Nearest Neighbor Classification

Machine Learning
Fall 2017

THE UNIVERSITY OF UTAH

This lecture

- K-nearest neighbor classification
  - The basic algorithm
  - Different distance measures
  - Some practical aspects
- Voronoi Diagrams and Decision Boundaries
  - What is the hypothesis space?
- The Curse of Dimensionality

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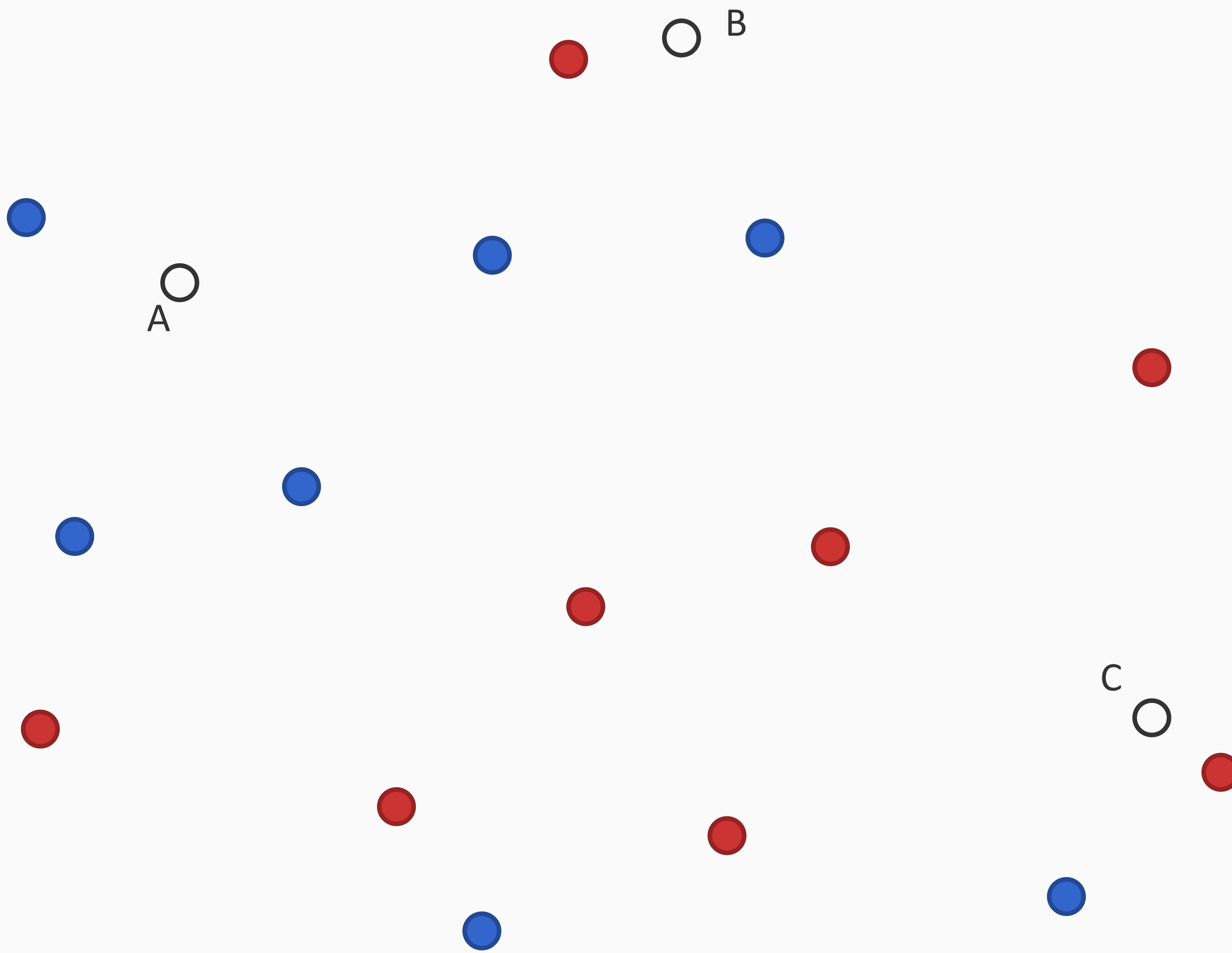
How would you color the blank circles?



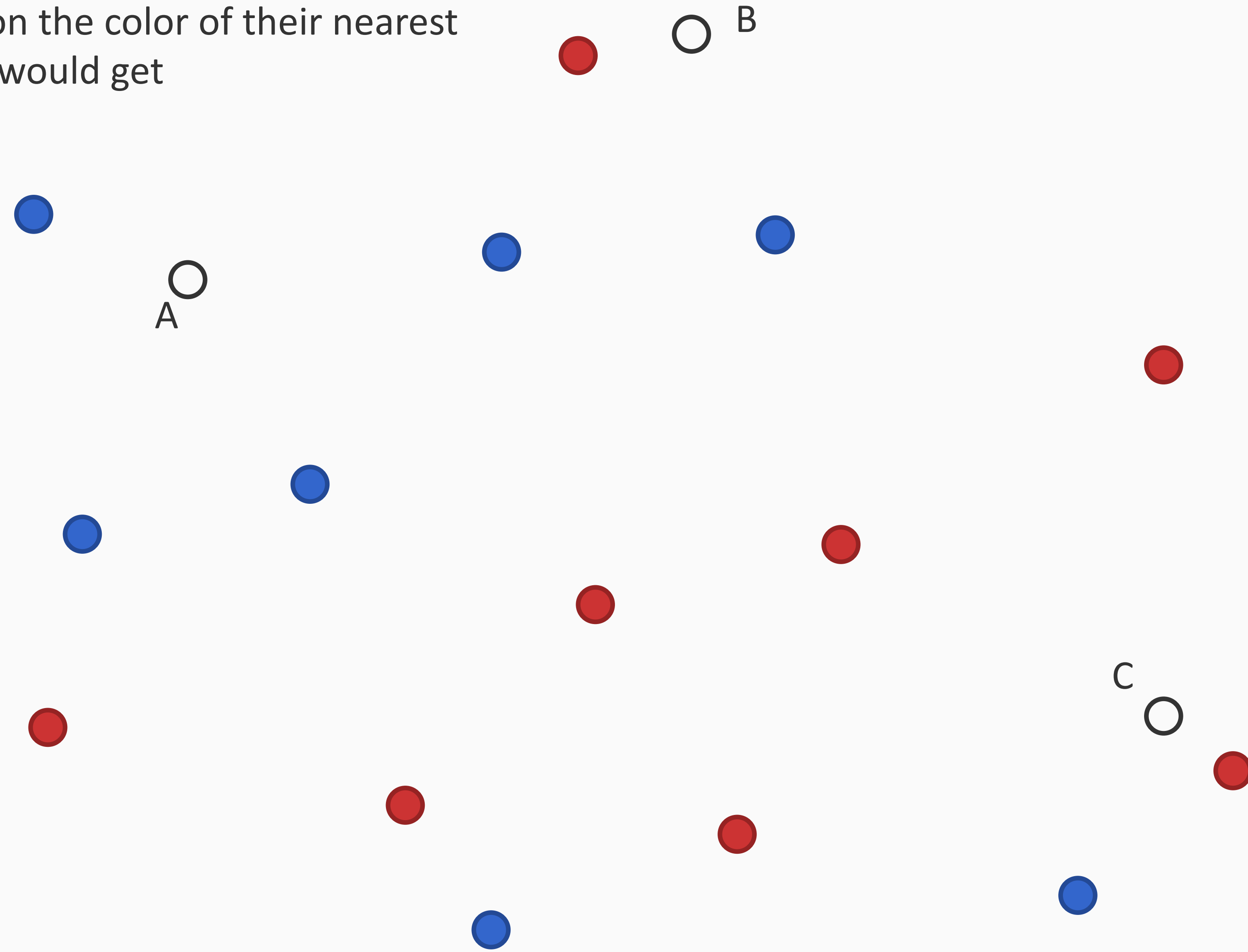
How would you color the blank circles?

If we based it on the color of their nearest neighbors, we would get

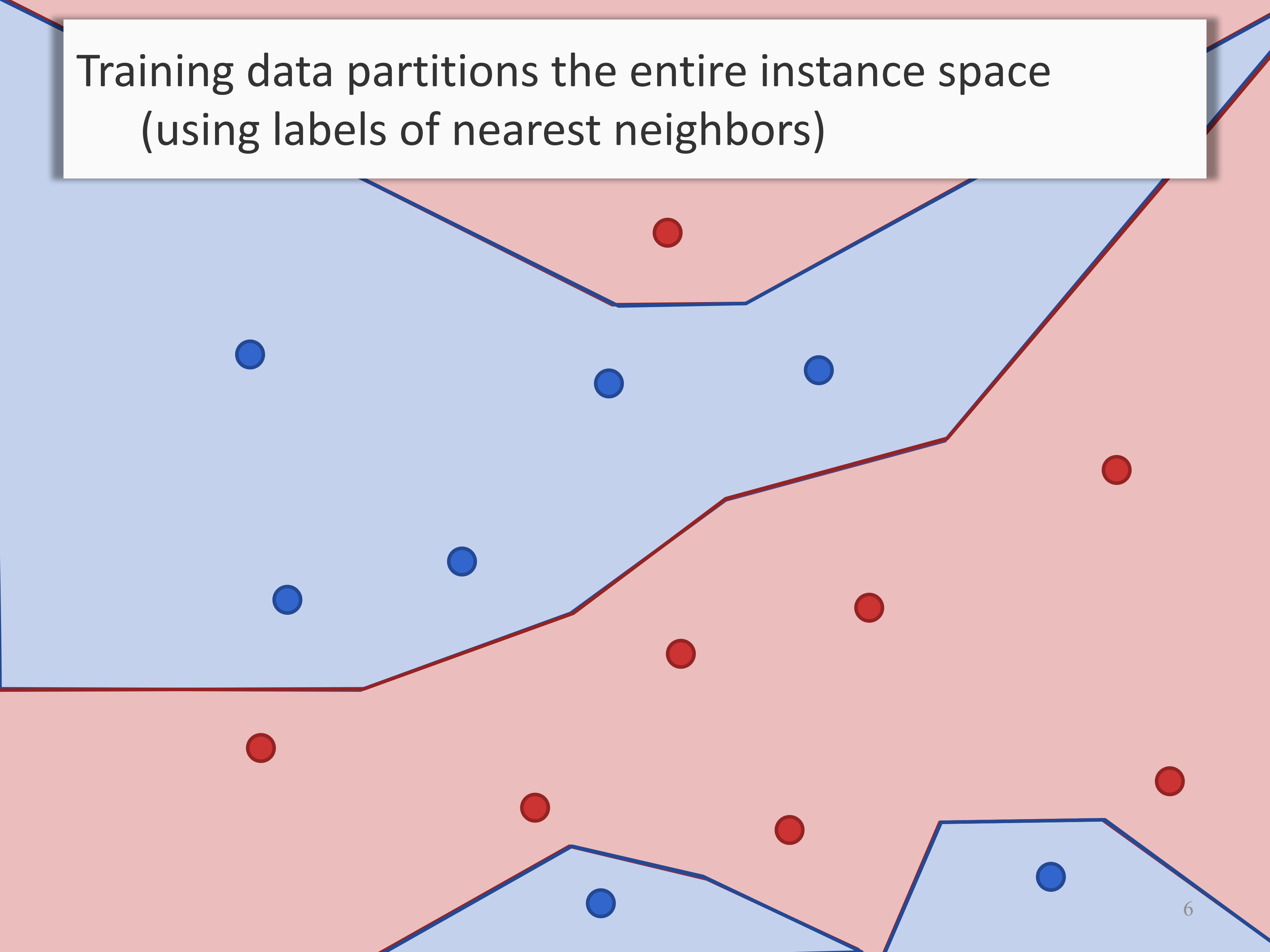
A: Blue

B: Red

C: Red



Training data partitions the entire instance space (using labels of nearest neighbors)



Nearest Neighbors: The basic version

- Training examples are vectors $\mathbf{x}_i$ associated with a label y_i
  - E.g. $\mathbf{x}_i$ = a feature vector for an email, $\mathbf{y}_i$ = SPAM

- Learning: Just store all the training examples

- Prediction for a new example $\mathbf{x}$
  - Find the training example $\mathbf{x}_i$ that is *closest* to $\mathbf{x}$
  - Predict the label of $\mathbf{x}$ to the label y_i associated with $\mathbf{x}_i$

K-Nearest Neighbors

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  - For classification: ?

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  - For classification: Every neighbor votes on the label. Predict the most frequent label among the neighbors.
  - For regression: ?

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  - Construct the label of $\mathbf{x}$ using these k points. *How?*
  - For classification: Every neighbor votes on the label. Predict the most frequent label among the neighbors.
  - For regression: Predict the mean value

Instance based learning

- A class of learning methods
  - Learning: Storing examples with labels
  - Prediction: When presented a new example, classify the labels using *similar* stored examples

- K-nearest neighbors algorithm is an example of this class of methods

- Also called *lazy* learning, because most of the computation (in the simplest case, all computation) is performed only at prediction time

Questions?

Distance between instances

- In general, a good place to inject knowledge about the domain

- Behavior of this approach can depend on this

- How do we measure distances between instances?

Distance between instances

Numeric features, represented as n dimensional vectors

Distance between instances

Numeric features, represented as n dimensional vectors

- Euclidean distance

$$||\mathbf{x}_1 - \mathbf{x}_2||_2 = \sqrt{\sum_{i=1}^{n} (\mathbf{x}_{1,i} - \mathbf{x}_{2,i})^2}$$

Distance between instances

Numeric features, represented as n dimensional vectors

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$$||\mathbf{x}_1 - \mathbf{x}_2||_2 = \sqrt{\sum_{i=1}^{n} (\mathbf{x}_{1,i} - \mathbf{x}_{2,i})^2}$$

- Manhattan distance

$$||\mathbf{x}_1 - \mathbf{x}_2||_1 = \sum_{i=1}^{n} |\mathbf{x}_{1,i} - \mathbf{x}_{2,i}|$$

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- L_p-norm
  - Euclidean = L_2
  - Manhattan = L_1
  - Exercise: What is L_∞?

$$||\mathbf{x}_1 - \mathbf{x}_2||_p = \left(\sum_{i=1}^{n} |\mathbf{x}_{1,i} - \mathbf{x}_{2,i}|^p\right)^{\frac{1}{p}}$$

Distance between instances

What about symbolic/categorical features?

Distance between instances

Symbolic/categorical features

Most common distance is the *Hamming distance*

- Number of bits that are different
- Or: Number of features that have a different value
- Also called the *overlap*
- Example:

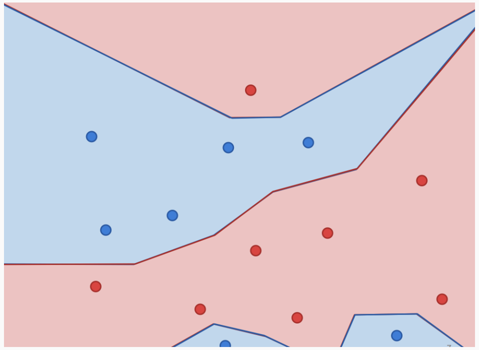
  $\mathbf{X_1}$: {Shape=Triangle, Color=Red, Location=Left, Orientation=Up}

  $\mathbf{X_2}$: {Shape=Triangle, Color=Blue, Location=Left, Orientation=Down}

  Hamming distance = 2

Advantages

- Training is *very fast*
  - Just adding labeled instances to a list
  - More complex indexing methods can be used, which slow down learning slightly to make prediction faster



- Can learn very complex functions
- We always have the training data
  - For other learning algorithms, after training, we don't store the data anymore. What if we want to do something with it later…

Disadvantages

- Needs a lot of storage
  - Is this really a problem now?

- Prediction can be slow!
  - Naïvely: O(dN) for N training examples in d dimensions
  - More data will make it slower
  - Compare to other classifiers, where prediction is very fast

- Nearest neighbors are fooled by irrelevant attributes
  - Important and subtle

Questions?

Summary: K-Nearest Neighbors

- Probably the first "machine learning" algorithm
  - Guarantee: If there are enough training examples, the error of the nearest neighbor classifier will converge to the error of the optimal (i.e. best possible) predictor
- In practice, use an odd K. Why?

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- Feature normalization could be important
  - Often, good idea to center the features to make them zero mean and unit standard deviation. Why?

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- How to choose K? Using a held-out set or by cross-validation
- Feature normalization could be important
  - Often, good idea to center the features to make them zero mean and unit standard deviation. Why?
  - Because different features could have different scales (weight, height, etc); but the distance weights them equally
- Variants exist
  - Neighbors' labels could be weighted by their distance

Where are we?

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  - Some practical aspects
- Voronoi Diagrams and Decision Boundaries
  - What is the hypothesis space?
- The Curse of Dimensionality

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The decision boundary for KNN

Is the K nearest neighbors algorithm explicitly building a function?

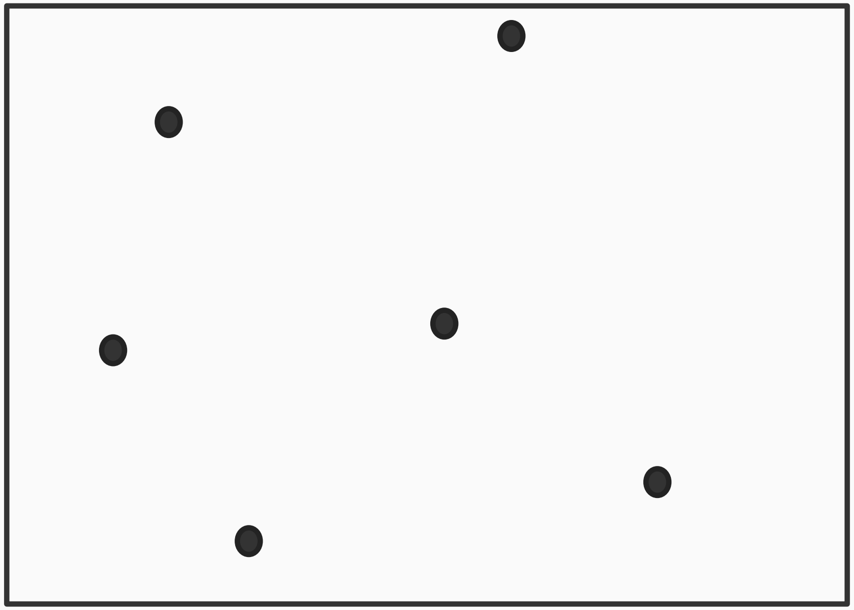
The decision boundary for KNN

Is the K nearest neighbors algorithm explicitly building a function?

- **No,** it never forms an explicit hypothesis

But we can still ask: Given a training set what is the implicit function that is being computed

The Voronoi Diagram

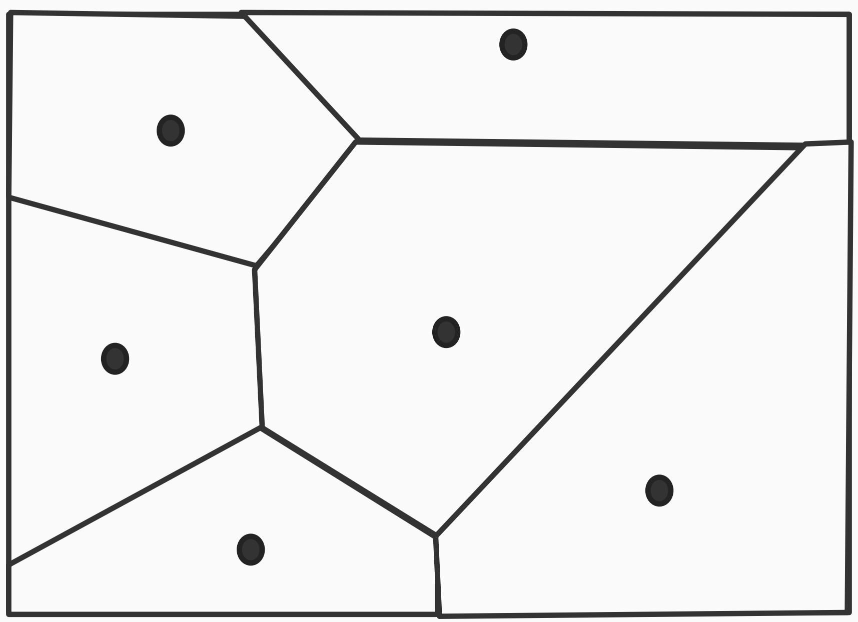


For any point **x** in a training set S, the Voronoi Cell of **x** is a polyhedron consisting of all points closer to **x** than any other points in S

The Voronoi diagram is the union of all Voronoi cells

- Covers the entire space

The Voronoi Diagram



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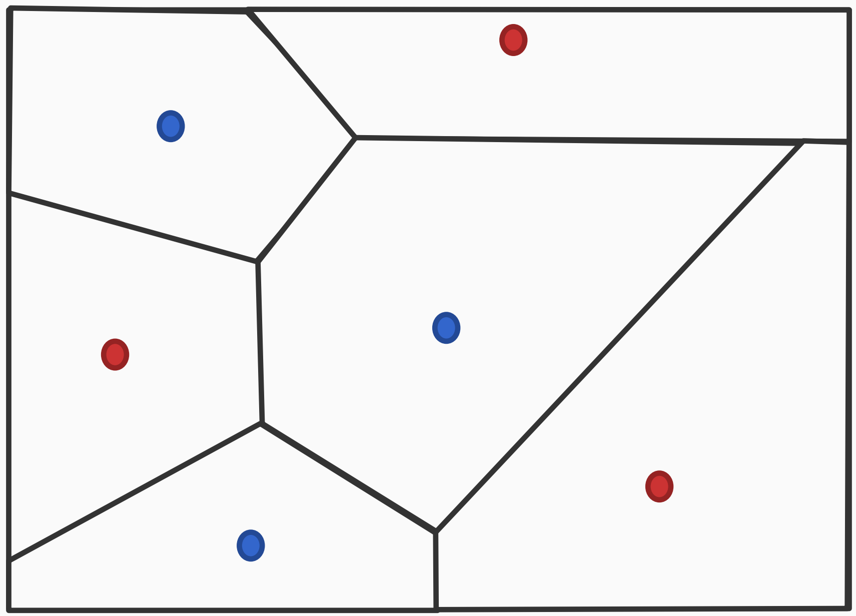
Voronoi diagrams of training examples



Points in the Voronoi cell of a training example are closer to it than any others

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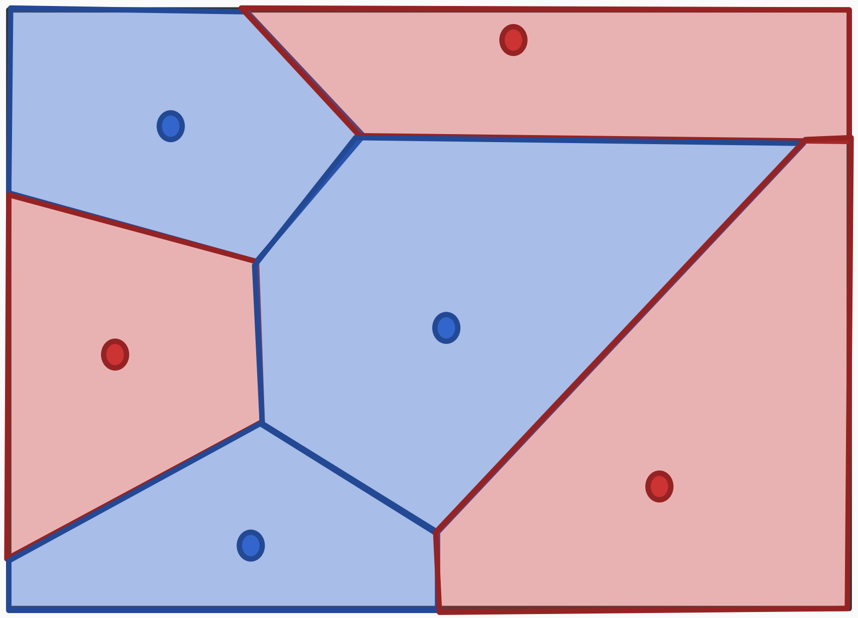

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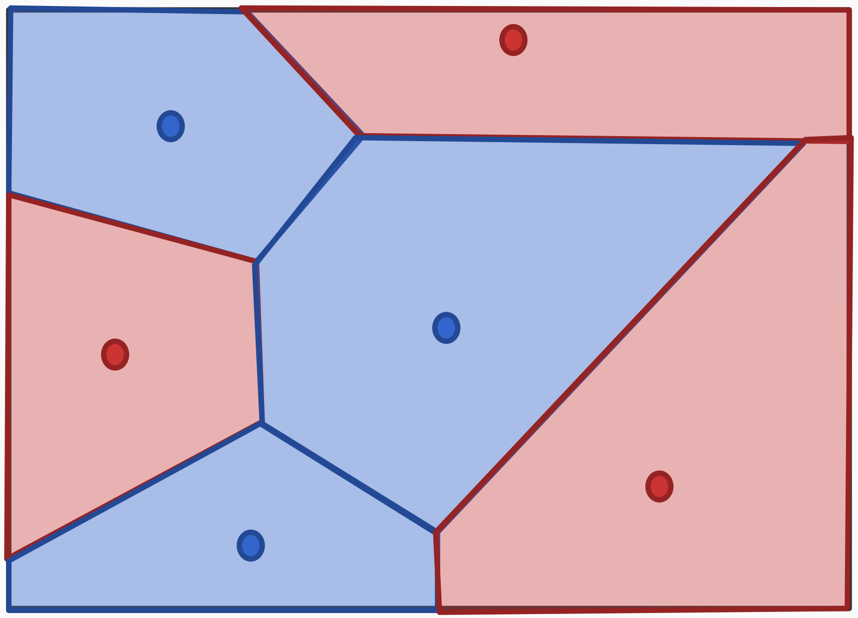


Points in the Voronoi cell of a training example are closer to it than any others

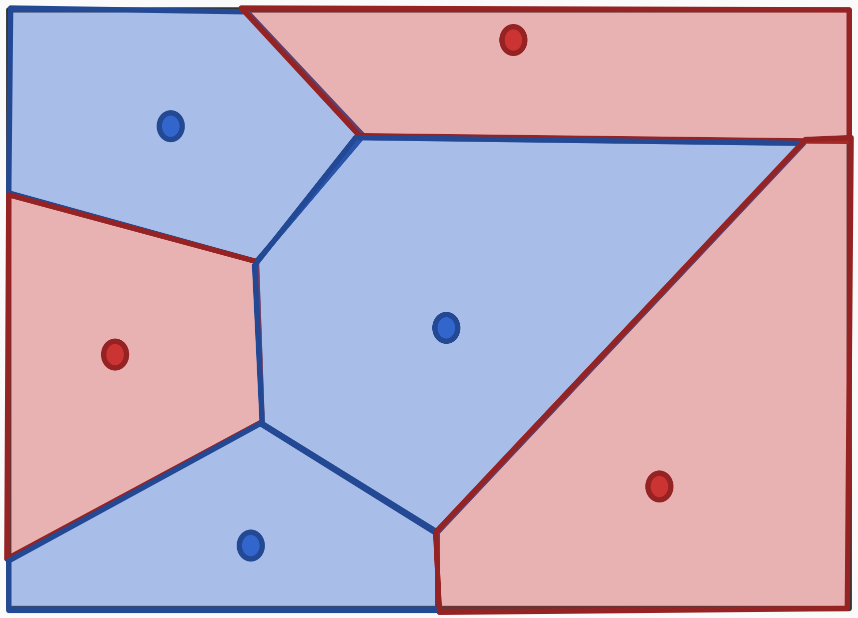
Picture uses Euclidean distance with 1-nearest neighbors.

What about K-nearest neighbors?

Also partitions the space, but much more complex decision boundary

Voronoi diagrams of training examples

What about points on the boundary? What label will they get?



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Exercise

If you have only two training points, what will the decision boundary for 1-nearest neighbor be?

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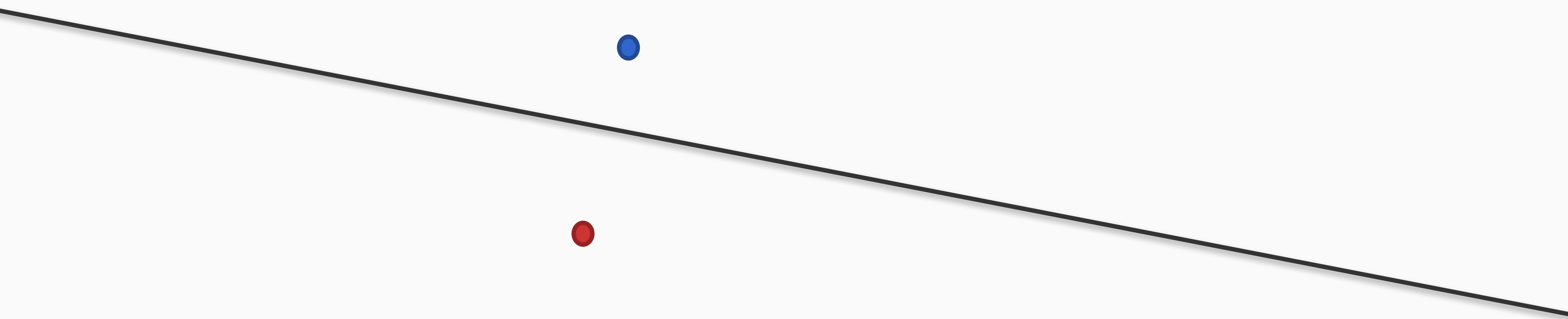

– A line bisecting the two points

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Why your classifier might go wrong

Two important considerations with learning algorithms

- Overfitting: We have already seen this
- The curse of dimensionality
  - Methods that work with low dimensional spaces may fail in high dimensions
  - What might be intuitive for 2 or 3 dimensions do not always apply to high dimensional spaces

Check out the 1884 book *Flatland: A Romance of Many Dimensions* for a fun introduction to the fourth dimension

Of course, irrelevant attributes will hurt

Suppose we have 1000 dimensional feature vectors

- But only 10 features are relevant

- Distances will be dominated by the large number of irrelevant features

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Suppose we have 1000 dimensional feature vectors

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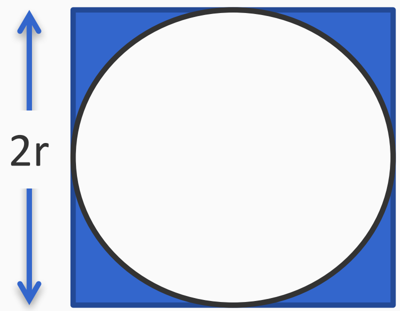
But even with only relevant attributes, high dimensional spaces behave in odd ways

The Curse of Dimensionality

Intuitions that are based on 2 or 3 dimensional spaces do not always carry over to high dimensional spaces

Example 1: What fraction of the points in a cube lie outside the sphere inscribed in it?

In two dimensions



What fraction of the square (i.e the cube) is outside the inscribed circle (i.e the sphere) in two dimensions?

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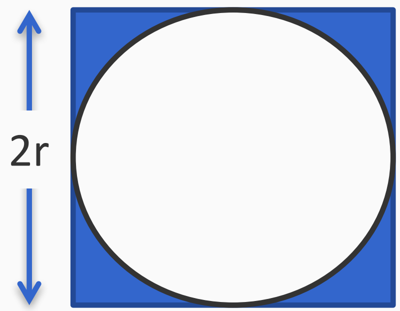

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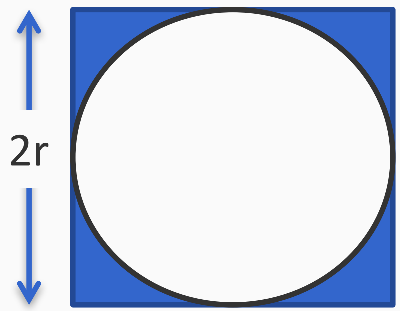

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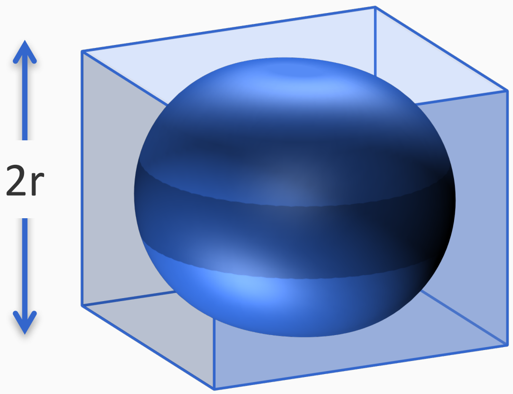

What fraction of the cube is outside the inscribed sphere in three dimensions?

$$1 - \frac{\frac{4}{3}\pi r^3}{8r^3} = 1 - \frac{\pi}{6}$$

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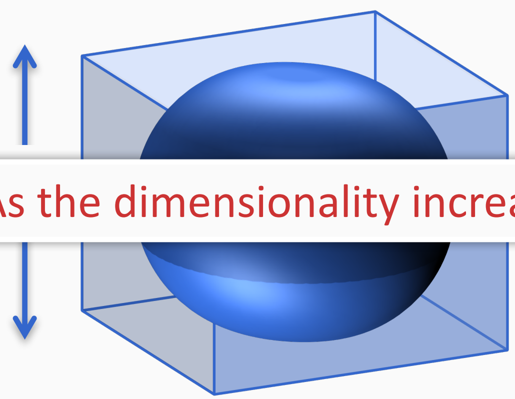

What fraction of the cube is outside the inscribed sphere in three dimensions?

$$\frac{\frac{4}{3}\pi r^3}{8r^3} = \frac{\pi}{6}$$

As the dimensionality increases, this fraction approaches 1!!

In high dimensions, most of the volume of the cube is far away from the center!

The Curse of Dimensionality

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Example 2: What fraction of the volume of a unit sphere lies between radius 1 - ϵ and radius 1?

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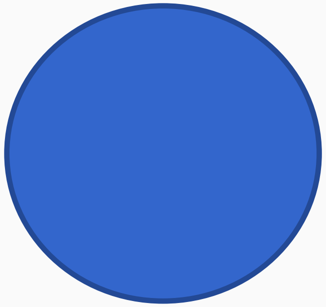

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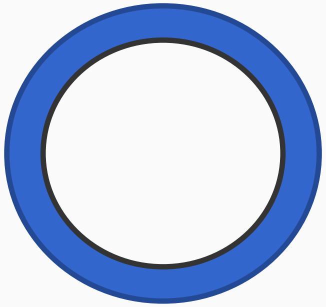

What fraction of the area of the circle is in the blue region?

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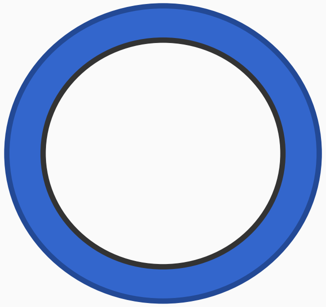

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$$\frac{\pi \cdot 1^2 - \pi(1-\epsilon)^2}{\pi \cdot 1^2} = 1 - (1-\epsilon)^2$$

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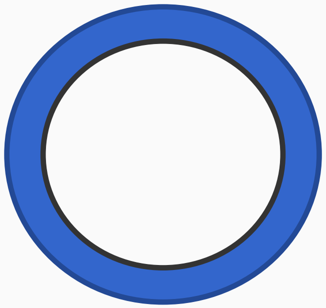

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Example 2: What fraction of the volume of a unit sphere lies between radius 1 - ϵ and radius 1?

But, distances do not behave the same way in high dimensions

In d dimensions, the fraction is $1 - (1 - \epsilon)^d$

As d increases, this fraction goes to 1!

In high dimensions, most of the volume of the sphere is far away from the center!

Questions?

The Curse of Dimensionality

- Most of the points in high dimensional spaces are far away from the origin!
  - In 2 or 3 dimensions, most points are near the center
  - Need more data to "fill up the space"

- Bad news for nearest neighbor classification in high dimensional spaces

Even if most/all features are relevant, in high dimensional spaces, most points are equally far from each other!

"Neighborhood" becomes very large

Presents computational problems too

Dealing with the curse of dimensionality

- Most "*real-world*" data is not uniformly distributed in the high dimensional space
  - Different ways of capturing the *underlying dimensionality* of the space
  - We will see dimensionality reduction later in the semester

- Feature selection, an art
  - Different methods exist
  - Select features, maybe by information gain
  - Try out different feature sets of different sizes and pick a good set based on a validation set

- Prior knowledge or preferences about the hypotheses can also help

Questions?

Summary: Nearest neighbors classification

- Probably the oldest and simplest learning algorithm
  - Prediction is expensive.
    - Efficient data structures help. k-D trees: the most popular, works well in low dimensions
    - Approximate nearest neighbors may be good enough some times. Hashing based algorithms exist

- Requires a distance measure between instances
  - Metric learning: Learn the “right” distance for your problem

- Partitions the space into a Voronoi Diagram

- Beware the curse of dimensionality

Questions?

Exercises

1. What will happen when you choose K to the number of training examples?

2. Suppose you want to build a nearest neighbors classifier to predict whether a beverage is a coffee or a tea using two features: the volume of the liquid (in milliliters) and the caffeine content (in grams). You collect the following data:

Volume (ml)	**Caffeine (g)**	**Label**
238	0.026	Tea
100	0.011	Tea
120	0.040	Coffee
237	0.095	Coffee

What is the label for a test point with Volume = 120, Caffeine = 0.013?

Why might this be incorrect?

How would you fix the problem?

Exercises

1. What will happen when you choose K to the number of training examples? *The label will always be the most common label in the training data*

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What is the label for a test point with Volume = 120, Caffeine = 0.013?
Coffee
Why might this be incorrect?
Because Volume will dominate the distance
How would you fix the problem?
Rescale the features. Maybe to zero mean, unit variance