DSC 190
DATA STRUCTURES & ALGORITHMS

Lecture 7 | Part 1

Today's Lecture

Approximate Nearest Neighbor

▶ **Given**: a set of n points in $\mathbb{R}^d$ and query point p.

▶ **Compute**: (approximate) nearest neighbor of p.

▶ Last time: k-d trees do not scale well with d.

Today

▶ Slightly different problem: given a distance *r* and query *p*.

▶ Return (approximately) all of the points within distance *r* of *p*.

▶ Can use to compute ANN.

Today

▶ We'll introduce **locality sensitive hashing**.

▶ An important idea.

▶ We'll see similar themes in remainder of course.

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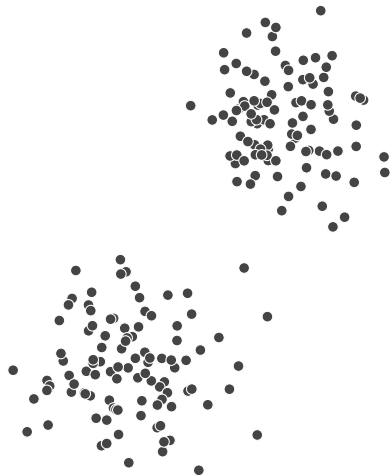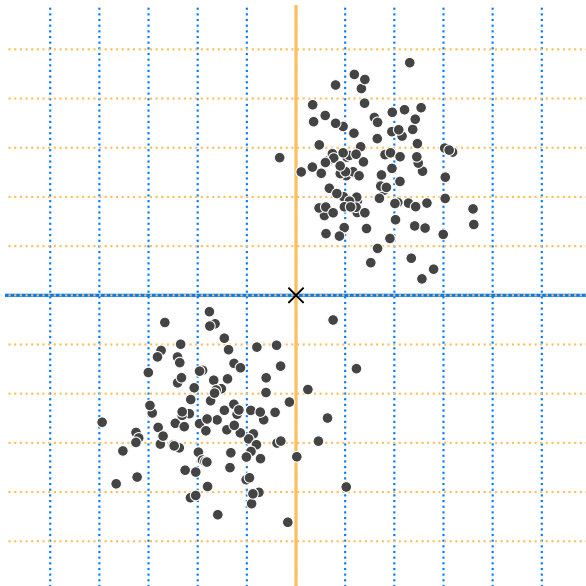
DATA STRUCTURES & ALGORITHMS

Lecture 7 | Part 2

Implementing a NN Grid

Grids

- ▶ Given input point *p*, want quick way to find nearby points.

- ▶ Idea: divide space into cells using grid.

- ▶ Find cell containing *p*, search it.

- ▶ How would we implement this?

Grid Cells

▶ Each point (x, y) given cell id: $(\lfloor x \rfloor, \lfloor y \rfloor)$
  ▶ Example: $(1.2, 6.7)$ given cell id $(1, 6)$.

▶ Store (x, y) in dictionary with cell id as key.
  ▶ Discretization allows multiple points in same cell.
  ▶ Store collisions in list.

▶ Generalizes naturally to d-dimensions.

```python
class NNGrid:

    def __init__(self, width):
        self.width = width
        self.cells = {}

    def cell_id(self, p):
        p = np.asarray(p)
        cell_id = np.floor(p / self.width).astype(int)
        return tuple(cell_id)

    def insert(self, p):
        """Insert p into the grid."""
        cell_id = self.cell_id(p)
        if cell_id not in self.cells:
            self.cells[cell_id] = []
        self.cells[cell_id].append(p)

    ...
```
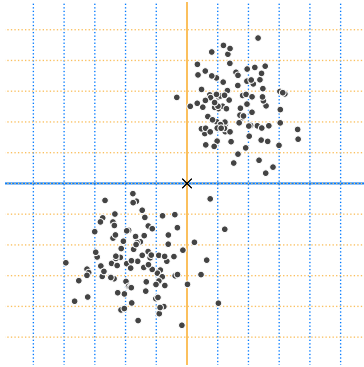
```python
...

def points_in_cell(self, p):
    cell_id = self.cell_id(p)
    if cell_id not in self.cells:
        return []
    points_in_cell = self.cells[cell_id]
    # turn into an array
    return np.vstack(points_in_cell)

def query(self, p):
    return brute_force_nn(self.points_in_cell(p), p)
```

Note

▶ This may **fail** – NN could be in different cell.

Problems

▶ In *d* dimensions, cell id has *d* entries.

$$\text{cell-id}(p) = (\lfloor x_1/w \rfloor, \lfloor x_2/w \rfloor, \ldots, \lfloor x_d/w \rfloor)$$

▶ All entries must be **exactly** the same for two points to have same cell id.

▶ This is **very unlikely**. Most cells are empty or contain one point.

High-Dimensional Cuboids

- ► One "fix": increase cell width parameter.

- ► Suppose we want to ensure any points within distance r are in same cell.

- ► Then cell width must be $2r$.[1]

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[1]Note: Jan 2022, this isn't actually true... but idea of next slide still holds.

High-Dimensional Cuboids

► But a *d*-dimensional cuboid of width 2*r* can contain points at distance $2\sqrt{d}r$ from one another!

► For even modest *r*, the whole data set is in one cell.

Main Idea

Dividing into a grid of cuboids fails in high dimensions. Either the cells are empty, or contain everything, depending on the width!
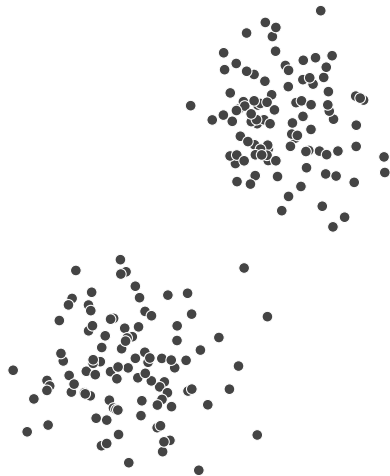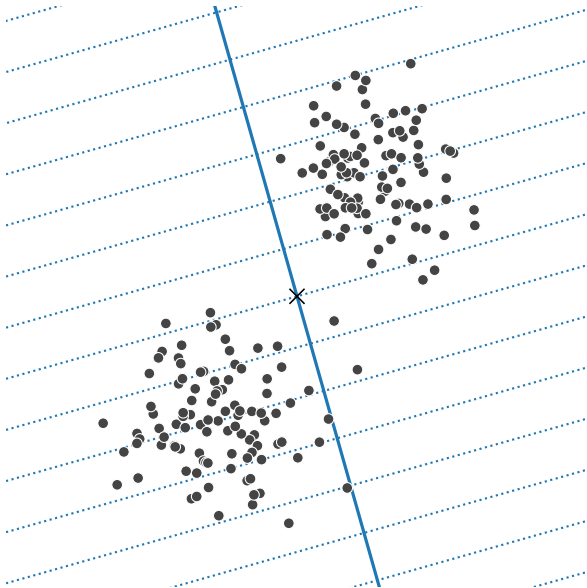
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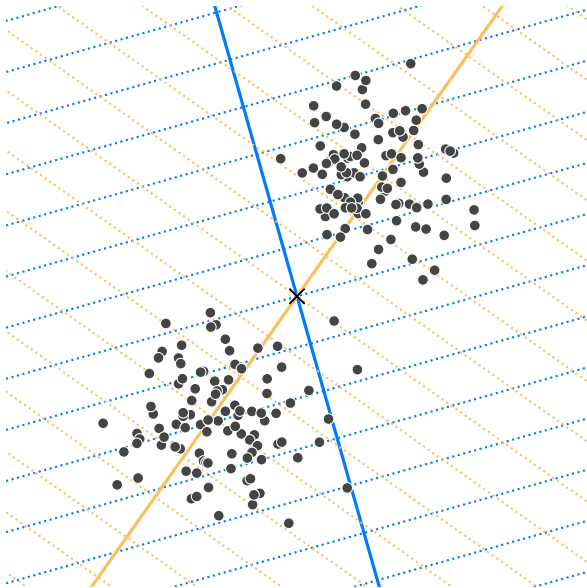## DATA STRUCTURES & ALGORITHMS

Lecture 7 | Part 3

A Randomized "Grid"

A Randomized "Grid"

▶ Idea: Instead of axis-aligned grid, divide into cells using $k \ll d$ random directions.
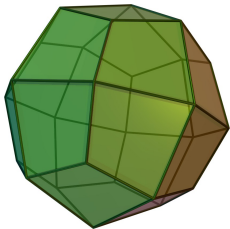
Cell Shape

▶ Cells are no longer d-dimensional cuboids.

▶ They are random k-dimensional **polytopes**.
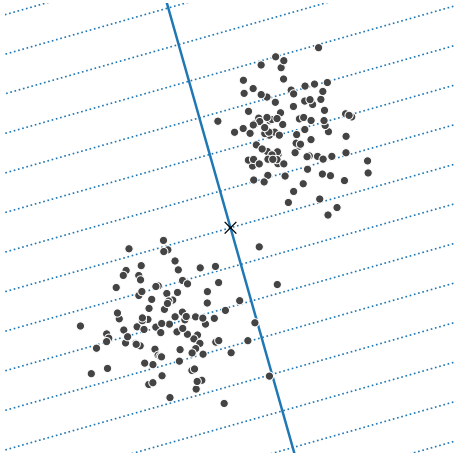
Question

- ▶ Why is this better? We'll see in the next sections.

Projection

▶ How do we determine which cell a point lies in?

Cell IDs

- ▶ Pick k random unit vectors, $\vec{u}^{(1)}, \ldots, \vec{u}^{(k)} \in \mathbb{R}^d$.

- ▶ Pick a width parameter, w.

- ▶ Given any point $\vec{p}$, its cell id is[2]:

$$\text{cell-id}(\vec{p}) = \left(\left\lfloor \frac{\vec{u}^{(1)} \cdot \vec{p}}{w} \right\rfloor, \left\lfloor \frac{\vec{u}^{(2)} \cdot \vec{p}}{w} \right\rfloor, \ldots, \left\lfloor \frac{\vec{u}^{(k)} \cdot \vec{p}}{w} \right\rfloor, \right)$$

---

[2]use same width and unit vectors for all points

Example
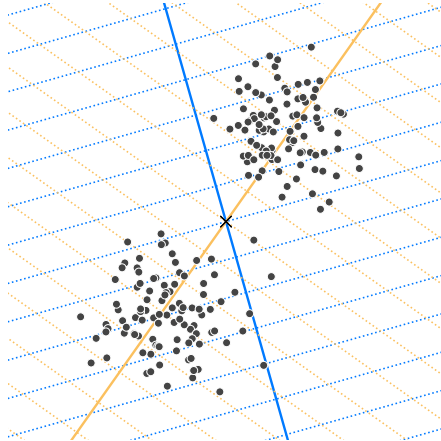
Quick Cell-ID Calculation

▶ Place $\vec{u}^{(1)}, \ldots, \vec{u}^{(k)}$ into a matrix:

$$U = \begin{pmatrix} \leftarrow & (\vec{u}^{(1)})^T & \rightarrow \\ \leftarrow & (\vec{u}^{(2)})^T & \rightarrow \\ \vdots & \vdots & \vdots \\ \leftarrow & (\vec{u}^{(k)})^T & \rightarrow \end{pmatrix}$$

▶ Then cell-id($\vec{p}$) = entrywise-floor($U\vec{p}/w$)

Generating Random Unit Vectors

```python
def gaussian_projection_matrix(k, d):
    X = np.random.normal(size=(k, d))
    U = X / np.linalg.norm(X, axis=1)[:,None]
    return U
```

```python
class NNProjectionGrid

    def __init__(self, projection_matrix, width):
        self.width = width
        self.projection_matrix = projection_matrix
        self.cells = {}

    def cell_id(self, p):
        projection = self.projection_matrix @ p
        cell_id = np.floor(projection / self.width)
        return tuple(cell_id.astype(int))

    # insert, query, points_in_cell same as for NNGrid
```

But wait…

▶ In high dimensions, still **very unlikely** for cell to contain >1 point.

▶ Idea: **banding**. Try, try again.

▶ Build multiple `NNProjectionGrids` with different random projections.

▶ Find `points_in_cell` for each, pool them together.

Multiple Random Projections
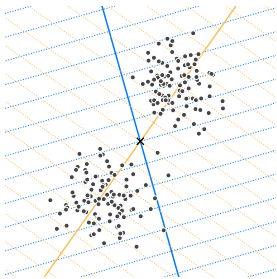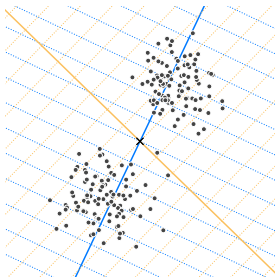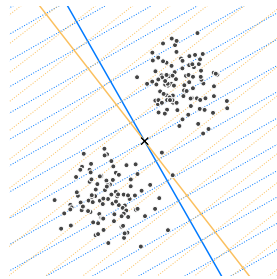
U_1 U_2 U_3

Locality Sensitive Hashing

► This idea (multiple random projections) is an example of **Locality Sensitive Hashing** (LSH).

► We'll explore it more in the next section.

```python
class LocalitySensitiveHashing:

    def __init__(self, l, k, d, w):
        self.randomized_grids = []
        for i in range(l):
            U = gaussian_projection_matrix(k, d)
            randomized_grid = NNProjectionGrid(U, w)
            self.randomized_grids.append(randomized_grid)

    def insert(self, p):
        for randomized_grid in self.randomized_grids:
            randomized_grid.insert(p)

    ...
```

```
...

def query_close(self, p):
    nearby = []
    for randomized_grid in self.randomized_grids:
        points_in_cell = randomized_grid.points_in_cell(p)
        nearby.append(points_in_cell)
    return np.vstack(nearby)

def query_nn(self, point):
    results = self.query_close(point)
    pool = np.vstack([r for r in results])
    if len(pool) == 0:
        raise ValueError('No points nearby.')
    return brute_force_nn(pool, point)
```

Parameters

- l: number of randomized "grids"

- k: number of random directions in each "grid"

- w: bin width

Tuning Parameters

▶ Choose so that `.query_close` returns a small # of points.

▶ If # is very small (or zero), either:
  ▶ increase w or ℓ
  ▶ decrease k

Note

▶ This is an approximate NN technique!

▶ May not find **the** NN.

▶ May not return **anything**!

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DATA STRUCTURES & ALGORITHMS

Lecture 7 | Part 4

Theory of Locality Sensitive Hashing

Why does LSH work?

- ▶ Two approaches to understanding LSH.

- ▶ **1) Hashing view.**

- ▶ 2) Dimensionality reduction view.

Standard Hashing

▶ A **hash function** $h : \mathcal{X} \rightarrow \mathbb{Z}$ takes in an object from $\mathcal{X}$ and returns a bucket number.

Standard Hashing

▶ **Collision**: two different objects have same hash.

▶ Usually, collisions are **bad**.

▶ Want similar things to have very different hashes.

Locality Sensitive Hashing

▶ But in NN search, we want "close" items to be in the **same bucket** (have same hash).

▶ "Far" items should be in **different buckets** (have different hash).

Locality Sensitive Hashing

▶ Let r be a distance we consider "close".

▶ Let cr (with $c > 1$) be a distance we consider "far".

▶ Suppose H is a **family** of hash functions.

LSH Family

▶ *H* is an **LSH family** if when *h* is randomly drawn from *H*:

$$\mathbb{P}(h(x) = h(y)) \geq p_1 \quad \text{when } d(x, y) \leq r$$
$$\mathbb{P}(h(x) = h(y)) \leq p_2 \quad \text{when } d(x, y) \geq cr$$

where $p_1 > p_2$.

Main Idea

If x and y are close, the probability that they hash to the **same** bin is not too small. If they are far, the probability is not too large.

Example: Random Projections

▶ We have seen one LSH family: random projections followed by binning.

▶ *H* has infinitely-many hash functions, one for each direction $\vec{u}$:

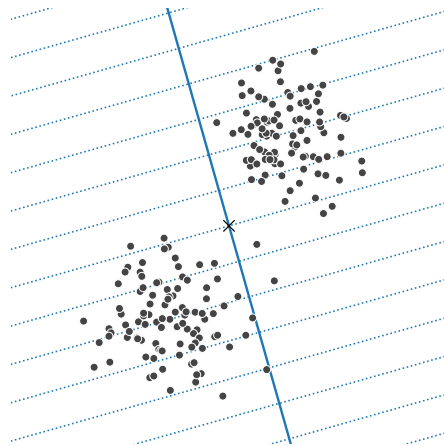$$h_{\vec{u}}(\vec{p}) = \left\lfloor \frac{\vec{u} \cdot \vec{p}}{w} \right\rfloor,$$

Example: Random Projections

▶ Suppose a random hash function h is chosen.

▶ Claim:

$$\mathbb{P}(h(x) = h(y)) \geq \frac{1}{2} \quad \text{when } d(x, y) \leq w/2$$
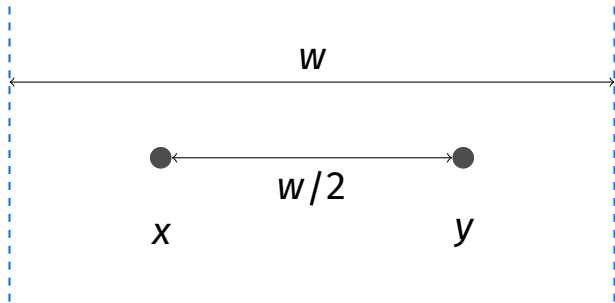
$$\mathbb{P}(h(x) = h(y)) \leq \frac{1}{3} \quad \text{when } d(x, y) \geq 2w$$
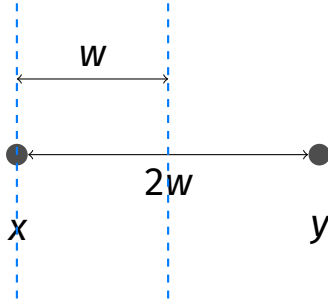
Intuition

Proof: Close

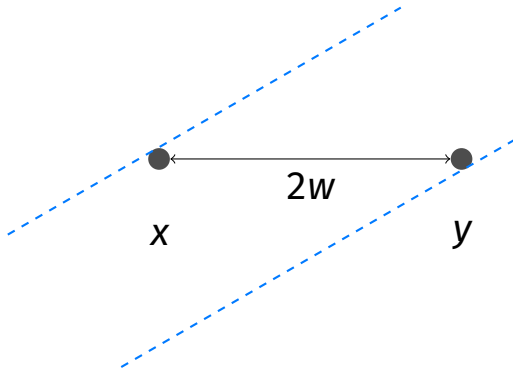▶ In worst case, grid is orthogonal to line between
points.

Proof: Far

▶ Only possible if grid is close to parallel.

Proof: Far

▶ Angle must be below 30˚.

Amplification

- ▶ Lots of points have same hash.

- ▶ To be more selective, randomly select k hash functions for cell id.

$$\text{cell-id}(x) = (h_1(x), h_2(x), \ldots, h_k(x))$$

Example: Random Projections

► In case of random projections.

$$\text{cell-id}(\vec{p}) = \left(\underbrace{\left\lfloor \frac{\vec{u}^{(1)} \cdot \vec{p}}{w} \right\rfloor}_{h_1}, \underbrace{\left\lfloor \frac{\vec{u}^{(2)} \cdot \vec{p}}{w} \right\rfloor}_{h_2}, \ldots, \underbrace{\left\lfloor \frac{\vec{u}^{(k)} \cdot \vec{p}}{w} \right\rfloor}_{h_k} \right)$$

Collision Probability

▶ Remember:

$$P(h(x) = h(y)) \geq p_1 \text{ if close.}$$
$$P(h(x) = h(y)) \leq p_2 \text{ if far.}$$

▶ Collision occurs if $h_i(x) = h_i(y)$ $\forall i \in \{1, \dots, k\}$.

▶ Probability of collision…
  ▶ if close: $\geq p_1^k$
  ▶ if far: $\leq p_2^k$

Choosing k

▶ Want prob. of far points colliding to be small.

▶ Say, $1/n$.

▶ Set $p_2^k = 1/n$. Then

$$k = \log_{p_2} \frac{1}{n} = \frac{\log n}{\log 1/p_2}$$

Main Idea

We can use $k = \Theta(\log n)$ hash functions.

Main Idea

When using random projections as hash functions, we can use $k = \Theta(\log n)$ directions. This is usually much less than d.

But wait…

▸ Probability of close points colliding is p_1^k.

▸ Let $p_1 = p_2^\rho$. We'll have $\rho < 1$, since $p_2 < p_1$.

▸ Since $p_2^k = \frac{1}{n}$, we have $p_1^k = \frac{1}{n^\rho}$.

▸ This is **very small**.

Banding

▶ Before: one set of k hash functions.

▶ With **banding**: keep ℓ sets (**bands**) of k hash functions.

▶ To query NN of p, find points that are in the same cell as p in *any* of the bands.

Banding

▶ Probability of at least one match:

$$\underbrace{\frac{1}{n^\rho}}_{\text{collision in band 1}} + \underbrace{\frac{1}{n^\rho}}_{\text{collision in band 2}} + \dots + \underbrace{\frac{1}{n^\rho}}_{\text{collision in band } \ell} = \frac{\ell}{n^\rho}$$

▶ Want this to be ≈ 1, so:

$$\ell = n^\rho$$

Main Idea

We should set the number of bands to be n^ρ. ρ depends on c, and is usually not small. For random projections, $\rho \approx .63$.

Analysis

▶ How efficient is LSH?

▶ Worst case, everything hashes to same bin: $O(n)$.

▶ In practice, much better.

▶ Requires **a lot** of memory. $\Theta(\ell n)$.

Other Distances

▶ LSH works for many different similarity measures.

▶ Random projections are for Euclidean distances.

▶ But other hashing approaches work for cosine distance, Jaccard distance, etc.

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Lecture 7 | Part 5

The Johnson-Lindenstrauss Lemma

Why does LSH work?

▶ Two approaches to understanding LSH.

▶ 1) Hashing view.

▶ **2) Dimensionality reduction view.**

Main Idea

The **Johnson-Lindenstrauss Lemma** says that, given n points in $\mathbb{R}^d$, you can reduce the dimensionality to $k \approx \log n$ while still preserving relative distances by randomly projecting onto a set of k unit vectors.

Claim

The **Johnson-Lindenstrauss Lemma** (Informal). Let X be a set of n points in $\mathbb{R}^d$. Let U be a matrix whose $k = O(\log(n)/\epsilon^2)$ rows are Gaussian random vectors in $\mathbb{R}^d$. Then for every $\vec{x}, \vec{y} \in X$,

$$\|\vec{x} - \vec{y}\| \le (1 \pm \epsilon)\|U\vec{x} - U\vec{y}\|$$

LSH and J-L

► In LSH, we use $k = O(\log n)$ hash functions.

► If these hash functions are random projections, the J-L lemma tells that distances are largely preserved.

A Different View of LSH

▶ Given $p \in \mathbb{R}^d$, randomly project to $\mathbb{R}^k$ with $k \approx \log n$.

▶ Let new coordinates be $(y_1, y_2, \dots, y_k)$.

▶ Use standard grid to assign cell id.

Main Idea

LSH (for Euclidean distances) (without banding) can be viewed as dimensionality reduction by random projections, followed by binning into a standard grid.

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Lecture 7 | Part 6

NN in Practice

In Practice

- ▶ LSH is an important idea.

- ▶ Good performance in practice.

- ▶ But heuristic approaches are often faster.

- ▶ `faiss` and `annoy`, among others.

Hierarchical k-Means

Product Quantization

Navigable Small Worlds