from the system after time  $t$  are of the form  $A(C_t, C)$  and  $A(C_t, C')$  for  $C \in \mathcal{C}_t - \{C_t, C'_t\}$ . Therefore,

$$\mathcal{D}_t = \{A(C_t, C'_t)\} \cup \{A(C, C') \mid C \in \{C_t, C'_t\}, C' \in \mathcal{C}_t - \{C_t, C'_t\}\},$$

$$\implies |\mathcal{D}_t| = 1 + 2(n - t - 1) = 2(n - t) - 1.$$

The arms added to the system before time  $t + 1$  are of the form  $A(\tilde{C}_{t+1}, C)$  for  $C \in \mathcal{C}_t - \{C_t, C'_t\}$ . Thus we have that the arms at time  $t + 1$  is given by,

$$\mathcal{A}_{t+1} = (\mathcal{A}_t - \mathcal{D}_t) \cup \mathcal{N}_{t+1},$$

where  $\mathcal{D}_t$  is the set of arms deleted after time  $t$  and  $\mathcal{N}_{t+1}$  is the set of arms that are added before time  $t + 1$ . Therefore

$$\mathcal{N}_t = \{A(\tilde{C}_t, C) \mid C \in \mathcal{C}_t - \{C_t, C'_t\}\},$$

$$\implies |\mathcal{N}_t| = n - t - 1.$$

Thus the total number of unique arms in the system at all times is  $M$

$$\begin{aligned} M &= \binom{n}{2} + \sum_{i=1}^{n-2} n - i - 1, \\ &= \binom{n}{2} + \binom{n-1}{2}, \\ &< n^2. \end{aligned}$$

To reiterate, an arm  $A^*(C_t, C'_t)$  is killed at step  $t$  of the algorithm if either  $A^*(C_t, C'_t)$  is the winner of the MAB at step  $t$  or the winning arm is of the form  $A^*(C_t, D)$  or  $A^*(C'_t, D)$  for some other cluster  $D$  which is in the system at time  $t$ .

Let the winning mean at step  $t$  be  $\mu_t^*$ .

**Lemma G.1.**  $\mu_1^* \leq \mu_2^* \leq \dots \leq \mu_{n-3}^* \leq \mu_{n-2}^*$

*Proof.* We first claim that the true means each of the arms added before step  $t$  is at least as large as one of the arms deleted after step  $t - 1$ . Once we show this, the proof is immediate as all arms in the system at time  $t - 1$  had their means to be at least  $\mu_{t-1}^*$ , and the new arms added have their true means to be at least  $\mu_{t-1}^*$ . So all the arms in the system at time  $t$  have their true means to be at least  $\mu_{t-1}^*$  giving us that the mean of the winning arm at time  $t$ ,  $\mu_t^*$  is at least  $\mu_{t-1}^*$ , that is  $\mu_t^* \geq \mu_{t-1}^*$  proving the result.

To see the claim, let  $A^*(C_t, C'_t)$  be the arm that won the MAB at time  $t - 1$ . For any cluster  $D$  (which is not  $C$  and  $C'$ ), we delete arms  $A^*(C_t, D)$  and  $A(C'_t, D)$  and add arm  $A(C_t \cup C'_t, D)$ . We note that as we are in the average linkage paradigm, the true mean of  $A(C_t \cup C'_t, D)$ ,  $\mu_{A(C_t \cup C'_t, D)}$  is a convex combination of the true means of  $A(C_t, D)$  and  $A(C'_t, D)$ . More concretely,

$$\begin{aligned} \mu_{A(C \cup C', D)} &= \frac{|C|}{|C| + |C'|} \mu_{A(C, D)} + \frac{|C'|}{|C| + |C'|} \mu_{A(C', D)}, \\ &\geq \min(\mu_{A(C, D)}, \mu_{A(C', D)}), \end{aligned}$$

where we have used the fact that as  $C$  and  $C'$  are two clusters in the system at the same time they are disjoint. This proves the claim and thus gives us the lemma.  $\square$

Let  $\tau(A(C, C'))$  denote the time at which arm  $A(C, C')$  goes out of the system. This can happen either because the arm wins that round of MAB or some arm containing one of cluster  $C$  or  $C'$  wins.

We note that if arm  $A(C, C')$  is introduced before step  $t_1$ , then following our previous analysis, the number of distance evaluations at step  $t_1$  is

$$\min \left( \frac{24\sigma^2 \log(nd)}{(\mu_{A(C, C')} - \mu_{t_1}^*)^2}, d|C||C'| \right)$$

The number of additional co-ordinate wise distance evaluations at time  $t_1 + 1$  (if  $A(C, C')$  is not delete after time  $t_1$ ) is then

$$\left[ \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{t_1+1}^*)^2}, d|C||C'| \right) - \min \left( \frac{24\sigma^2 \log n}{(\mu_{A(C, C')} - \mu_{t_1}^*)^2}, d|C||C'| \right) \right]$$

where Lemma G.1 gives us that the quantity above is non-negative.

This gives us that the total number of distance evaluations at time  $\tau(A(C, C'))$ , continuing in this manner is thus

$$\begin{aligned} n(A(C, C')) &= \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{t_1}^*)^2}, d|C||C'| \right) \\ &\quad + \sum_{i=t_1+1}^{\tau(A(C, C'))} \left[ \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{t_i+1}^*)^2}, d|C||C'| \right) - \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{t_i}^*)^2}, d|C||C'| \right) \right], \\ &= \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{\tau(A(C, C'))}^*)^2}, d|C||C'| \right), \end{aligned}$$

We note that following all our previous analysis we have that if the number of distance evaluations on  $A(C, C')$  is at most

$$\min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_{\tau(A(C, C'))}^*)^2}, d|C||C'| \right),$$

If  $\mu_{A(C, C')} - \mu_{\tau(A(C, C'))}^*$  can be thought of as constants independent of  $n$ , then this gives us that the algorithm needs  $O(n^2 \log n)$  co-ordinate wise distance computations.

More generally at step  $t$ , if  $A(C_t, C'_t)$  is the winning arm, then the number of evaluations in arms discarded at step  $t$  apart from the winners is given by

$$\sum_{A(C, C') \in \mathcal{D}_t - A(C_t, C'_t)} \min \left( \frac{24\sigma^2 \log nd}{(\mu_{A(C, C')} - \mu_t^*)^2}, d|C||C'| \right)$$

If we assume that  $\mu_{A(C, C')} \sim \mathcal{N}(\mu, 1)$  then this is  $O(n \log n)$  at each step. This gives us that the total number of distance evaluations on non-winning arms is  $O(n^2 \log nd)$ . We further note that the total number of distance evaluations is also at most the twice the number distance evaluations spent on the non-winning arms because the cost of the winning and the second best arms are the same. This gives us that we have  $O(n^2 \log nd)$  co-ordinate wise distance evaluations.

While the above model is not a very compelling model of our problem, it does give us some intuition as to why the algorithm is observed to run with  $O(n^2 \log nd)$  co-ordinate wise distance evaluations.

**Remark 4.** We note that if we reuse the distances evaluated in the deleted arms which are not winners, all distances evaluated end up being used in distinguishing one of the winners or a second best arm. This intuitively tells us that we are not wasting distance evaluations.

## H Details on Maximum Mutual Information based feature selection

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### Algorithm 4 MMI UCB

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- 1:  $d$  features with  $n$  samples:  $x_1, \dots, x_d$  are and a response  $y$  input to the algorithm.
  - 2: Consider arms  $\mathcal{A}_\ell, 1 \leq \ell \neq i \leq n$  with estimators defined as in Eq. (??).
  - 3: The most relevant feature to the response is given by  $\text{UCB}(\{\mathcal{A}_\ell, 1 \leq \ell \neq i \leq n\}, n, 1)$ , using maximum instead of minimum.  $\triangleright \text{MAX\_PULLS} = d$
- 

Let  $i^*$  be the feature whose mutual information with the target is the largest. Define

$$\Delta_i = f(i^*) - f(i),$$

where  $f(i)$  is the empirical estimate of the mutual information of the feature  $i$  with the target.

**Theorem H.1.** With probability  $1 - \frac{1}{d^2}$ , Algorithm 4 returns the feature of maximum mutual information of point 1 with at most

$$M \leq \sum_{i=2}^n \left( \left( \frac{24\sigma^2}{\Delta_i^2} \log(nd) \right) \wedge 2n \right) \quad (16)$$

effective number of computations (which is the total number of points used in estimating the mutual information). This takes

$$O \left( \sum_{i=1}^d \log(d) \left( \left( \frac{\sigma^2 \log(nd)}{\Delta_i^2} \right) \wedge n \right) \right) \quad (17)$$

time.

**Theorem H.2.** If we further assume that  $\Delta_i \sim \mathcal{N}(\gamma, 1)$ , for some  $\gamma$ , and  $d = cn$ , for  $c \in [0, 1]$ , then we have that the expected number of effective number of computations (over randomness in  $\Delta_i$ ),

$$\mathbb{E}[M] \leq O(d \log(nd) + n).$$

with probability  $1 - \Theta(\frac{1}{d^2})$  over randomness in the algorithm of returning the correct answer. This takes  $O(d \log(nd) \log(d) + n \log(d))$

## I Comparison with projection based dimensionality reduction

A natural algorithm for improving the scaling of  $k$ -nearest neighbors is to project the data into lower dimensional space using Johnson-Lindenstrauss and computing the  $k$ -nearest neighbors.

If one projects a set of  $n$  points onto  $\frac{\log n}{\epsilon^2}$  dimensional space (obtained by a random linear transformation), then one preserves the distances between any two points to a multiplicative factor of  $(1 \pm \epsilon)$ . Thus using this method, we obtain a  $(1 + \epsilon)$  approximation for  $k$ -nearest neighbors. This algorithm would need  $O(nd \frac{\log n}{\epsilon^2})$  computations for projecting data down, and then would require  $O(n^2 \frac{\log n}{\epsilon^2})$  to obtain the  $k$ -nearest neighbors.

On the other hand the adaptive sampling based algorithm would take  $O(n^2 \frac{\log n}{\epsilon})$  (assuming  $n > d$ ) to obtain an  $1 + \epsilon$  approximation, giving it a better scaling. However we note that this comes at the expense of assuming mild regularity conditions (which we have shown that the data satisfies) that the Johnson-Lindenstrauss based algorithm (which only assumes boundedness).