K-Nearest Neighbors

Nipun Batra

IIT Gandhinagar

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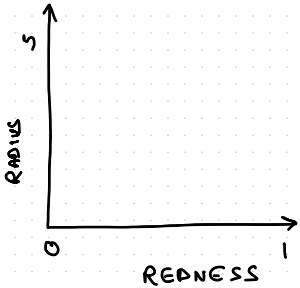
Introduction and Fundamentals

CLASSIFICATION



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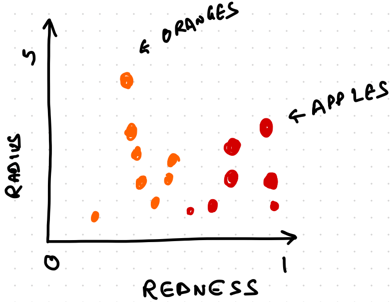

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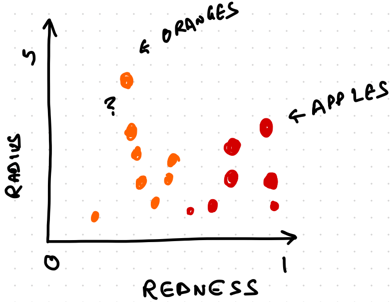

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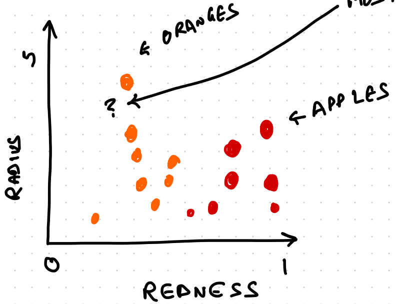
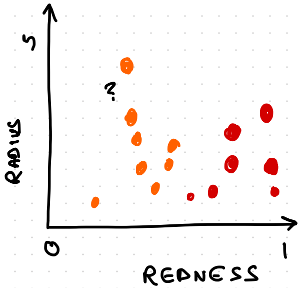
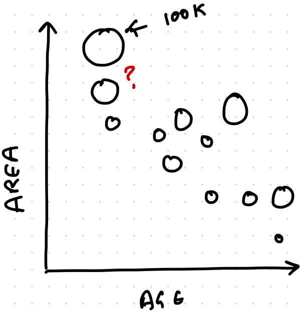


MOST LIKELY AN ORANGE ∵ "SIMILAR" TO ORANGES IN ATTRIBUTES

CLASSIFICATION



REGRESSION



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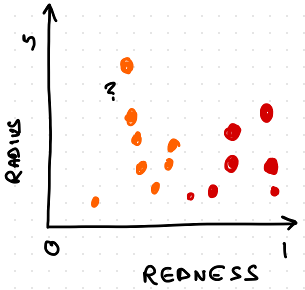
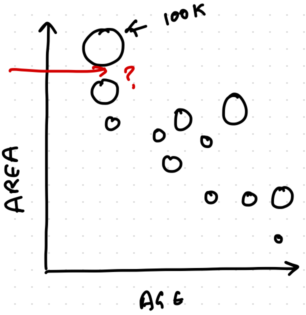
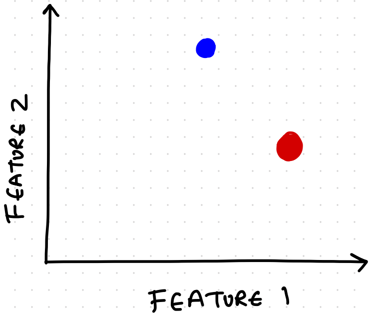


REGRESSION

LIKELY CLOSE to 100K AS "SIMILAR" TO HOMES OF THAT PRICE



VORONOI DIAGRAM FOR 1-NN



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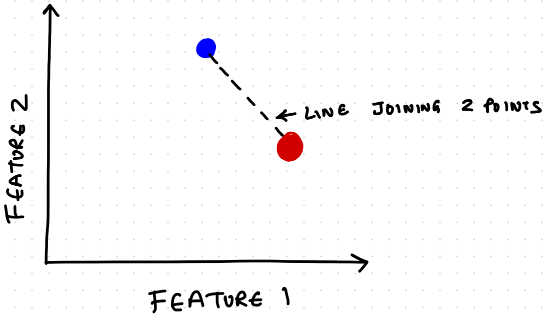

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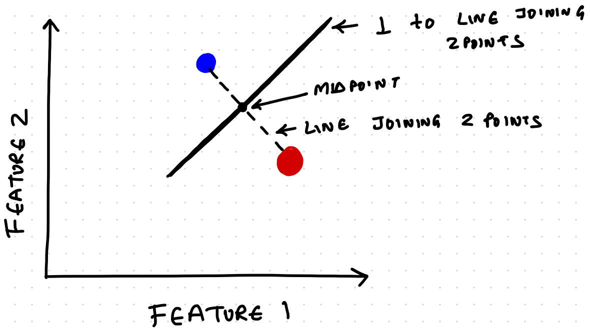

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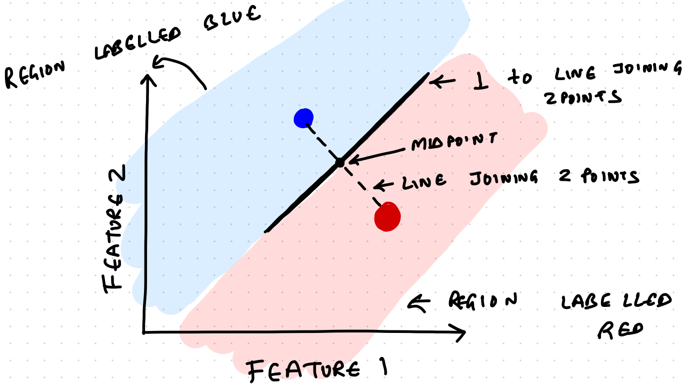

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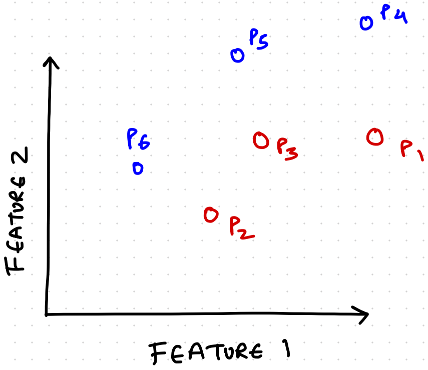

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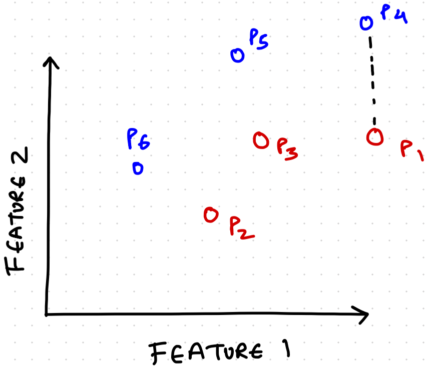
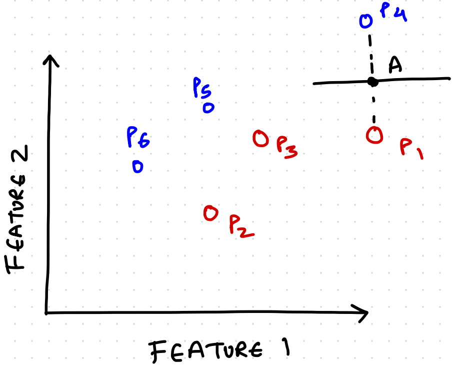


VORONOI DIAGRAM FOR 1-NN

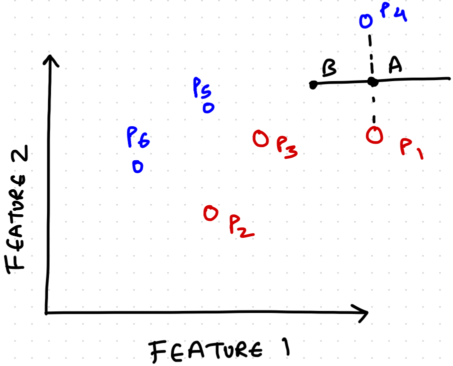
A: MID PT B/W P_1 & P_4



VORONOI DIAGRAM FOR 1-NN

A: MID PT B/W P_1 & P_4

B: CLOSER TO P_3 than P_1



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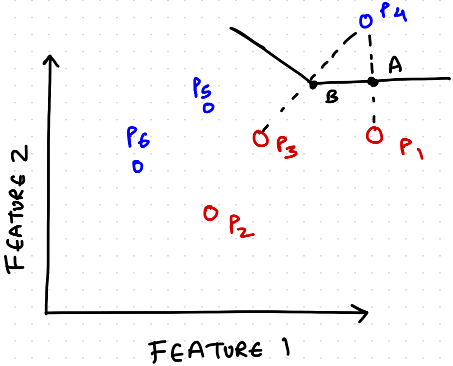
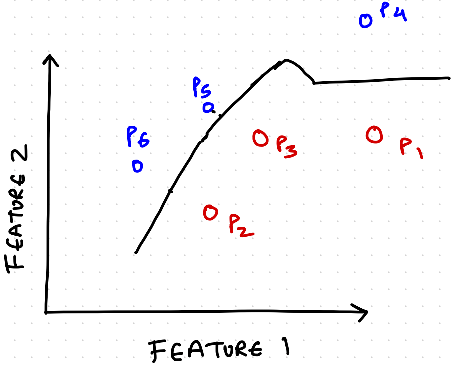


VORONOI DIAGRAM FOR 1-NN

DECISION BOUNDARY IS PIECE-WISE LINEAR



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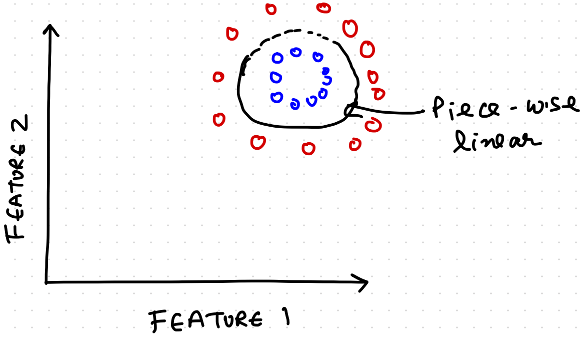
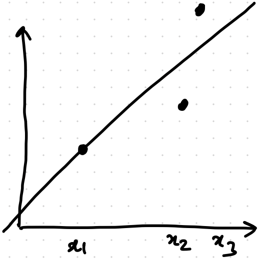
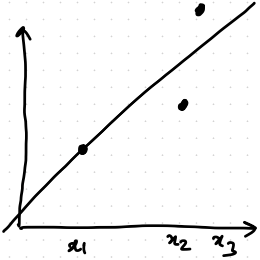


LINEAR REGRESSION



1NN REGRESSION

LINEAR REGRESSION



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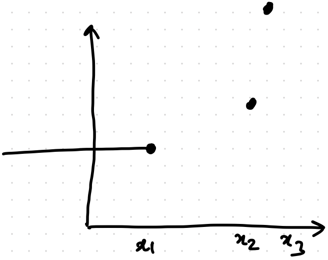

$x < x_1$: NN is (x_1, y_1)

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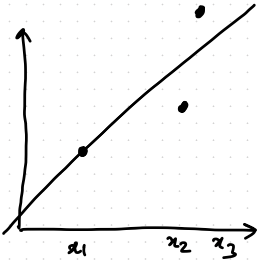

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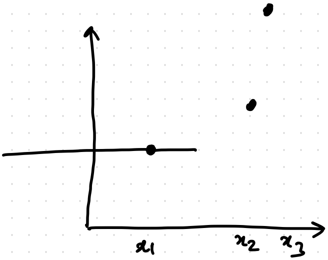
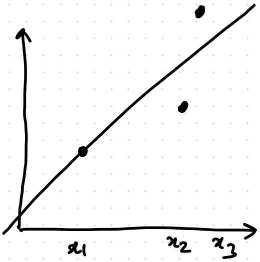


$x < x_1$: NN is (x_1, y_1)

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

LINEAR REGRESSION



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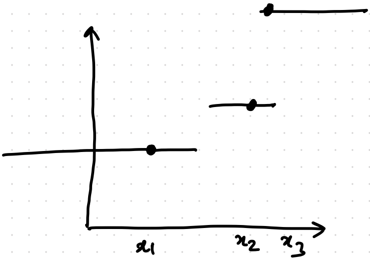

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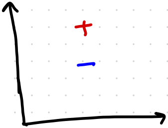
$x < \frac{x_1+x_2}{2}$: NN is (x_1, y_1)

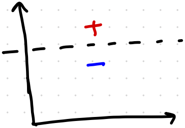
$\frac{x_1+x_2}{2} < x < \frac{x_2+x_3}{2}$: NN is (x_2, y_2)

KNN IS NON-PARAMETRIC



LINEAR MODEL

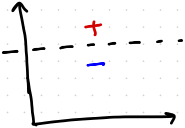
KNN IS NON-PARAMETRIC



LINEAR MODEL

DECSⁿ BOUNDARY $y = mx + c$ (# params = 2)

KNN IS NON-PARAMETRIC



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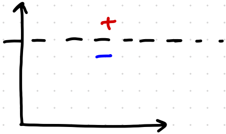
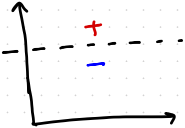
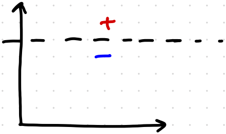


KNN (K=1)

Decs^n BOUNDARY (LIKE $y = mx + c$)

KNN IS NON-PARAMETRIC





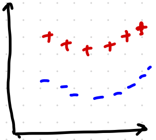
LINEAR MODEL

DECS^n BOUNDARY $y = mx + c$ (# params = 2)

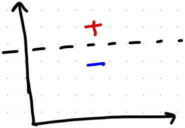
KNN (K=1)

DECS^n BOUNDARY (LIKE $y = mx + c$)

ADD DATA

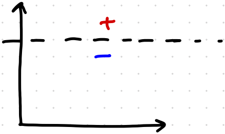


KNN IS NON-PARAMETRIC



LINEAR MODEL

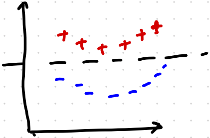
DECS^{N} BOUNDARY $y = mx + c$ (# params = 2)



KNN (K=1)

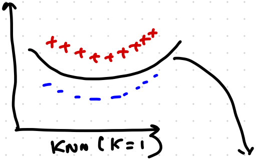
DECS^{N} BOUNDARY (LIKE $y = mx + c$)

ADD DATA



LINEAR MODEL

DECS^{N} BOUNDARY $y = mx + c$ (2 params)



KNN (K=1)

PARAMS >> 2 (AT LEAST CUBIC)

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 **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.

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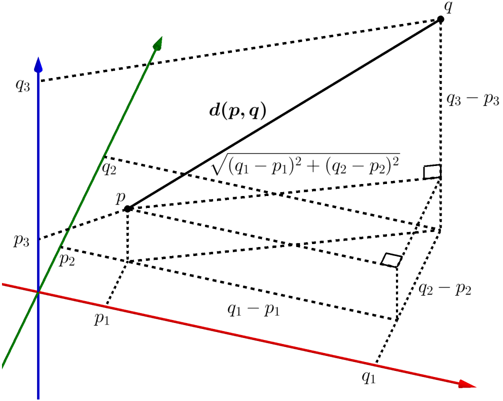

Euclidean Distance

Important Considerations: Distance Metric

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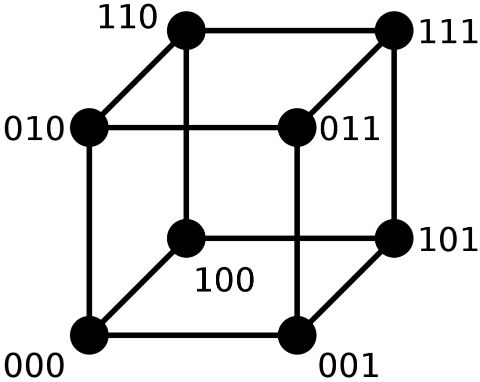

Hamming Distance

Important Considerations: Distance Metric

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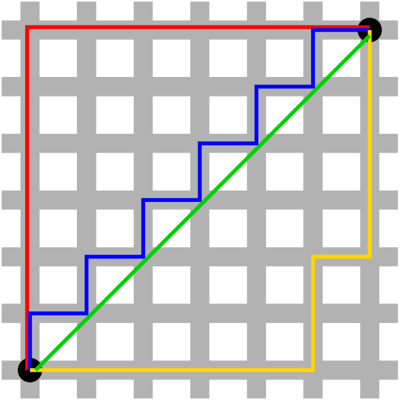

Manhattan Distance

Important Considerations: Value of K

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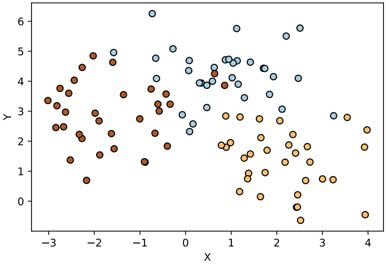
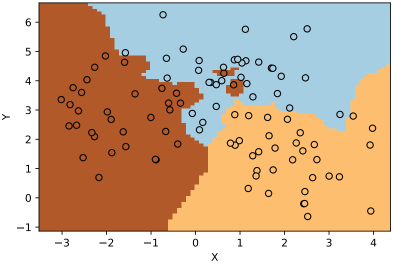
Low values of K will result in each point having a very high influence on the final output $\implies$ noise will influence the result
High values of K will result in smoother decision boundaries $\implies$ lower variance but also higher bias

Important Considerations: Value of K

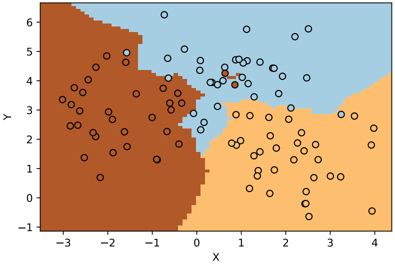


Dataset

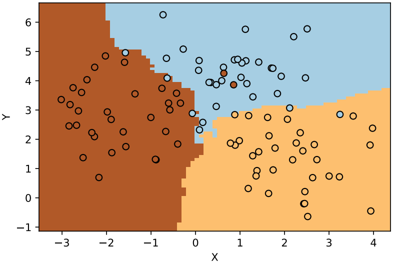


K = 1 High Variance

Important Considerations: Value of K



K = 3



K = 9 High Bias

Aggregating data

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

- 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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  2. Predict y^*

Challenges and Extensions

Curse of Dimensionality

With an increase in the number of dimensions:

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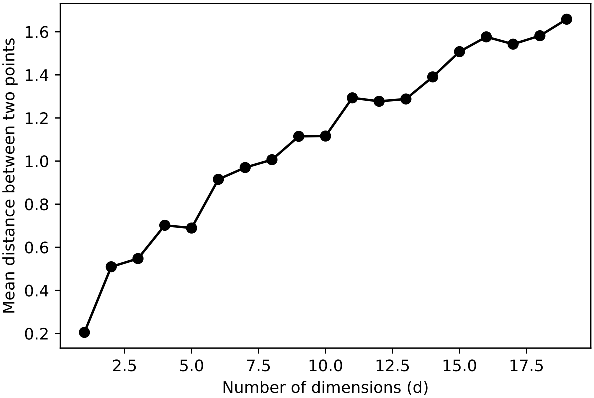
1. the distance between points starts to increase



For a unifromly random dataset

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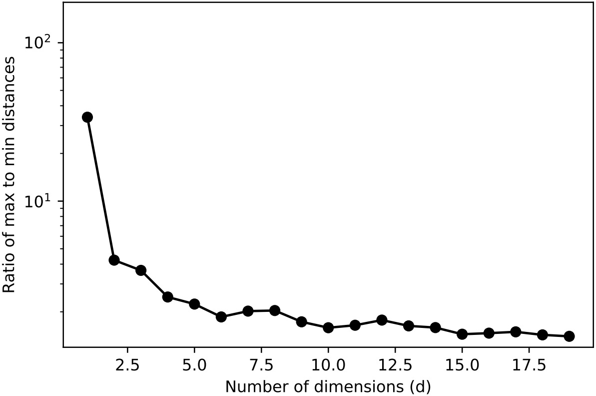


For a unifromly random dataset

Curse of Dimensionality

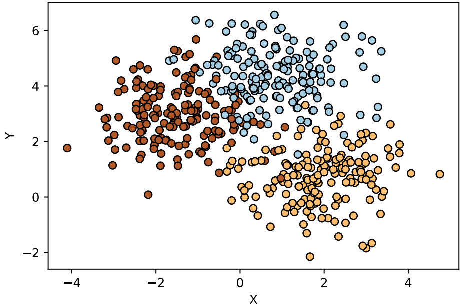
With an increase in the number of dimensions:

1. the distance between points starts to increase
2. the variation in distances between points starts to decrease

Due to this, distance metrics lose their efficacy as a similarity metric.

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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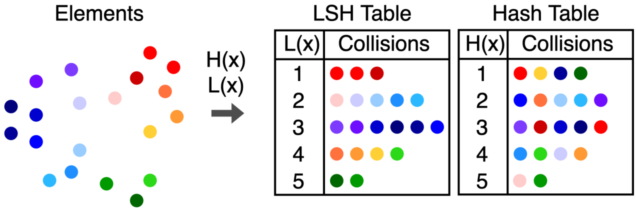
- Locality sensitive hashing
- Vector approximation files
- Greedy search in proximity neighborhood graphs

Locality sensitive hashing

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



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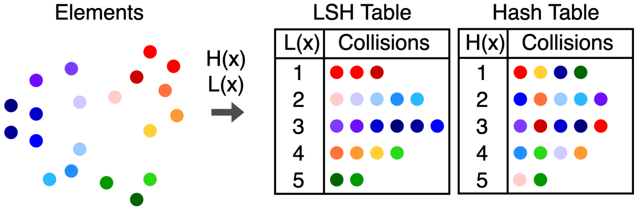
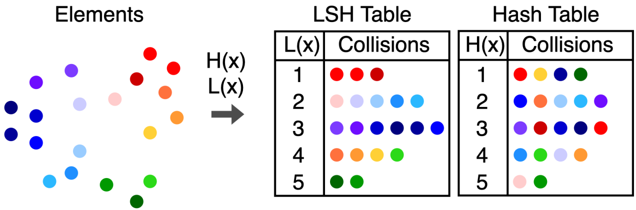
A locality sensitive hash (LSH) function $L(x)$ would be designed such that similar values are mapped to similar bins.



Example of a big dataset

Locality sensitive hashing

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



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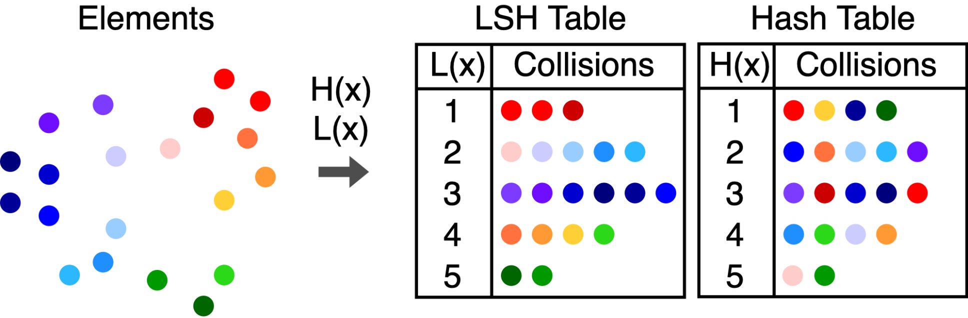
Elements
H(x)
L(x)
LSH Table
L(x)
Collisions
1
2
3
4
5
Hash Table
H(x)
Collisions
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2
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Practice and Summary

Pop Quiz: KNN Concepts

1. What happens to KNN performance as k approaches n (total data points)?

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4. What is the time complexity of finding k nearest neighbors naively?

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- **Scalability**: Approximate methods needed for large datasets