

K-Nearest Neighbors

Nipun Batra

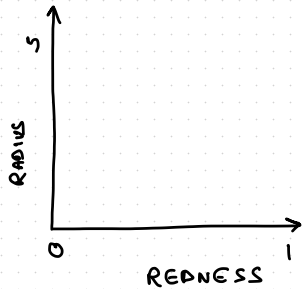
July 26, 2025

IIT Gandhinagar

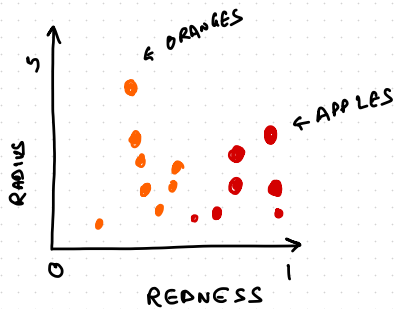
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Introduction and Fundamentals

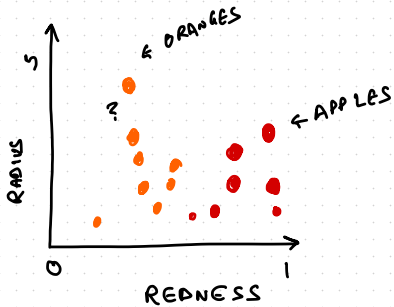
CLASSIFICATION



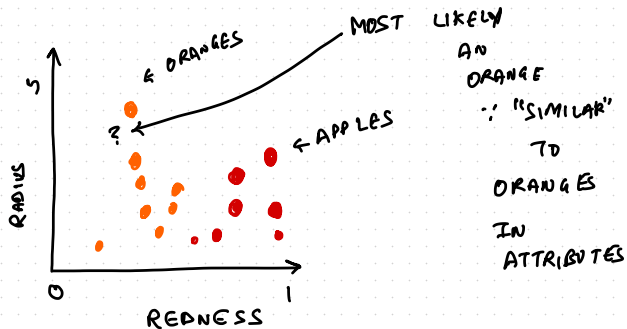
CLASSIFICATION



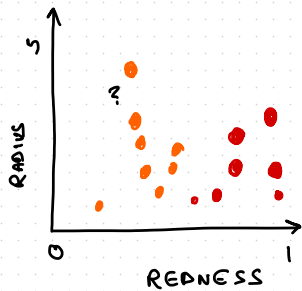
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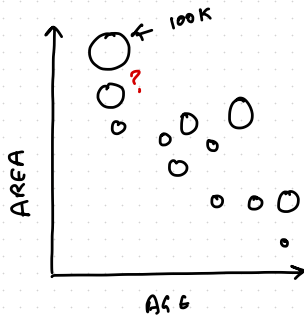
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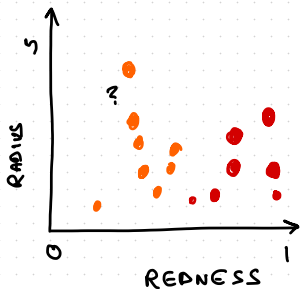
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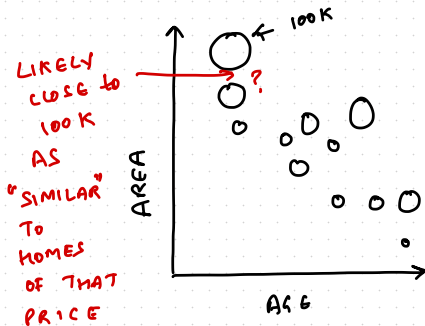
REGRESSION



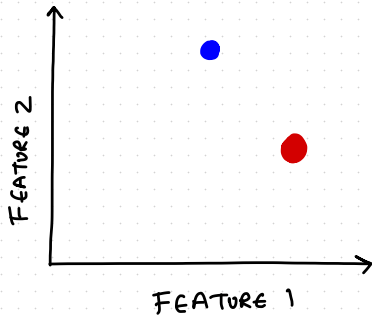
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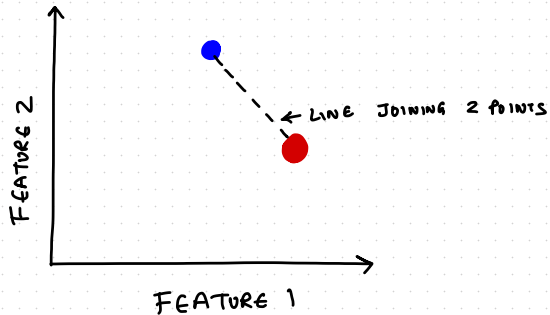
REGRESSION



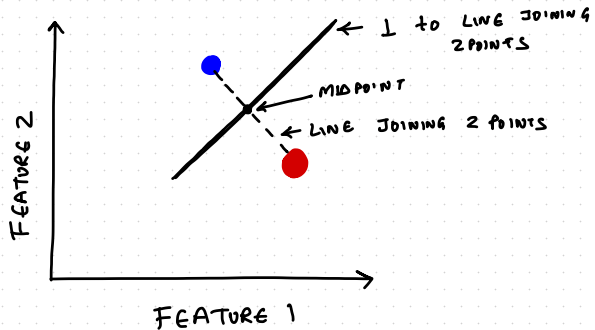
VORONOI DIAGRAM FOR 1-NN



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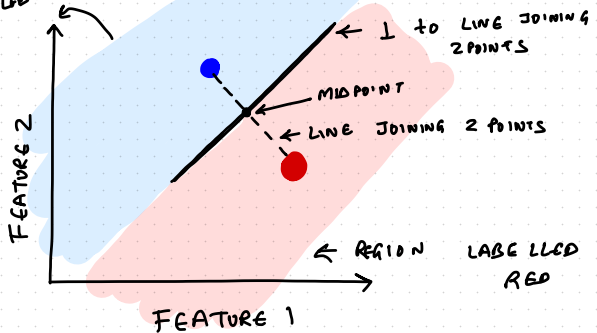


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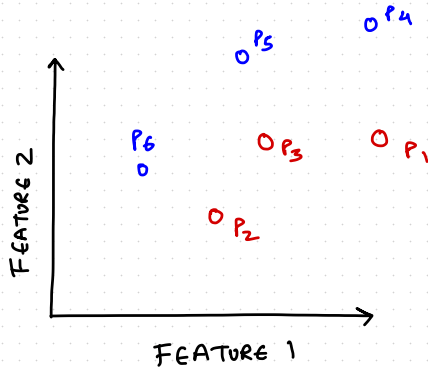


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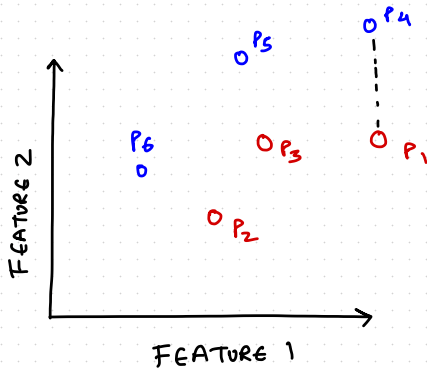
REGION LABELLED BLUE



VORONOI DIAGRAM FOR 1-NN

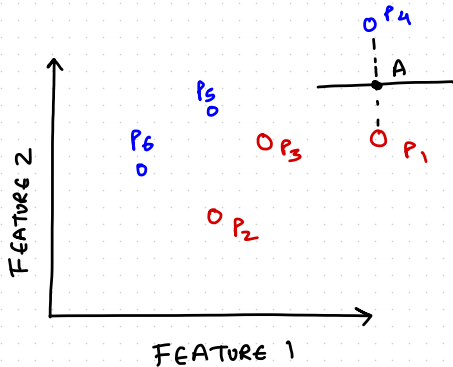


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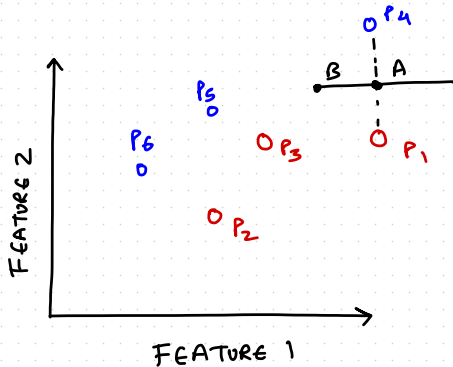
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A: MID PT B/W P_1 & P_4



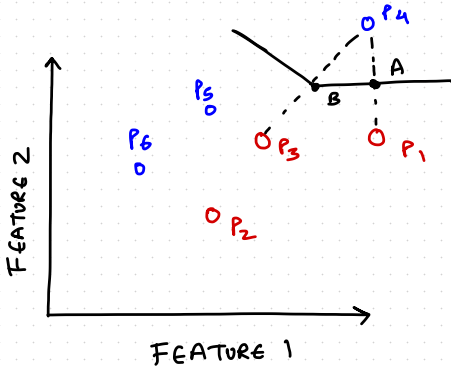
VORONOI DIAGRAM FOR 1-NN

A: MID PT B/W P_3 & P_4
B: CLOSER TO P_3 than P_1



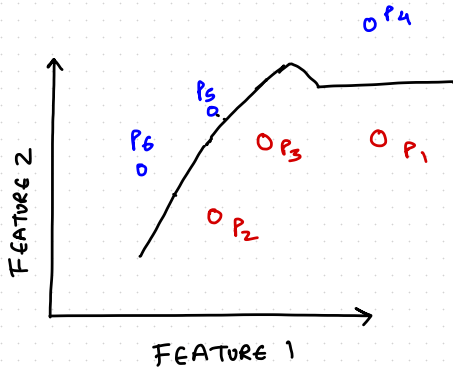
VORONOI DIAGRAM FOR 1-NN

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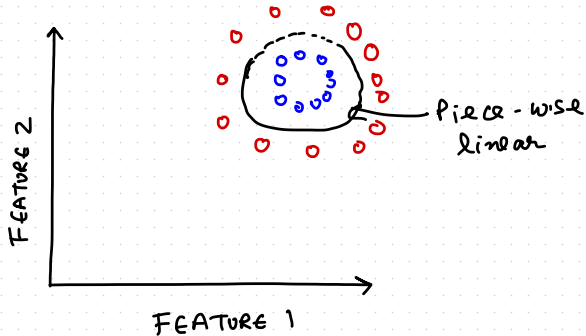
VORONOI DIAGRAM FOR 1-NN

DECISION
BOUNDARY IS
PIECE-WISE
LINEAR

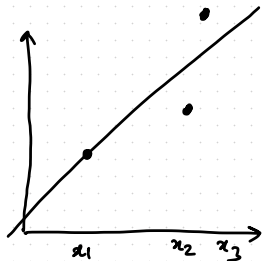


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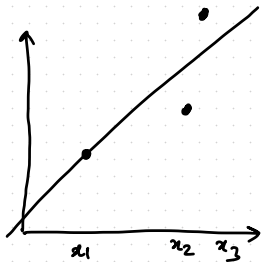


LINEAR REGRESSION

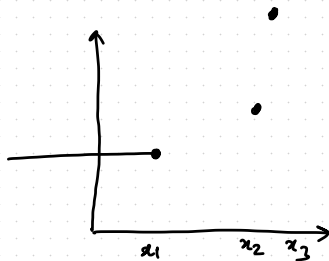


1NN REGRESSION

LINEAR REGRESSION

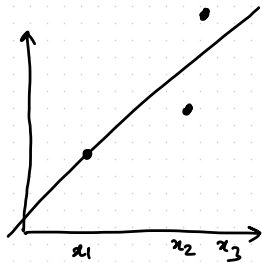


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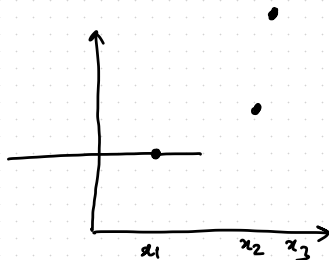


$x < x_1$: NN is (x_1, y_1)

LINEAR REGRESSION



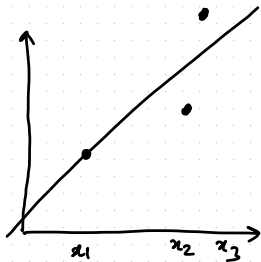
1NN REGRESSION



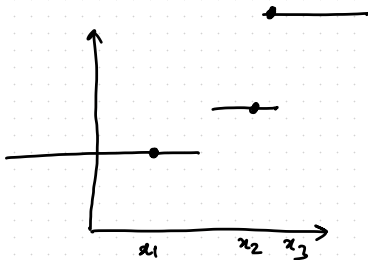
$x < x_1$: NN is (x_1, y_1)

$x < \frac{x_1 + x_2}{2}$: NN is (x_1, y_1)

LINEAR REGRESSION



1NN REGRESSION

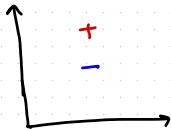


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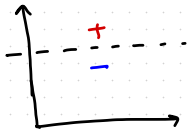
$\frac{x_1 + x_2}{2} < x < \frac{x_2 + x_3}{2}$: NN is (x_2, y_2)

KNN IS NON-PARAMETRIC



LINEAR MODEL

KNN IS NON-PARAMETRIC

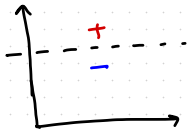


DECISION
BOUNDARY

LINEAR MODEL

$$y = mx + c \quad (\# \text{ params} = 2)$$

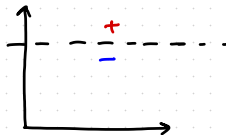
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LINEAR MODEL

DECISION
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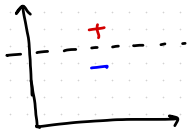


KNN (K=1)

DECISION
BOUNDARY

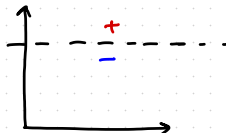
$$(\text{LIKE } y = mx + c)$$

KNN IS NON-PARAMETRIC



DECISION
BOUNDARY

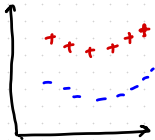
LINEAR MODEL
 $y = mx + c$ (# params = 2)



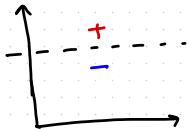
KNN (K=1)

DECISION
BOUNDARY (LIKE $y = mx + c$)

ADD DATA

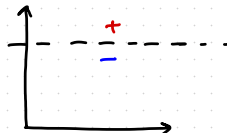


KNN IS NON-PARAMETRIC



DECISION
BOUNDARY

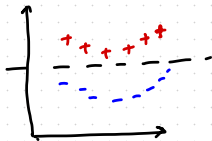
LINEAR MODEL
 $y = mx + c$ (#params = 2)



KNN (K=1)

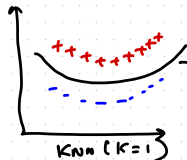
DECISION
BOUNDARY (LIKE $y = mx + c$)

ADD DATA



DECISION
BOUNDARY

LINEAR MODEL
 $y = mx + c$ (2 params)



KNN (K=1)

#PARAMS ≥ 2 (AT LEAST QUADRATIC)

PARAMETRIC

#PARAMS FIXED
WRT DATASET SIZE

MAKE ASSUMPTIONS
(LIKE FUNCTIONAL FORM)

USUALLY QUICKER

Eg: LINEAR MODELS,
SVM (LINEAR, POLYNOMIAL)

NON-PARAMETRIC

#PARAMS GROWS
WRT DATASET SIZE

LESSER ASSUMPTIONS

USUALLY SLOWER

Eg: KNN, DT,
SVM (with
RBF)

Parametric vs Non-Parametric Models

	Parametric	Non-Parametric
Parameter	Number of parameters is fixed w.r.t dataset size	Number of parameters grows w.r.t. to an increase in dataset size
Speed	Quicker (as the number of parameters are less)	Longer (as number of parameters are less)
Assumptions	Strong Assumptions (like linearity in Linear Regression)	Very few (sometimes no) assumptions
Examples	Linear Regression	KNN, Decision Tree

Lazy vs Eager Strategies

	Lazy	Eager
Train Time	0	$\neq 0$
Test	Long (due to comparison with train data)	Quick (as only "parameters" are involved)
Memory	Store/Memorise entire data	Store only learnt parameters
Utility	Useful for online settings	
Examples	KNN	Linear Regression, Decision Tree

Important Considerations

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- What is the **distance metric** that will be used to calculate data similarity?
- What is the **aggregation function** that is going to be used?
- What are the **number of neighbors** that you are going to take into consideration?
- What is the **computational complexity** of the algorithm that you are implementing?

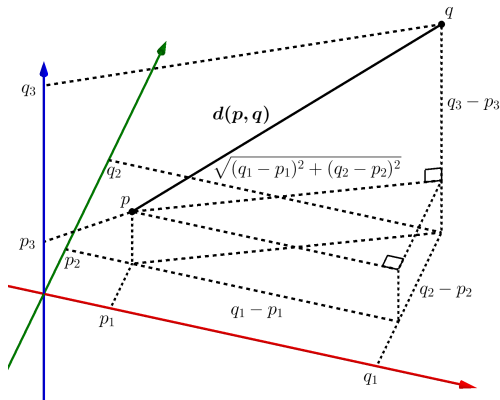
Distance Metrics and Considerations

Important Considerations: Distance Metric

The Distance Metric acts as a *measure of similarity* between the points.

Important Considerations: Distance Metric

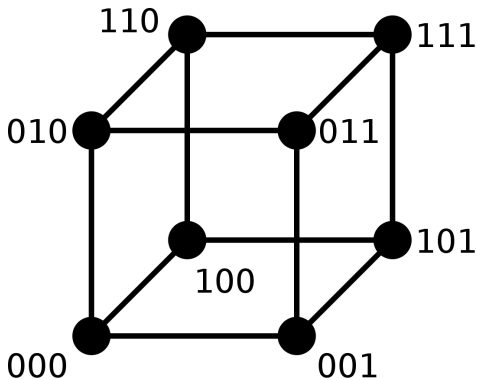
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Euclidean Distance

Important Considerations: Distance Metric

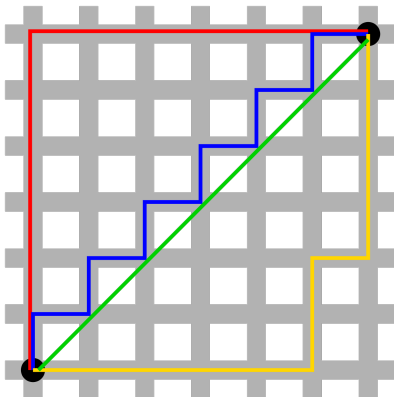
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Hamming Distance

Important Considerations: Distance Metric

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Manhattan Distance

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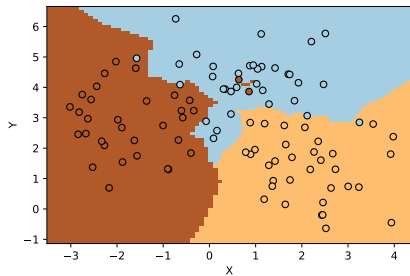
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High values of K will result in smoother decision boundaries
 \implies lower variance but also higher bias

Important Considerations: Value of K

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$K = 3$

Important Considerations: Value of K

Aggregating data

There are different ways to go about aggregating the data from the K nearest neighbors.

- Median

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- Median
- Mean
- Mode

KNN Algorithm and Implementation

KNN Algorithm

- Keep the entire dataset: (x, y)

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KNN Algorithm

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- For a query vector q :
 1. Find the k -closest data point(s) x^*
 2. Predict y^*

Challenges and Extensions

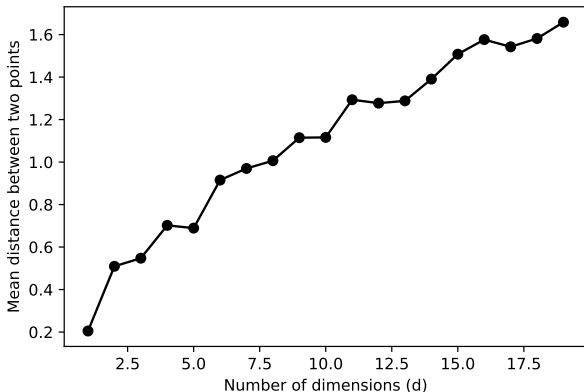
Curse of Dimensionality

With an increase in the number of dimensions:

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1. the distance between points starts to increase



For a uniformly random dataset

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Curse of Dimensionality

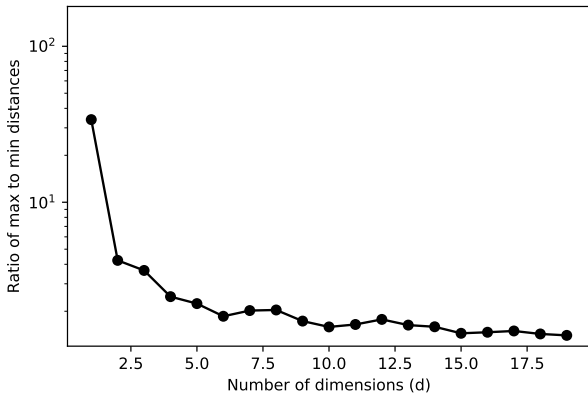
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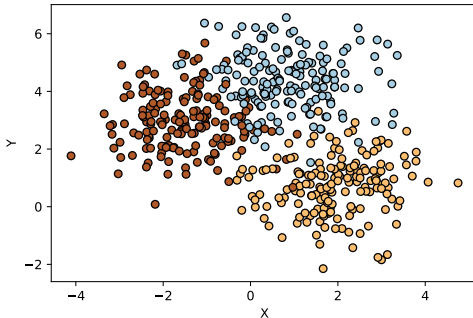
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Approximate Nearest Neighbors

Doing an exhaustive search over all the points is time consuming, especially if you have a large number of data points.



Example of a big dataset

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Such techniques include:

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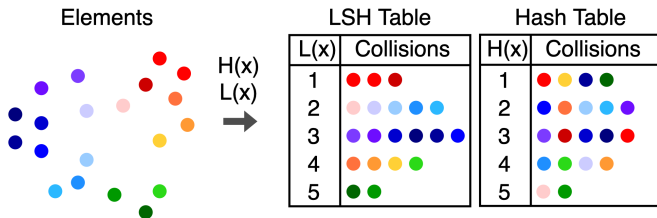
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- Vector approximation files
- Greedy search in proximity neighborhood graphs

Locality sensitive hashing

Normal hash functions $H(x)$ try to keep the collision of points across bins uniform.

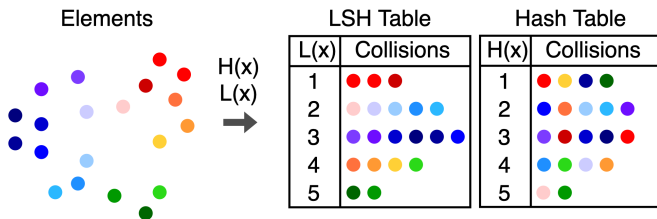


Example of a big dataset

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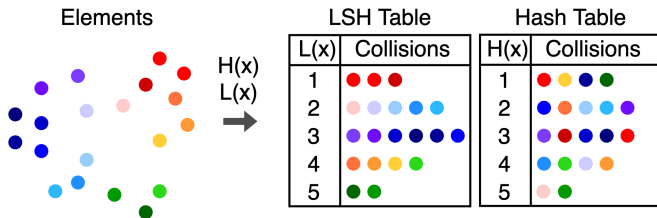


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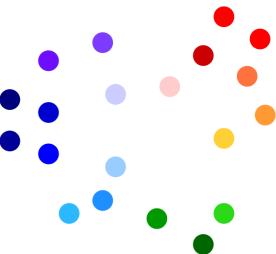
A locality sensitive hash (LSH) function $L(x)$ would be designed such that similar values are mapped to similar bins.

For such cases, all elements in a bin would be given the same label, which again can be decided on the basis of different aggregation methods



Example of a big dataset

Elements



$H(x)$
 $L(x)$



LSH Table

L(x)	Collisions
1	
2	
3	
4	
5	

Hash Table

H(x)	Collisions
1	
2	
3	
4	
5	

Practice and Summary

Pop Quiz: KNN Concepts

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2. Why is feature scaling important for KNN?
3. In which scenarios would you prefer KNN over parametric methods?
4. What is the time complexity of finding k nearest neighbors naively?

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- **Distance Metrics:** Choice affects performance significantly
- **Curse of Dimensionality:** Performance degrades in high dimensions
- **Scalability:** Approximate methods needed for large datasets