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

$$
\min _{p \in P} \operatorname{dist}(p, q) .
$$

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 $O\left(2^{d}\right)$ 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

$$
\operatorname{dist}(p, q) \leq c \cdot \min _{s \in P} \operatorname{dist}(s, q),
$$

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 $\operatorname{ANNS}(c, r)$ 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 $\operatorname{dist}(p, q) \leq r$, it returns a point $p^{\prime}$ such that

$$
\operatorname{dist}\left(p^{\prime}, q\right) \leq c \cdot r
$$

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 $\operatorname{ANNS}(c, r)$. In fact, all we need to do is to guess $\min _{p \in P} \operatorname{dist}(p, q)$ up to a multiplicative factor of $1 \pm \epsilon$. By an approporiate scaling assume

$$
\operatorname{diam}(P)=\max _{p, p^{\prime} \in P} \operatorname{dist}\left(p, p^{\prime}\right) \leq 1
$$

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 $\operatorname{ANNS}(c(1-\epsilon), r)$ 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 $O\left(\log \frac{1}{\delta}\right)$ 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 $\operatorname{ANNS}(c, r)$. 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 $\operatorname{dist}(p, q) \leq r$ we want them to map to the same value, with a high probability, and if $\operatorname{dist}(p, q)>c \cdot r$ 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 $\left(c, c \cdot r, p_{1}, p_{2}\right)$-LSH if: for all $p, q \in P$ :

$$
\begin{aligned}
& \operatorname{dist}(p, q) \leqslant r \Longrightarrow \mathbb{P}[h(p)=h(q)] \geqslant p_{1} \\
& \operatorname{dist}(p, q) \geqslant c \cdot r \Longrightarrow \mathbb{P}[h(p)=h(q)] \leqslant p_{2}
\end{aligned}
$$

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

$$
\operatorname{dist}(p, q)=\|p-q\|_{1}
$$

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

$$
\mathbb{P}[h(p)=h(q)]= \begin{cases}\geq 1-\frac{r}{d} \approx e^{-r / d} & \text { if } \operatorname{dist}(p, q) \leq r \\ \leq 1-\frac{c \cdot r}{d} \approx e^{-c \cdot r / d} & \text { if } \operatorname{dist}(p, q) \geq c \cdot r\end{cases}
$$

So, $\mathcal{H}$ is $\left(c, c \cdot r, e^{-r / d}, e^{-c \cdot r / d}\right)$-LSH.

### 6.4 Reduction to LSH

Now let us discuss the reduction from ANNS $(c, r)$ to LSH? Well if we had a $\left(r, c \cdot r, p_{1}, p_{2}\right)$-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 $h \sim \mathcal{H}$ 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 $\left(r, c \cdot r, p_{1}, p_{2}\right)$-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 $\mathcal{H}$, and hash each point $p \in P$ to a $k$-dimensional vector,

$$
h(p)=\left[h_{1}(p), \ldots, h_{k}(p)\right] .
$$

Then, by the independence of $h_{1}, \ldots, h_{k}$, for any two points $p, q$,

$$
\operatorname{dist}(p, q) \geqslant c \cdot r \Longrightarrow \mathbb{P}[h(p)=h(q)] \leqslant p_{2}^{k}
$$

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 $p_{1}^{k}$. 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,

$$
\begin{aligned}
f_{1}(p) & =\left[h_{1,1}(p), \ldots, h_{1, k}(p)\right] \\
& \vdots \\
f_{\ell}(p) & =\left[h_{\ell, 1}(p), \ldots, h_{\ell, k}(p)\right]
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbb{P}\left[\exists i \mid f_{i}(p)=f_{i}(q)\right] & =1-\mathbb{P}\left[\forall i, f_{i}(p) \neq f_{i}(q)\right] \\
& =1-\mathbb{P}\left[f_{i}(p) \neq f_{i}(q)\right]^{\ell} \\
& \geqslant 1-\left(1-p_{1}^{k}\right)^{\ell}
\end{aligned}
$$

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

$$
\begin{equation*}
p_{1}=p_{2}^{\rho} \tag{6.1}
\end{equation*}
$$

for some $\rho<1$. As we will see $\rho$ is the main parameter that determines the running time/memory of our algorithm. We choose $\ell \propto n^{-\rho} \ln n$.

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

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

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 $\operatorname{dist}(p, q) \leq r$ for some $p \in P$, then

$$
\mathbb{P}\left[\exists i: f_{i}(p)=f_{i}(q)\right] \geq 1-\left(1-p_{1}^{k}\right)^{\ell}=1-\left(1-p_{2}^{\rho k}\right)^{\ell}=1-\left(1-n^{-\rho}\right)^{\ell} \approx 1-e^{\ell n^{-\rho}}=1-1 / n
$$

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 $c \cdot r$ form $q$.

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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 \(f_{i}(p)=\left(h_{i, 1}(p), \ldots, h_{i, k}(p)\right)\) for all \(p \in P\) in the \(i\)-th has
    table.
Query \((q)\) :
    for \(i=1 \rightarrow \ell\) do
        Compute \(f_{i}(q)\).
        Go over all points \(p\) where \(f_{i}(p)=f_{i}(q)\). For all such points if \(\operatorname{dist}(p, q) \leq c \cdot r\), 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

$$
O(\ell \cdot n \cdot k)=O\left(n^{1+\rho} \log \frac{n}{p_{2}}\right)
$$

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 $\operatorname{dist}(p, q)$. 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

$$
O(d(\ell+|O|)+\ell \cdot k)=O\left(n^{\rho}\left(d+\log \frac{n}{p_{2}}\right)+|O| d\right)
$$

Ignoring lower order terms, the algorithm runs with memory $O\left(n^{1+\rho}\right)$ and querytime $O\left(n^{\rho}\right)$.
Let us calculate $\rho$ for the binary vector example that we described at the beginning. Recall that $\rho$ is chosen such that $p_{1}^{\rho}=p_{2}$, 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 $O\left(n^{1.5}\right)$ 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

[IM98] P. Indyk and R. Motwani. "Approximate nearest neighbors: towards removing the curse of dimensionality". In: STOC. ACM. 1998, pp. 604-613 (cit. on pp. 6-1, 6-2).

