

Distance based models

Chapter 8



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Measuring distance

How to measure closeness?

Distance measures for continuous data:

The Euclidean distance:

$$Dis_2(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \sqrt{\sum_{i=1}^d (x_i - y_i)^2} = \sqrt{(\mathbf{x} - \mathbf{y})^\top (\mathbf{x} - \mathbf{y})}$$

(based on the 2-norm)

Distance based methods

- Supervised learning methods (nearest neighbor methods)
- Clustering (K-means and hierarchical clustering)

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More distance measures

The Manhattan distance:

$$Dis_1(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^d |x_i - y_i|$$

This is the distance if we can only travel along coordinate axes.

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The Minkowski distance

The Minkowski distance of order p :

$$\text{Dis}_p(\mathbf{x}, \mathbf{y}) = \left(\sum_{j=1}^d |x_j - y_j|^p \right)^{1/p} = \|\mathbf{x} - \mathbf{y}\|_p$$

where $\|\mathbf{z}\|_p = \left(\sum_{j=1}^d |z_j|^p \right)^{1/p}$ is the **p -norm** (sometimes denoted L_p norm) of the vector \mathbf{z} . We will often refer to Dis_p simply as the p -norm.

The Euclidean and Manhattan distances are special cases

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What happens when p goes to infinity?

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What happens when p goes to infinity?

$$\text{Dis}_{\infty}(\mathbf{x}, \mathbf{y}) = \max_i |x_i - y_i|$$

We get the **Chebyshev distance**

a	b	c	d	e	f	g	h	8
5	4	3	2	2	2	2	2	8
5	4	3	2	1	1	1	2	7
5	4	3	2	1	1	1	2	6
5	4	3	2	1	1	1	2	5
4	5	4	3	2	2	2	2	4
3	5	4	3	3	3	3	3	3
2	5	4	4	4	4	4	4	2
1	5	5	5	5	5	5	5	1
a	b	c	d	e	f	g	h	7

The Minkowski distance

The unit sphere for various values of p

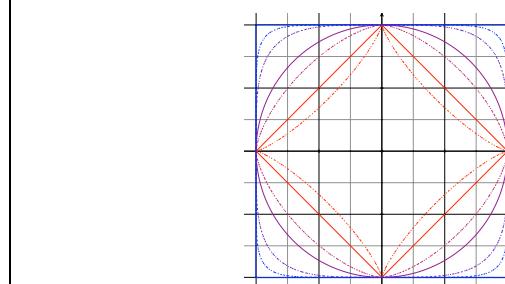


Figure 8.3

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Properties of a distance

Given an instance space \mathcal{X} , a *distance metric* is a function $\text{Dis} : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ such that for any $x, y, z \in \mathcal{X}$:

- ☒ distances between a point and itself are zero: $\text{Dis}(x, x) = 0$;
- ☒ all other distances are larger than zero: if $x \neq y$ then $\text{Dis}(x, y) > 0$;
- ☒ distances are symmetric: $\text{Dis}(y, x) = \text{Dis}(x, y)$;
- ☒ detours can not shorten the distance: $\text{Dis}(x, z) \leq \text{Dis}(x, y) + \text{Dis}(y, z)$.

The last condition is called the *triangle inequality*

The Minkowski distance with $p < 1$ does not satisfy the triangle inequality.

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The Mahalanobis distance

Sometimes it's useful to use different scales for different coordinates.

Therefore: use an ellipse rather than a circle to identify points that are a fixed distance away.

Also consider rotating the ellipse.

$$\mathbf{R} = \begin{pmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{pmatrix}$$

45 degree clockwise rotation

$$\mathbf{S} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix}$$

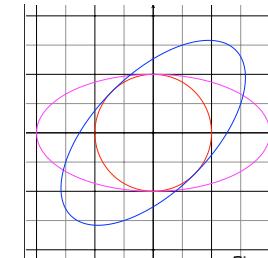


Figure 8.3

$$\mathbf{x}^T \mathbf{R}^T \mathbf{S}^2 \mathbf{R} \mathbf{x} = 1/4; \text{ the axis-parallel ellipse } \mathbf{x}^T \mathbf{S}^2 \mathbf{x} = 1/4; \text{ and the circle } \mathbf{x}^T \mathbf{x} = 1/4.$$

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The Mahalanobis distance

The shape of the ellipse is estimated from data as the inverse of the covariance matrix:

$$\text{Dis}_M(\mathbf{x}, \mathbf{y} | \Sigma) = \sqrt{(\mathbf{x} - \mathbf{y})^T \Sigma^{-1} (\mathbf{x} - \mathbf{y})}$$

(The inverse of the covariance matrix has the effect of decorrelating and normalizing features)

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The closest centroid classifier revisited

Theorem 8.1 (The arithmetic mean minimizes the squared Euclidean distance).

The arithmetic mean of a set of data points D is the unique point that minimizes the sum of squared Euclidean distances to those data points.

In other words:

$$\operatorname{argmin}_{\mathbf{y}} \sum_{\mathbf{x} \in D} \|\mathbf{x} - \mathbf{y}\|^2 = \mu$$

Proof: Find the minimum by taking the derivative and setting to 0.
(page 238 in the book)

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The closest centroid classifier revisited

The arithmetic mean is a representative example (exemplar) that is used to represent each class.

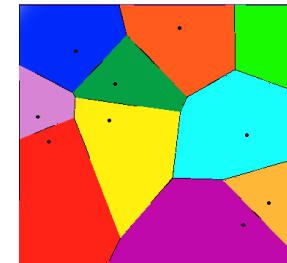
The closest centroid classifier works for multi-class data - classify a point according to which mean is closest in Euclidean distance.

How does the decision boundary look like?

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Voronoi diagrams

Voronoi diagram with respect to a collection of points m_1, \dots, m_k :



The Voronoi cell associated with point m_i is the set of points that are closer to m_i than every other point in the collection

Image from http://en.wikipedia.org/wiki/Voronoi_diagram

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Voronoi diagrams

Decision boundary of the closest centroid algorithm when using L2 and L1 norms:

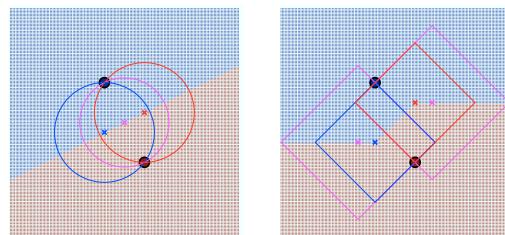
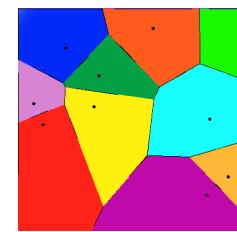


Figure 8.6

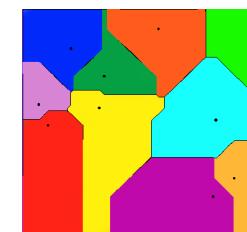
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Voronoi diagrams

The Voronoi diagram depends on the distance measure that is used:



Voronoi diagram computed from Euclidean distance (L2 norm)



Voronoi diagram computed from Manhattan distance (L1 norm)

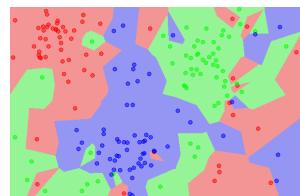
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Nearest neighbor classification

The **nearest neighbor classifier**:

Classify a given test example to the class of the nearest training example.

Decision boundary is the result of fusing adjacent Voronoi cells that are associated with the same class.



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Nearest neighbor classification

The **nearest neighbor classifier**:

Classify a given test example to the class of the nearest training example.

What is the accuracy of the nearest neighbor classifier when it is tested on the training set?

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Nearest neighbor classification

The **nearest neighbor classifier**:

Classify a given test example to the class of the nearest training example.

Running time for testing an example when dataset has n examples?

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Nearest neighbor classification

The **nearest neighbor classifier**:

Classify a given test example to the class of the nearest training example.

Running time for testing an example when dataset has n examples?

$O(n)$. Expensive when dealing with large datasets.

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Nearest neighbor classification in high dimensions

Distance functions lose their usefulness in high dimensions.

Consider the Euclidean distance for example:

$$Dis_2(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^d (x_i - y_i)^2}$$

We expect that if d is large, many of the features won't be relevant, and so the signal contained in the informative dimensions can easily be corrupted by the noise.

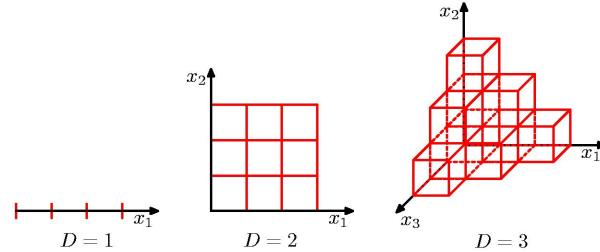
This can lead to low accuracy of a nearest neighbor classifier.

Solution: feature selection, dimensionality reduction (chapter 10)

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The curse of dimensionality

An umbrella term for the issues that can arise in high dimensional data.



The curse of dimensionality

Some of our intuition from low dimensional spaces breaks in high dimensions.

Example: In high dimensions, most of the volume of the unit sphere is very close to its surface.

Let's compute the fraction of the volume that is between $r=1-\epsilon$ and $r=1$.

$$V_d(r) = k_d \cdot r^d$$

The required fraction is:

$$\frac{V_d(1) - V_d(1-\epsilon)}{V_d(1)} = 1 - (1-\epsilon)^d$$

Related fact:

The ratio of the volume of the unit sphere and unit cube tends to 0 as d goes to infinity.

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k-NN

Use the closest k neighbors to make a decision instead of a single nearest neighbor

Choose the label that occurs among the majority of the k nearest neighbors

Why do you expect this to work better?

k-NN

Use the closest k neighbors to make a decision instead of a single nearest neighbor
 Choose the label that occurs among the majority of the k nearest neighbors

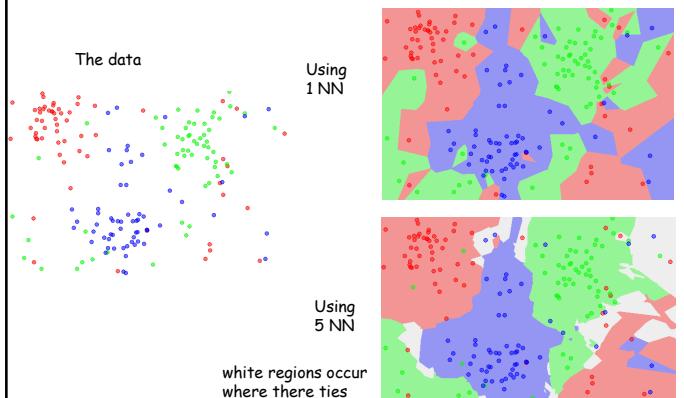
Can produce confidence scores. How?

k-NN

Use the closest k neighbors to make a decision instead of a single nearest neighbor
 Choose the label that occurs among the majority of the k nearest neighbors

Other refinements: an example's vote is inversely proportional to its distance

NN vs k-NN



Nearest neighbor regression

How do turn k-NN into a regression method?

Distances and kernels

The Euclidean distance can be expressed in terms of dot products:

$$Dis_2(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \sqrt{(\mathbf{x} - \mathbf{y})^\top (\mathbf{x} - \mathbf{y})} = \sqrt{\mathbf{x}^\top \mathbf{x} - 2\mathbf{x}^\top \mathbf{y} - \mathbf{y}^\top \mathbf{y}}$$

Replacing dot products with kernels:

$$Dis_K(\mathbf{x}, \mathbf{y}) = \sqrt{K(\mathbf{x}, \mathbf{x}) - 2K(\mathbf{x}, \mathbf{y}) - K(\mathbf{y}, \mathbf{y})}$$

As an alternative, consider kernels as measures of similarity, and rather than looking for the closest points, look for the most similar points, and use kernels directly.

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Distances and kernels

Replacing dot products with kernels:

$$Dis_K(\mathbf{x}, \mathbf{y}) = \sqrt{K(\mathbf{x}, \mathbf{x}) - 2K(\mathbf{x}, \mathbf{y}) - K(\mathbf{y}, \mathbf{y})}$$

If we consider a kernel that satisfies $K(\mathbf{x}, \mathbf{x}) = 1$, then nearest neighbor classification with kernels or distances is equivalent.

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