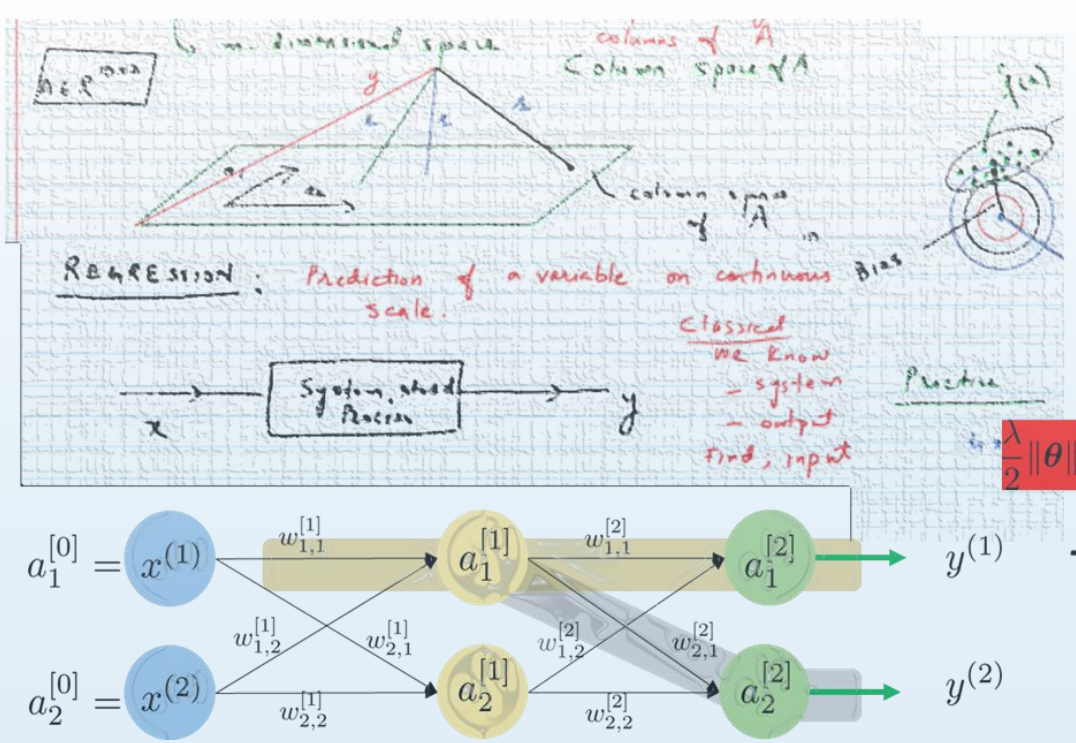
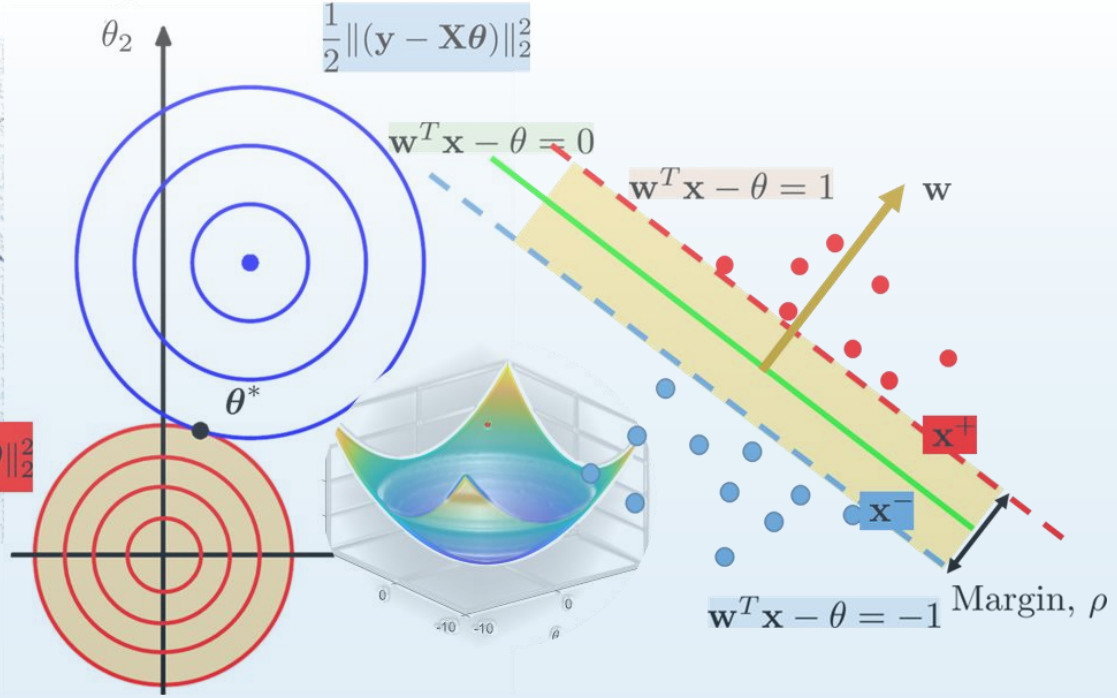




Machine Learning

kNN Algorithm: Overview, Analysis, and Convergence

School of Science and Engineering

https://www.zubairkhalid.org/ee514_2025.html

LUMS
A Not-for-Profit University

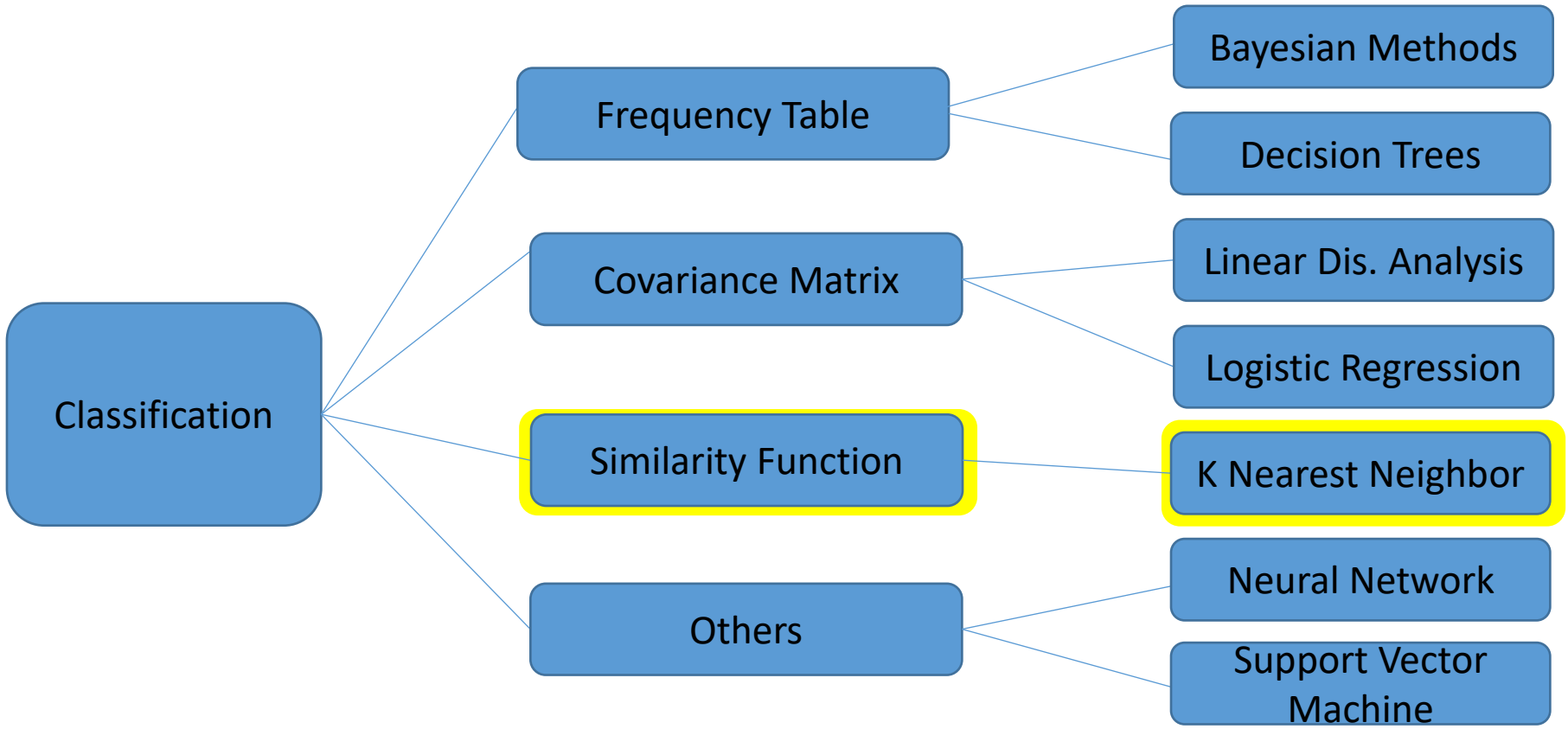
Outline

- k-Nearest Neighbor (kNN) Algorithm Overview
- Algorithm Formulation
- Distance Metrics
- Choice of k
- Algorithm Convergence
- Storage, Time Complexity Analysis
- The Curse of Dimensionality

Supervised Learning

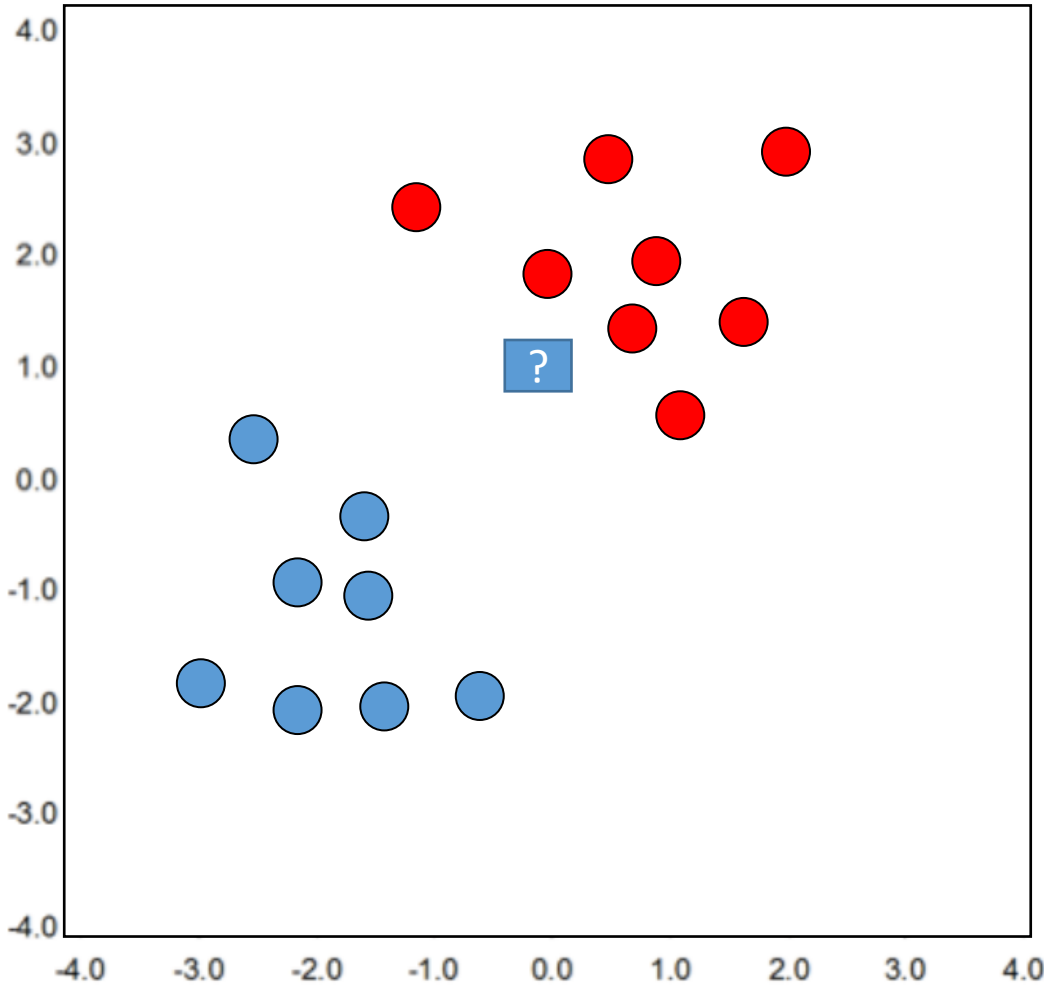
Classification Algorithms or Methods

Predicting a categorical output is called classification



k-Nearest Neighbor (kNN) Algorithm

Idea:



- Two classes, two features
- We want to assign label to unknown data point?
- Label should be red.

k-Nearest Neighbor (kNN) Algorithm

Idea:

- We have similar labels for similar features.
- We classify new test point using similar training data points.

Algorithm overview:

- Given some new test point x for which we need to predict the class y.
- Find **most similar** data-points in the training data.
- Classify x "like" these **most** similar data points.

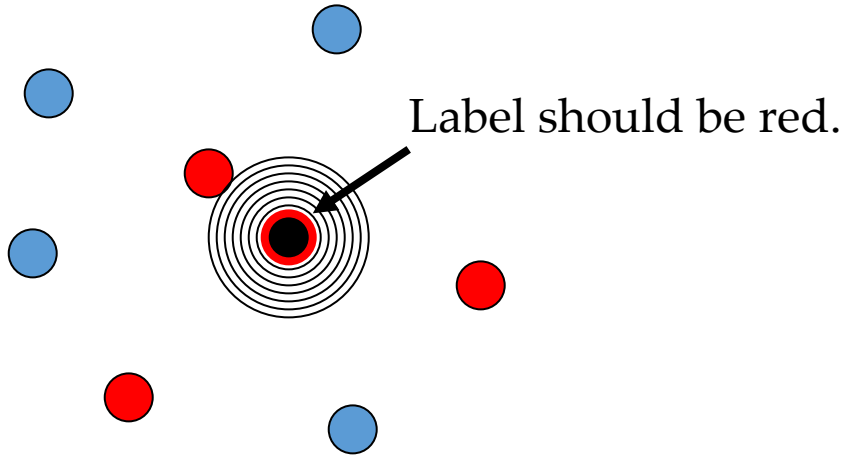
Questions:

- How do we determine the similarity?
- How many similar training data points to consider?
- How to resolve inconsistencies among the training data points?

k-Nearest Neighbor (kNN) Algorithm

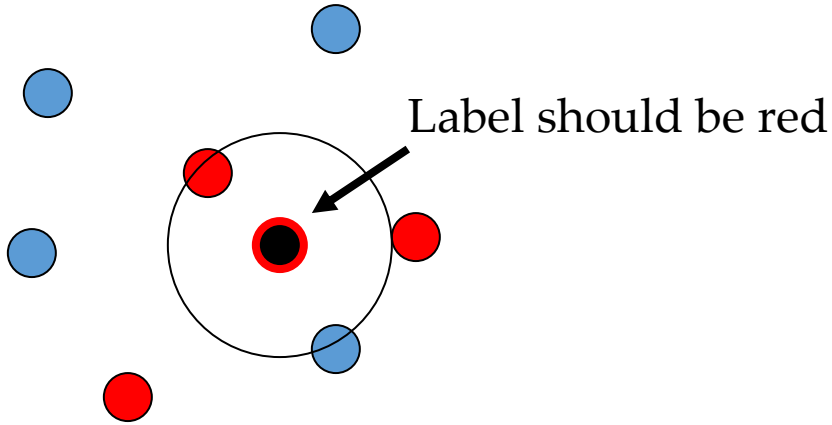
1-Nearest Neighbor:

Simplest ML Classifier
*Idea: Use the label of the **closest** known point*

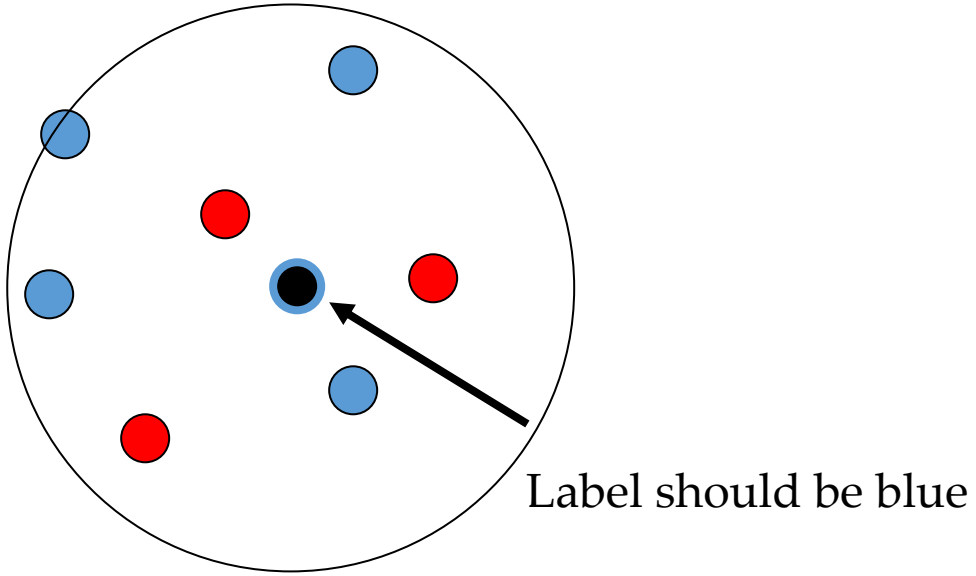


Generalization:

*Determine the label of **k** nearest neighbors and assign the most frequent label*



k=3



k=7

k-Nearest Neighbor (kNN) Algorithm

Formal Definition:

- We assume we have training data D given by

$$D = \{(\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), \ldots, (\mathbf{x_n}, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

- $\mathcal{Y} = \{1, 2, \ldots, M\}$ (M-class classification)
- For a point $\mathbf{x} \in \mathcal{X}^d$, we define a set $S_\mathbf{x} \subseteq D$ as a set of k neighbors.
- Using the function 'dist' that computes the distance between two points in $\mathcal{X}^d$, we can define a set $S_\mathbf{x}$ of size k as

$$\text{dist}(\mathbf{x}, \mathbf{x}') \geq \max_{(\mathbf{x}'', y'') \in S_\mathbf{x}} \text{dist}(\mathbf{x}, \mathbf{x}''), \quad \forall (\mathbf{x}', y') \in D \backslash S_\mathbf{x}$$

Interpretation:

Every point in D but not in $S_\mathbf{x}$ is at least as far away from $\mathbf{x}$ as the furthest point in $S_\mathbf{x}$.

k-Nearest Neighbor (kNN) Algorithm

Formal Definition:

- Using the $S_{\mathbf{x}}$, we can define a classifier as a function that gives us most frequent label of the data points in $S_{\mathbf{x}}$

$$h(\mathbf{x}) = \text{mode}(\{y'' : (x'', y'') \in S_{\mathbf{x}}\})$$

- *Instance-based learning algorithm; easily adapt to unseen data*

k-Nearest Neighbor (kNN) Algorithm

Decision Boundary:

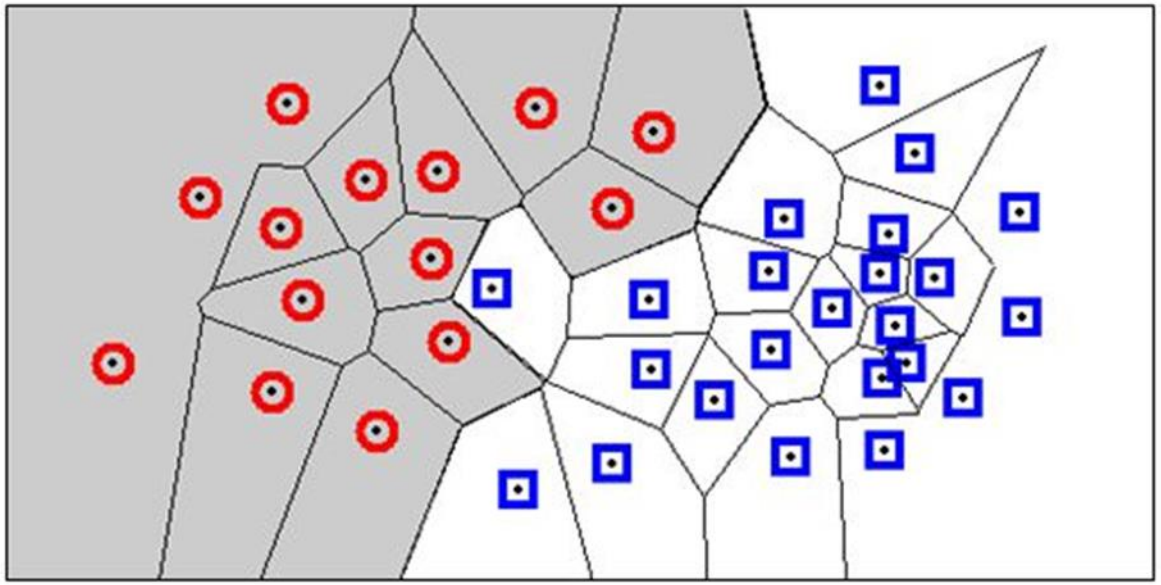
For $k = 1$, kNN defines a region, called decision boundary or region, in the space. Such division of the featue space is referred to as Voronoi partitioning.

We can define a region R_i associated with the feature point $\mathbf{x}_i$ as

$$R_i = \{\mathbf{x} : \text{dist}(\mathbf{x}, \mathbf{x}_i) < \text{dist}(\mathbf{x}, \mathbf{x}_j),\ i \neq j\}$$

For example, Voronoi partitioning using Euclidean distance in two-dimensional space.

Classification boundary changes with the change in k and the distance metric.



k-Nearest Neighbor (kNN) Algorithm

Decision Boundary:

Demonstration

https://demonstrations.wolfram.com/KNearestNeighborKNNClassifier/

k-Nearest Neighbor (kNN) Algorithm

Characteristics of kNN:

- No assumptions about the distribution of the data
- Non-parametric algorithm
  - No parameters

- Hyper-Parameters
  - k (number of neighbors)
  - Distance metric (to quantify similarity)

k-Nearest Neighbor (kNN) Algorithm

Characteristics of kNN:

- Complexity (both time and storage) of prediction increases with the size of training data.

- Can also be used for regression (average or inverse distance weighted average)
  - For example,

$$y = \frac{1}{k}\sum_{i=1}^{k} y_i, \quad (\mathbf{x}_i, y_i) \in S_{\mathbf{x}}$$

k-Nearest Neighbor (kNN) Algorithm

Practical issues:

- For binary classification problem, use odd value of k. Why?

- In case of a tie:
  - Use prior information
  - Use 1-nn classifier or k-1 classifier to decide

- Missing values in the data
  - Average value of the feature.

Outline

- k-Nearest Neighbor (kNN) Algorithm Overview
- Algorithm Formulation
- **Distance Metrics**
- Choice of k
- Algorithm Convergence
- Storage, Time Complexity Analysis
- The Curse of Dimensionality

k-Nearest Neighbor (kNN) Algorithm

We need to define distance metric to find the set of k nearest neighbors, S_x

- Recall we defined a set $S_{\mathbf{x}}$ of size k as

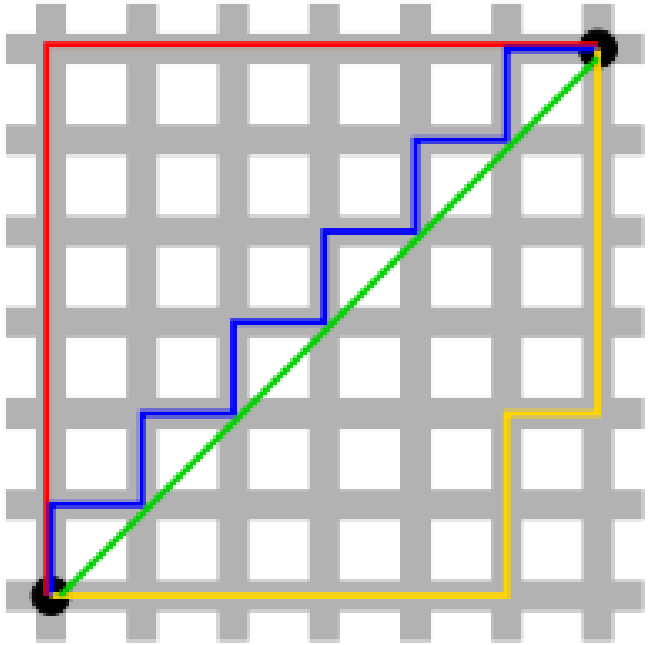
$$\text{dist}(\mathbf{x}, \mathbf{x}') \geq \max_{(\mathbf{x}'', y'') \in S_{\mathbf{x}}} \text{dist}(\mathbf{x}, \mathbf{x}''), \quad \forall (\mathbf{x}', y') \in D \backslash S_{\mathbf{x}}$$

k-Nearest Neighbor (kNN) Algorithm

Distance Metric:

- Euclidean $$\text{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_2 = \sqrt{\sum_{i=1}^{d} (x_i - x'_i)^2}$$

- Manhattan $$\text{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_1 = \sum_{i=1}^{d} |x_i - x'_i|$$



Euclidean

Manhattan
Manhattan
Manhattan

k-Nearest Neighbor (kNN) Algorithm

Norm of a vector

- p-norm of a vector $\mathbf{x} \in \mathbf{R}^d$

$$\|\mathbf{x}\|_p = \Big(\sum_{i=1}^{d} |x_i|^p\Big)^{1/p}, \quad p \geq 1$$

Properties of Norm

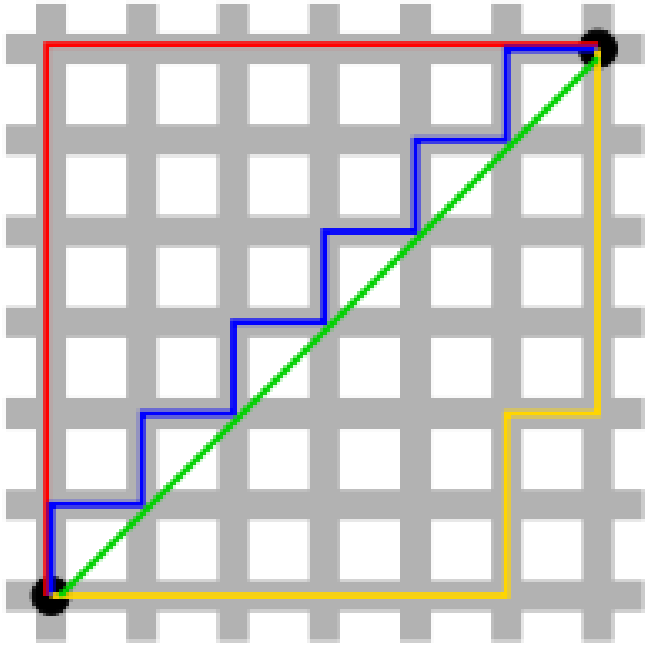
Non-negative, $\|\mathbf{x}\|_p \geq 0$

Absolutely homogenous: $\|\alpha\mathbf{x}\|_p = |\alpha|\|\mathbf{x}\|_p$

$\|\alpha\mathbf{x}\|_p = 0 \iff \mathbf{x} = 0$

Triangular inequality, $\|\mathbf{x} + \mathbf{x}'\|_p \leq \|\mathbf{x}\|_p + \|\mathbf{x}'\|_p$

$$\|\mathbf{x}\|_q \leq \|\mathbf{x}\|_p, \quad p \leq q$$



Euclidean $6\sqrt{2}$

Manhattan
Manhattan 12
Manhattan

k-Nearest Neighbor (kNN) Algorithm

Distance Metric:

- Euclidean $\quad \mathrm{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_2 = \sqrt{\sum_{i=1}^{d} (x_i - x_i')^2}$

- Manhattan $\quad \mathrm{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_1 = \sum_{i=1}^{d} |x_i - x_i'|$

- Minkowski

$$\mathrm{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_p = \Big(\sum_{i=1}^{d} (|x_i - x_i'|)^p\Big)^{1/p}, \quad p \geq 1$$

$p = 2$

$p = 1$

$p = \infty$

$$\mathrm{dist}(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|_\infty = \max_{i=1,2,\ldots,d} (|x_i - x_i'|)$$ Chebyshev Distance

k-Nearest Neighbor (kNN) Algorithm

Distance Metric:

Properties of Distance Metrics:

Non-negative, $\text{dist}(\mathbf{x}, \mathbf{x}') \geq 0$

Symmetric, $\text{dist}(\mathbf{x}, \mathbf{x}') = \text{dist}(\mathbf{x}', \mathbf{x})$

$\text{dist}(\mathbf{x}, \mathbf{x}') = 0 \iff \mathbf{x} = \mathbf{x}'$

Triangular inequality, $\text{dist}(\mathbf{x}, \mathbf{x}') \leq \text{dist}(\mathbf{x}', \mathbf{x}'') + \text{dist}(\mathbf{x}'', \mathbf{x})$

k-Nearest Neighbor (kNN) Algorithm

Distance Metric:

- For categorical vaiable, use Hamming Distance

$$\text{dist}(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^{d} 1 - \delta_{x_i - x_i'}$$

k-Nearest Neighbor (kNN) Algorithm

Cosine Distance

- Cosine distance, though does not satisfy the properties we defined for distance metric, is however used to meaasure the angular distance between the vectors.
- It follows from the standard definition of inner (dot) product between the vectors, that is,

$$\mathbf{x}^T\mathbf{x}' = \|\mathbf{x}\|_2\|\mathbf{x}'\|_2 \cos\theta$$

or

$$\cos\theta = \frac{\mathbf{x}^T\mathbf{x}'}{\|\mathbf{x}\|_2\|\mathbf{x}'\|_2}$$

What is the range of values of angular distance and what is the interpretation of these values?

k-Nearest Neighbor (kNN) Algorithm

Practical issues in computing distance:

- Mismatch in the values of data
  - Issue: Distance metric is mapping from d-dimensional space to a scaler. The values should be of the same order along each dimension.

  - Solution: Data Normalization

Outline

- k-Nearest Neighbor (kNN) Algorithm Overview
- Algorithm Formulation
- Distance Metrics
- **Choice of k**
- Algorithm Convergence
- Storage, Time Complexity Analysis
- The Curse of Dimensionality

k-Nearest Neighbor (kNN) Algorithm

Choice of k:

- k=1

Sensitive to noise

High variance

Increasing k makes algorithm less sensitive to noise

- k=n

Decreasing k enables capturing finer structure of space

Idea: Pick k not too large, but not too small (depends on data)

How?

k-Nearest Neighbor (kNN) Algorithm

Choice of k:

- Learn the best hyper-parameter, k using the data.
- Split data into training and validation.
- Start from k=1 and keep iterating by carrying out (5 or 10, for example) cross-validation and computing the loss on the validation data using the training data.
- Choose the value for k that minimizes validation loss.
- This is the only learning required for kNN.

Outline

- k-Nearest Neighbor (kNN) Algorithm Overview
- Algorithm Formulation
- Distance Metrics
- Choice of k
- **Algorithm Convergence**
- Storage, Time Complexity Analysis
- The Curse of Dimensionality

k-Nearest Neighbor (kNN) Algorithm

Error Convergence:

We wish to analyze the error rate of the kNN classifier.

We will show that the error of 1-NN classifer converges as number of points in D increases.

To show the convergence, we will derive that 1-NN classifier is only a factor 2 worse than the best possible classifier.

k-Nearest Neighbor (kNN) Algorithm

Learning Problem

We represent the entire training data as

$$D = \{(\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), \ldots, (\mathbf{x_n}, y_n)\} \subseteq \mathcal{X}^d \times \mathcal{Y}$$

Recall a problem in hand. We want to develop a model that can predict the label for the input for which label is unknown using kNN.

We assume that the data points $(\mathbf{x_i}, y_i)$ are drawn from some (unknown) distribution $P(X, Y)$.

k-Nearest Neighbor (kNN) Algorithm

Bayes Optimal Classifier

If we assume that we know $P(y|\mathbf{x})$, we can predict the most likely label as follows:

$$y^* = h(\mathbf{x}) = \max_y P(y|\mathbf{x})$$

Error Rate:

Probability of misclassification or error rate can be computed as

$$\epsilon_{\text{Bayes Classifier}} = 1 - P(h(\mathbf{x})|\mathbf{x}) = 1 - P(y^*|\mathbf{x})$$

k-Nearest Neighbor (kNN) Algorithm

Error Convergence:

We want to determine 1-NN classification error as $n \to \infty$.

For a test-point $\mathbf{x}$, we assume 1-NN classifier assigns label of $\mathbf{x}_{NN}$ to $\mathbf{x}$.

We can easily show that (consequence of filling of space)

$$\lim_{n \to \infty} \text{dist}(\mathbf{x}, \mathbf{x}_{\text{NN}}) \to 0$$

Error Rate:

We want to determine probability of misclassification, that is, the probability of having different labels of $\mathbf{x}$ and $\mathbf{x}_{NN}$.

Reference: Cover, Thomas, and, Hart, Peter. Nearest neighbor pattern classification[J]. IEEE Transactions on Information Theory, 1967, 13(1): 21-27

k-Nearest Neighbor (kNN) Algorithm

Error Convergence:

Probability that y is the correct label of $\mathbf{x}$ but $\mathbf{x}_{NN}$ has a different label:

$$P(y|\mathbf{x})\big(1 - P(y|\mathbf{x}_{NN})\big)$$

Probability that y is the incorrect label of $\mathbf{x}$ but $\mathbf{x}_{NN}$ has y label:

$$P(y|\mathbf{x}_{NN})\big(1 - P(y|\mathbf{x})\big)$$

Error Rate:

Probability of misclassification or error rate can be computed using the law of total probability

$$\epsilon_{\text{NN}} = P(y|\mathbf{x}_{NN})\big(1 - P(y|\mathbf{x})\big) + P(y|\mathbf{x})\big(1 - P(y|\mathbf{x}_{NN})\big)$$

k-Nearest Neighbor (kNN) Algorithm

Error Convergence:

Bound on Error Rate:

$$\epsilon_{\text{NN}} = P(y|\mathbf{x}_{NN})\big(1 - P(y|\mathbf{x})\big) + P(y|\mathbf{x})\big(1 - P(y|\mathbf{x}_{NN})\big)$$

Using

$$\lim_{n\to\infty} \text{dist}(\mathbf{x}, \mathbf{x}_{\text{NN}}) \to 0 \Rightarrow \mathbf{x} \to \mathbf{x}_{NN}$$

We obtain

$$\epsilon_{\text{NN}} = 2P(y|\mathbf{x})\big(1 - P(y|\mathbf{x})\big)$$

$$\epsilon_{\text{NN}} \leq 2\big(1 - P(y|\mathbf{x})\big)$$

Noting $P(y|\mathbf{x}) \leq 1$

$$\epsilon_{\text{NN}} \leq 2\epsilon_{\text{Bayes Classifier}}$$

1-NN classifier is only a factor 2 worse than the best possible classifier.

Outline

- k-Nearest Neighbor (kNN) Algorithm Overview
- Algorithm Formulation
- Distance Metrics
- Choice of k
- Algorithm Convergence
- **Storage, Time Complexity Analysis**
- The Curse of Dimensionality

k-Nearest Neighbor (kNN) Algorithm

Algorithm Computational and Storage Complexity:

Input/Output:

- We have a feature vector, $\mathbf{x}$ for which we want to predict label y.
- We have k and dist function.

Steps:

- We defined a set $S_{\mathbf{x}}$ of size k as

$$\text{dist}(\mathbf{x}, \mathbf{x}') \geq \max_{(\mathbf{x}'', y'') \in S_{\mathbf{x}}} \text{dist}(\mathbf{x}, \mathbf{x}''), \quad \forall (\mathbf{x}', y') \in D \backslash S_{\mathbf{x}}$$

- Classifier that gives us most frequent label of the data points in $S_{\mathbf{x}}$

$$h(\mathbf{x}) = \text{mode}(\{y'' : (x'', y'') \in S_{\mathbf{x}}\})$$

k-Nearest Neighbor (kNN) Algorithm

Algorithm:

Steps:

Computational Complexity

1. *Find distance between given test point and feature vector of every point in D.*

   Noting n number of data points we have and each feature vector $\mathbf{x}$ is d-dimensional. $\mathcal{O}(dn)$

2. *Find k points in D closest to the given test point vector to form a set S_X.*

   Finding k-th smallest distance using median of medians method. $\mathcal{O}(n)$

   Finding k data-points in D with distance less than the k-th smallest distance $\mathcal{O}(n)$

3. *Find the most frequent label in the set S_x and assign it to the test point.* $\mathcal{O}(k)$

Computational Complexity: $\mathcal{O}(dn)$

Space Complexity: $\mathcal{O}(dn)$

Outline

- k-Nearest Neighbor (kNN) Algroithm Overview
- Algorithm Formulation
- Distance Metrics
- Choice of k
- Algorithm Convergence
- Storage, Time Complexity Analysis
- **The Curse of Dimensionality**

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality:

- Refers to the problems or phenomena associated with classifying, analyzing and organizing the data in high-dimensional spaces that do not arise in low-dimensional settings.

- For high-dimensional datasets, the **size** of data **space** is **huge**.

- In other words, the size of the feature space grows exponentially with the number of dimensions (d) of the data sets.

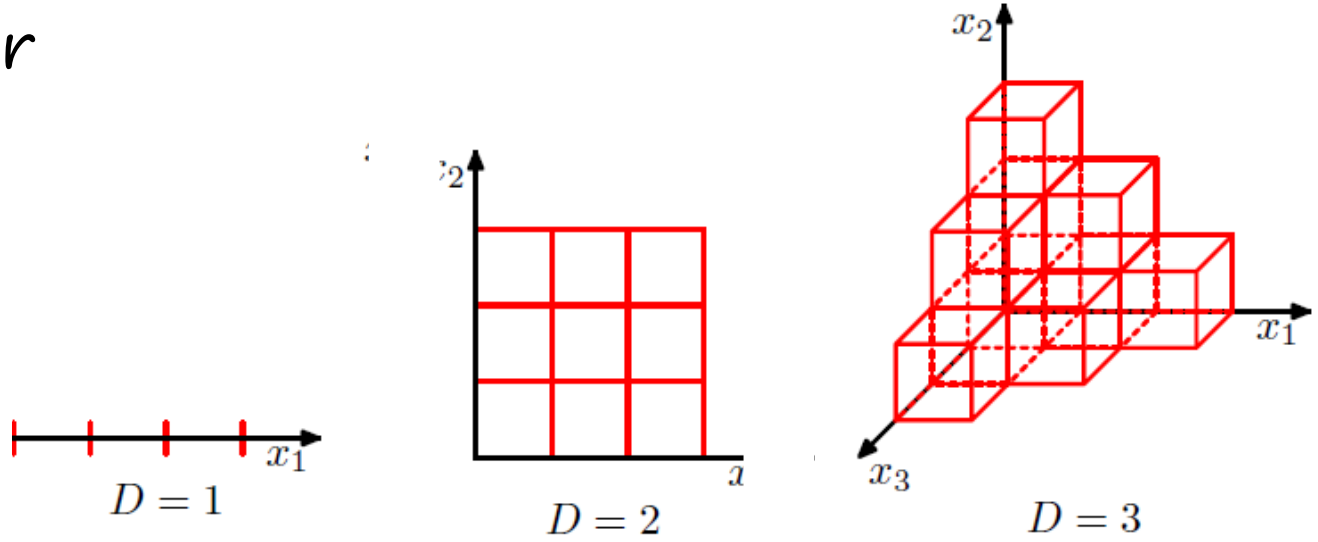
- To ensure the points stay close to each other, the size (n) of the data set must also have exponential growth. That means, we need a very large dataset to maintain the density of points in the high dimensional space.

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality:

- For high-dimensional datasets, the **size** of data **space** is **huge**.

For an exponentially large number of cells, we need an exponentially large amount of training data to ensure that the cells are not empty.



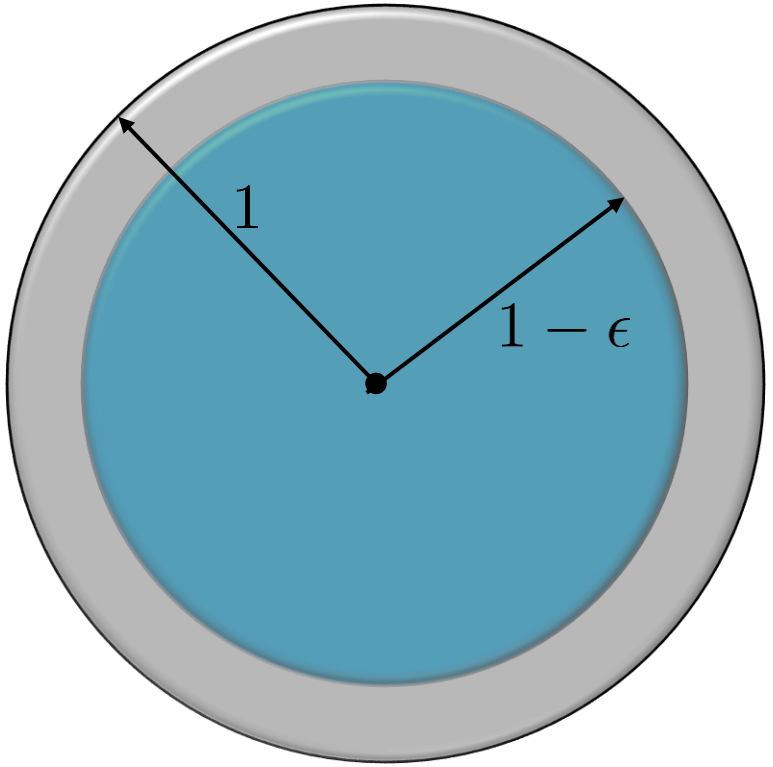
Ref: CB

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality:

Consider a ball of radius r defined as

$$B(r) = \{\|\mathbf{x}\|_2 \leq r \,|\, \mathbf{x} \in \mathbf{R}^d\}$$



Volume of a ball of radius r

$$V(d) = K_D r^D$$

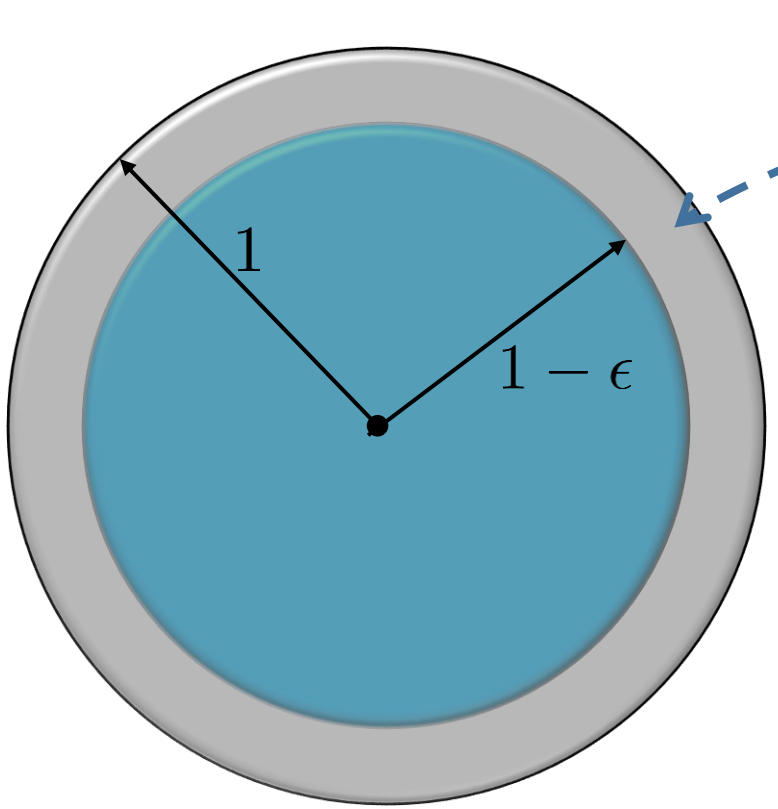
Fraction of a volume between the balls of radius 1 and radius $1-\epsilon$

$$\frac{V(1) - V(1-\epsilon)}{V(1)} = 1 - (1-\epsilon)^D$$

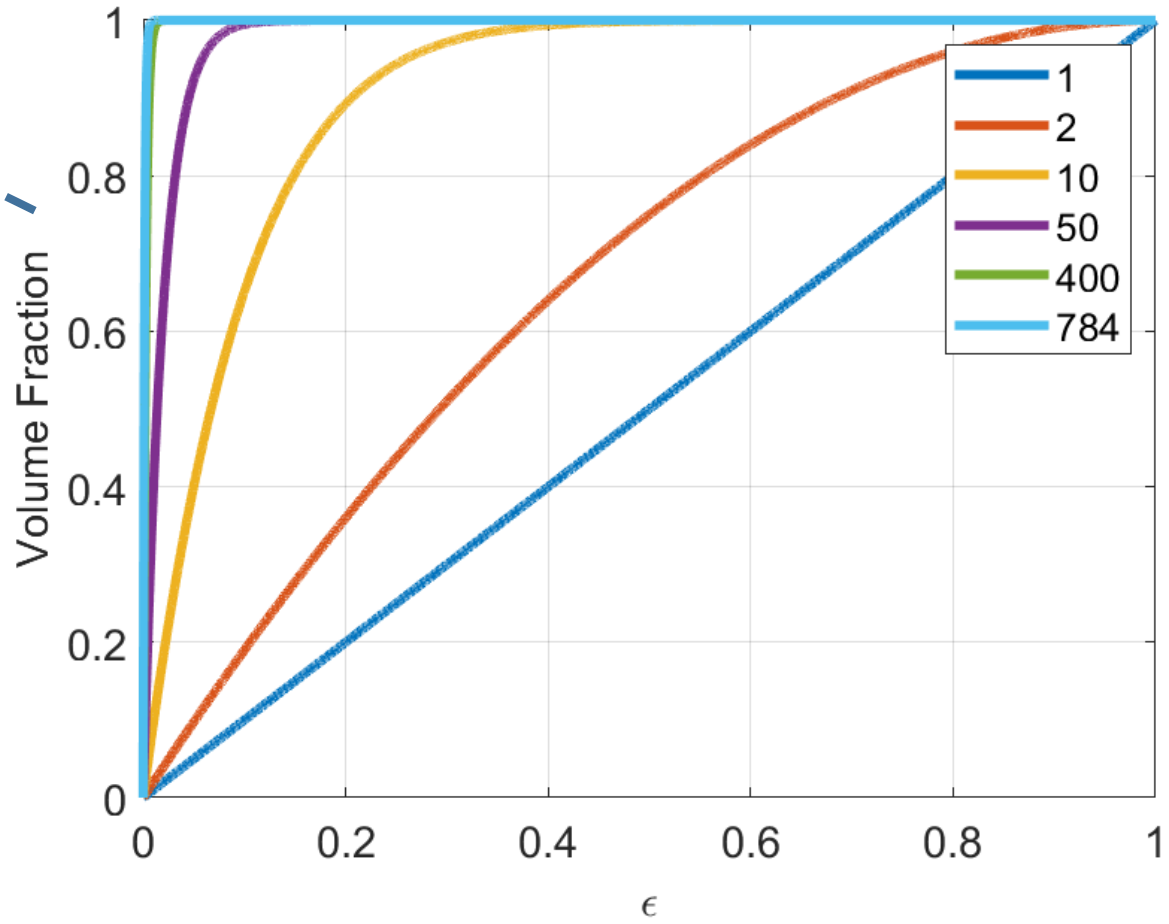
$$K_D = \frac{\pi^{D/2}}{\Gamma(\frac{n}{2}+1)}$$

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality:

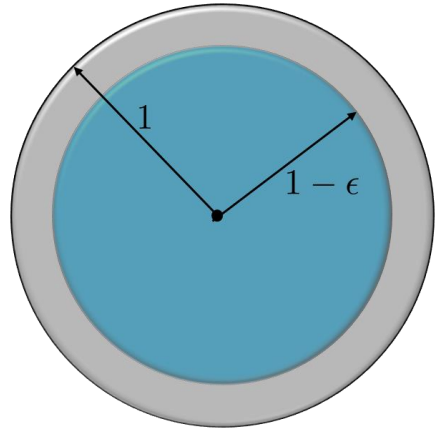


$$1-(1-\epsilon)^D$$



k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality (Another viewpoint):



Calculate Probabilities that a uniformly distributed point is inside

$\epsilon = 0.1$

the shell: $1-(1-\epsilon)^D$

the inner ball: $(1-\epsilon)^D$

D = 1	2	10	50	400	784
0.1	0.19	0.65	0.995	1.000	1.000
0.9	0.81	0.35	0.005	0.000	0.000

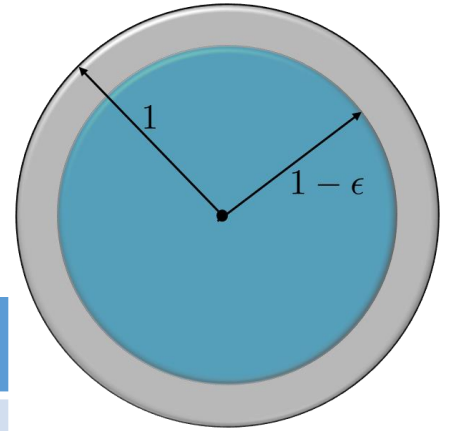
For $D = 50$, 5 out of 1000 data-points would be inside the inner ball.

For $D = 400$, $(1-\epsilon)^D = 4.9774e-19$; almost all points lie on the surface of the ball.

If you take a test point on the origin and $D = 400$, (almost) every point is at the same (Euclidean) distance from the origin.

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality (Another viewpoint):



Calculate Probabilities that a uniformly distributed point is inside

$\epsilon = 0.01$

the shell: $1-(1-\epsilon)^D$

the inner ball: $(1-\epsilon)^D$

D = 1	2	10	50	400	784
0.01	0.02	0.096	0.395	0.982	0.999
0.99	0.98	0.904	0.605	0.018	0.0004

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality:

Connection with kNN:

- With the increase in the number of features or number of dimensions of the feature space, data-points are never near to one another.

- kNN algorithm carries out predictions about the test point assuming we have data-points near to the test point that are similar to the test point.

- As we do not have neighbors in the high dimensional space, kNN becomes vulnerable and sensitive to the Curse of Dimensionality.

k-Nearest Neighbor (kNN) Algorithm

The Curse of Dimensionality: **Why does kNN work?**

Two related explanations;

- Real-world data in the higher dimensional space is confined to a region with effective lower dimensionality.
  - Dimensionality Reduction (to be covered next)

- Real-world data exhibits smoothness that enables us to make predictions exploiting interpolation techniques.

- For example,
  - Data along a line or a plane in higher dimensional space
  - detection of orientation of object in an image; data lies on effectively 1 dimensional manifold in probably 1million dimensional space.
  - Face recognition in an image (50 or 71 features).
  - Spam filter

k-Nearest Neighbor (kNN) Algorithm

Reference:

Overall:

- https://www.cs.cornell.edu/courses/cs4780/2018fa/

- CB: sec 1.1

- HTF: 13.3 up to end of 13.3.2

- The curse of dimensionality
  - CB: 1.4
  - KM: 1.4.3
  - N. Kouiroukidis and G. Evangelidis, "The Effects of Dimensionality Curse in High Dimensional kNN Search," 2011 15th Panhellenic Conference on Informatics, Kastonia, 2011, pp. 41-45, doi: 10.1109/PCI.2011.45.