Disclaimer: These notes have not been subjected to the usual scrutiny reserved for formal publications.

In this lecture we will discuss a reduction of the nearest neighbor search (NNS) problem to that of finding a locally sensitive hashing function as invented in [IM98].

6.1 Introduction to the Nearest Neighbor Search Problem

The NNS problem is as follows: Suppose $P \subset \mathbb{R}^d$ is a set of $n$ points. Given any $q \in \mathbb{R}^d$ find

$$\min_{p \in P} \text{dist}(p, q).$$

The distance here could be any arbitrary distance function; in this lecture we will talk more about $\ell_1$ or $\ell_2$ distances even though the machinery that we describe can be generalized to a variety of distance functions. Some applications include: web search, document search, or clustering - these are all situations in which knowing how “far” an object is from other objects tells us important information.

A naive solution would be to store all of the points and simply loop over all $p \in P$ to find the minimum distance. This takes $O(n \cdot d)$ time and space, which is not good. Ideally we would like to have a query time that is sublinear in $n$; we may allow for a super-linear amount of memory to store the data structure.

If $d = 1$ we could pre-process the points by sorting them and then finding the distance minimizing point would simply reduce to binary searching for $p$ in a list, and returning the closest of the two adjacent elements in the list. This takes $O(\log n)$ query time and $O(n)$ bits of memory.

Extending the pre-processing idea to higher dimensions $d$ leads to what are known as $k$-d trees: here the idea is to partition the space by using coordinate-aligned planes chosen appropriately for the data at hand. Unfortunately $k$-d trees generally fail to beat the naive approach when $d = \Omega(\log n)$. It turns out that in all known approaches the size of the data structure (or the query-time) grows exponentially in $d$.

The main underlying difficulty is the well-known facts in high dimensions, which is usually referred to as the “curse of dimensionality”. Suppose we partition the space by a grid where each cell is a cube of side length $a$. Then, a cube of side length $a$ randomly positioned in the space intersects $2^d$ many cells of the grid. This phenomenon essentially implies that a NNS algorithm based on kd-trees takes time $O(2^d)$ in expectation to look into all of the nearby cells of a query point to find the closes point.

6.2 Reducing to Approximate Nearest Neighbors Search

We now describe the idea of [IM98]. Firstly, instead of solving the exact problem we will look for approximate solutions. That is instead of finding the closest point $p$ to a query point $q$, we are happy to find a point $p$ such that

$$\text{dist}(p, q) \leq c \cdot \min_{s \in P} \text{dist}(s, q),$$

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where $c > 1$ is the approximation factor of in our algorithm. As we will see the memory and the query time of our algorithm will be a function of $c$.

So, let us define the approximate NNS problem. For $c > 1, r > 0$, the ANNS($c, r$) is defined as follows: Given a set point of points $P$, construct a data structure such that for any query point $q$, if there is a point $p$ such that $\text{dist}(p, q) \leq r$, it returns a point $p'$ such that $\text{dist}(p', q) \leq c \cdot r$.

If there is no such $p$, then we return nothing.

It is not hard to see that we can give a $c$ approximation to the nearest neighbor search problem using the solution to ANNS($c, r$). In fact, all we need to do is to guess $\min_{p \in P} \text{dist}(p, q)$ up to a multiplicative factor of $1 \pm \epsilon$. By an appropriate scaling assume $\text{diam}(P) = \max_{p, p' \in P} \text{dist}(p, p') \leq 1$

Also, suppose $\delta > 0$ is the minimum possible distance for all pairs of points in our dataset. Roughly speaking, $1/\delta$ can represent the bit precision of the data points stored in our system. We solve ANNS($c(1 - \epsilon), r$) for the following values of $r$,

$$\delta, (1 + \epsilon)\delta, (1 + \epsilon)^2\delta, \ldots, 1.$$  

We report the minimal value of $r$ for which we find a point at distance $c(1 - \epsilon)$ of $q$. This reduction imposes an additional $O(\log \frac{1}{\delta})$ overhead to the query time and the memory of our algorithm. This is because we need to maintain a separate data structure for each possible value of $r$ in the above sequence.

### 6.3 Locally Sensitive Hashing functions

From now on we only focus on the ANNS($c, r$). The main interesting idea of [IM98] is a reduction from this problem to the design of a locally sensitive hash (LSH) function. Roughly speaking, an LSH is a hash function which is sensitive to distance. Ideally, we would like to have a hash function that maps “close points” to the same value with a high probability and maps “far points” to different values. To be more precise, if $\text{dist}(p, q) \leq r$ we want them to map to the same value, with a high probability, and if $\text{dist}(p, q) > c \cdot r$ we want them to map to different values with a high probability. Let us give a formal definition

Suppose we have a family a functions $\mathcal{H} = \{h: P \rightarrow \mathbb{Z}\}$ of maps from our points $P$ to the set of integers $\mathbb{Z}$; we say $\mathcal{H}$ is $(c, c \cdot r, p_1, p_2)$-LSH if: for all $p, q \in P$:

$$\text{dist}(p, q) \leq r \implies \Pr[h(p) = h(q)] \geq p_1$$

$$\text{dist}(p, q) \geq c \cdot r \implies \Pr[h(p) = h(q)] \leq p_2$$

where the probabilities are over $h \sim \mathcal{H}$. Ideally, we want to have $p_1 \gg p_2$, but as we see this highly depends on the magnitude of $c$. The main idea in the reduction of [IM98] is that even if $p_1$ is slightly larger than $p_2$ it is possible to use many independently chosen functions from $\mathcal{H}$ to boost $p_1$ to a number close to 1 and $p_2$ to $1/n$.

Before describing the reduction, let us give an example of LSH for binary vectors. We will see several examples in PS3. Suppose $P \subseteq \{0, 1\}^d$ with Manhattan distance function

$$\text{dist}(p, q) = \|p - q\|_1,$$

i.e. $\text{dist}(p, q)$ is the number of coordinates at which $p$ and $q$ have different bits. Consider the family $\mathcal{H} := \{h_i\}_{i=1}^d$ where

$$h_i(p) = p_i$$
is the $i$th bit of $p$. Then observe that for each $p, q \in \{0, 1\}^d$

$$\mathbb{P}[h(p) = h(q)] = \frac{\# \text{ bits in common}}{\text{total bits}} = \frac{d - \|p - q\|_1}{d} = 1 - \frac{\|p - q\|_1}{d}.$$ Therefore,

$$\mathbb{P}[h(p) = h(q)] = \left\{ \begin{array}{ll}
\geq 1 - \frac{r}{d} \approx e^{-r/d} & \text{if } \text{dist}(p, q) \leq r \\
\leq 1 - \frac{c \cdot r}{d} \approx e^{-c \cdot r/d} & \text{if } \text{dist}(p, q) \geq c \cdot r.
\end{array} \right.$$ So, $H$ is $(c, c \cdot r, e^{-r/d}, e^{-c \cdot r/d})$-LSH.

### 6.4 Reduction to LSH

Now let us discuss the reduction from ANNS($c, r$) to LSH? Well if we had a $(r, c \cdot r, p_1, p_2)$-LSH family such that $p_1 \approx 1$ and $p_2 \approx 0$ we could solve the problem as follows: We start by choosing a function $h \sim H$ uniformly at random and we store $h(p)$ for all points in $P$. Given a query point $q$, we compute $h(q)$ and see if there is any point $p \in P$ where $h(p) = h(q)$. Note that we can do the lookup in $O(1)$ time using a hash table as we discussed in previous lectures. If there is no such point $p$, then with high probability there is no point at distance $c \cdot r$ of $q$. Thus we only need to show that if we are given an $(r, c \cdot r, p_1, p_2)$-LSH family with the assumption $p_1 > p_2$, then we can boost it to get $p_1 \approx 1$ and $p_2 \approx 0$.

We do this boosting in two steps. First, we just try to make $p_2$ small. To do this it suffices to take $k$ independent hash functions from $H$, and hash each point $p \in P$ to a $k$-dimensional vector, $h(p) = [h_1(p), \ldots, h_k(p)]$.

Then, by the independence of $h_1, \ldots, h_k$, for any two points $p, q$,

$$\text{dist}(p, q) \geq c \cdot r \implies \mathbb{P}[h(p) = h(q)] \leq p_2^k.$$ But this doesn’t help us increase $p_1$. In fact, the above hash function maps two close points to the same vector with probability at least $p_2^k$. How do we do this? We choose $\ell$ independent copies of the above $k$-dimensional hash function, $f_1, f_2, \ldots, f_\ell$, for a sufficiently large $\ell$, with high probability there is an $i$ such that $f_i(p) = f_i(q)$. Assume,

$$f_1(p) = [h_{1,1}(p), \ldots, h_{1,k}(p)]$$

$$\vdots$$

$$f_\ell(p) = [h_{\ell,1}(p), \ldots, h_{\ell,k}(p)]$$

It follows that if $\text{dist}(p, q) \leq r$, then

$$\mathbb{P}\left[ \exists i \mid f_i(p) = f_i(q) \right] = 1 - \mathbb{P}\left[ \forall i, f_i(p) \neq f_i(q) \right] = 1 - \mathbb{P}\left[ f_i(p) \neq f_i(q) \right] \geq 1 - (1 - p_2^k)^\ell.$$ The details of the algorithm is described in Equation 6.4.

Next, we describe how to tune the parameters $k, \ell$. We choose $k$ such that $p_2^k = 1/n$. Also, assume

$$p_1 = p_2^\rho,$$ (6.1)
for some $\rho < 1$. As we will see $\rho$ is the main parameter that determines the running time/memory of our algorithm. We choose $\ell = \Theta n^{-\rho} \ln n$.

Fix a query point $q$; it follows by linearity of expectation that for any $i$,

$$\mathbb{P} \left[ \exists p : \text{dist}(p, q) > c \cdot r, f_i(p) = f_i(q) \right] = n \cdot p_{2k}^{\ell} \leq 1.$$  

Summing up over all $i$, in expectation there are $O(\ell)$ points in our data set which map to the same hash value as $q$ for some $i$. This implies an overhead of $O(\ell)$ in the query time.

On the other hand, if $\text{dist}(p, q) \leq r$ for some $p \in P$, then

$$\mathbb{P} \left[ \exists i : f_i(p) = f_i(q) \right] \geq 1 - (1 - p_{1k})^\ell = 1 - (1 - n^{-\rho})^\ell \approx 1 - e^{\ell n^{-\rho}} = 1 - 1/n.$$  

In summary, for any point $p$ at distance at most $r$, our algorithm outputs $p$ with probability at least $1 - 1/n$.

The algorithm in expectation had $O(\ell \cdot d)$ overhead to examine $O(\ell)$ points at distance more than $c \cdot r$ from $q$.

**Algorithm 1** LSH Algorithm

**Preprocessing:**
- Choose $k \cdot \ell$, $h_{1,1}, \ldots, h_{\ell,k}$ functions uniformly at random from $\mathcal{H}$.
- Construct $\ell$ hash tables; for all $1 \leq i \leq \ell$ store $f_i(p) = (h_{i,1}(p), \ldots, h_{i,k}(p))$ for all $p \in P$ in the $i$-th table.
- For all $i$, sort all values of $\{f_i(p) : p \in P\}$.

**Query**($q$):
- for $i = 1 \rightarrow \ell$ do
  - Compute $f_i(q)$.
  - Find all points $p$ where $f_i(p) = f_i(q)$ using a binary search on table $i$. For all such points if $\text{dist}(p, q) \leq c \cdot r$, output $p$.
- end for

6.5 Space and Time Complexity of the Reduction

The algorithm needs to maintain $O(\ell)$ hash tables. In each hash table we need to store $n = |P|$ hash values where each value is a $k$ dimensional vector. So, the space complexity of the algorithm is

$$O(\ell \cdot n \cdot k) = O(n^{1+\rho} \frac{\log n}{\log \frac{1}{p_2}}).$$

For any query point $q$ we need to spend The query time is $O(\ell \cdot k)$ time to compute $f_i(q)$ for all $1 \leq i \leq \ell$. For any candidate close point $p$ we spend $O(d)$ time to calculate $\text{dist}(p, q)$. Let $|O|$ be size of the output, i.e., the number of points at distance $c \cdot r$ from $q$. In expectation we examine $O(\ell)$ far points that we don’t output. So, the query time is $O(d(\ell + |O|))$ in expectation. So, the query time is

$$O(d(\ell + |O|) + \ell \cdot k) = O \left( n^{\rho} \left(d + \frac{\log n}{\log \frac{1}{p_2}}\right) + |O|d \right).$$

Ignoring lower order terms, in particular the size of the output and the dimension, the algorithm runs with memory $O(n^{1+\rho})$ and querytime $O(n^\rho)$.
Let us calculate $\rho$ for the binary vector example that we described at the beginning. Recall that $\rho$ is chosen such that $p_1 = p_2^\rho$, so

$$\rho = \frac{\ln \frac{1}{p_1}}{\ln \frac{1}{p_2}} = \frac{r/d}{c \cdot r/d} = \frac{1}{c}.$$ 

For example, if $c = 2$, we need $O(n^{1.5})$ to store hash tables and we have $O(\sqrt{n})$ query time. As we see the query time (and memory) get significantly better as we increase $c$. In practice, we may tune the parameter $c$ based on the amount of resources available to us.

It has been a very active area of research to design the best of LSH functions for many metrics. In PS3 we design LSH for $\ell_1, \ell_2$ distance where $\rho = 1/c$.

References