# CSC 411: Lecture 05: Nearest Neighbors

#### Raquel Urtasun & Rich Zemel

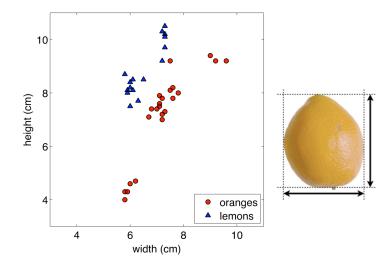
University of Toronto

Sep 28, 2015

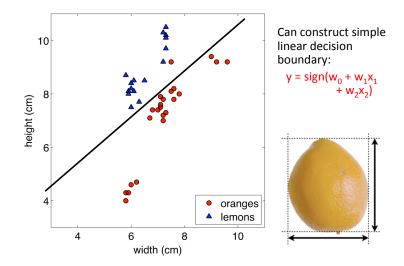
#### • Non-parametric models

- distance
- non-linear decision boundaries

## Classification: Oranges and Lemons



## Classification: Oranges and Lemons



- Classification is intrinsically non-linear
  - It puts non-identical things in the same class, so a difference in the input vector sometimes causes zero change in the answer

- Classification is intrinsically non-linear
  - It puts non-identical things in the same class, so a difference in the input vector sometimes causes zero change in the answer
- Linear classification means that the part that adapts is linear (just like linear regression)

$$z(x) = \mathbf{w}^T \mathbf{x} + w_0$$

with adaptive **w**, w<sub>0</sub>

- Classification is intrinsically non-linear
  - It puts non-identical things in the same class, so a difference in the input vector sometimes causes zero change in the answer
- Linear classification means that the part that adapts is linear (just like linear regression)

$$z(x) = \mathbf{w}^T \mathbf{x} + w_0$$

with adaptive **w**, *w*<sub>0</sub>

• The adaptive part is follow by a non-linearity to make the decision

$$y(\mathbf{x}) = f(z(\mathbf{x}))$$

- Classification is intrinsically non-linear
  - It puts non-identical things in the same class, so a difference in the input vector sometimes causes zero change in the answer
- Linear classification means that the part that adapts is linear (just like linear regression)

$$z(x) = \mathbf{w}^T \mathbf{x} + w_0$$

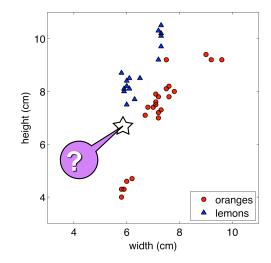
with adaptive **w**, w<sub>0</sub>

• The adaptive part is follow by a non-linearity to make the decision

$$y(\mathbf{x}) = f(z(\mathbf{x}))$$

• What f have we seen so far in class?

## Classification as Induction



#### • Alternative to parametric model is non-parametric

- Alternative to parametric model is non-parametric
- Simple methods for approximating discrete-valued or real-valued target functions (classification or regression problems)

- Alternative to parametric model is non-parametric
- Simple methods for approximating discrete-valued or real-valued target functions (classification or regression problems)
- Learning amounts to simply storing training data

- Alternative to parametric model is non-parametric
- Simple methods for approximating discrete-valued or real-valued target functions (classification or regression problems)
- Learning amounts to simply storing training data
- Test instances classified using similar training instances

- Alternative to parametric model is non-parametric
- Simple methods for approximating discrete-valued or real-valued target functions (classification or regression problems)
- Learning amounts to simply storing training data
- Test instances classified using similar training instances
- Embodies often sensible underlying assumptions:
  - Output varies smoothly with input
  - Data occupies sub-space of high-dimensional input space

• Assume training examples correspond to points in d-dimensional Euclidean space

- Assume training examples correspond to points in d-dimensional Euclidean space
- Target function value for new query estimated from known value of nearest training example(s)

- Assume training examples correspond to points in d-dimensional Euclidean space
- Target function value for new query estimated from known value of nearest training example(s)
- Distance typically defined to be Euclidean:

$$||\mathbf{x}^{(a)} - \mathbf{x}^{(b)}||_2 = \sqrt{\sum_{j=1}^{d} (x_j^{(a)} - x_j^{(b)})^2}$$

- Assume training examples correspond to points in d-dimensional Euclidean space
- Target function value for new query estimated from known value of nearest training example(s)
- Distance typically defined to be Euclidean:

$$||\mathbf{x}^{(a)} - \mathbf{x}^{(b)}||_2 = \sqrt{\sum_{j=1}^d (x_j^{(a)} - x_j^{(b)})^2}$$

Algorithm

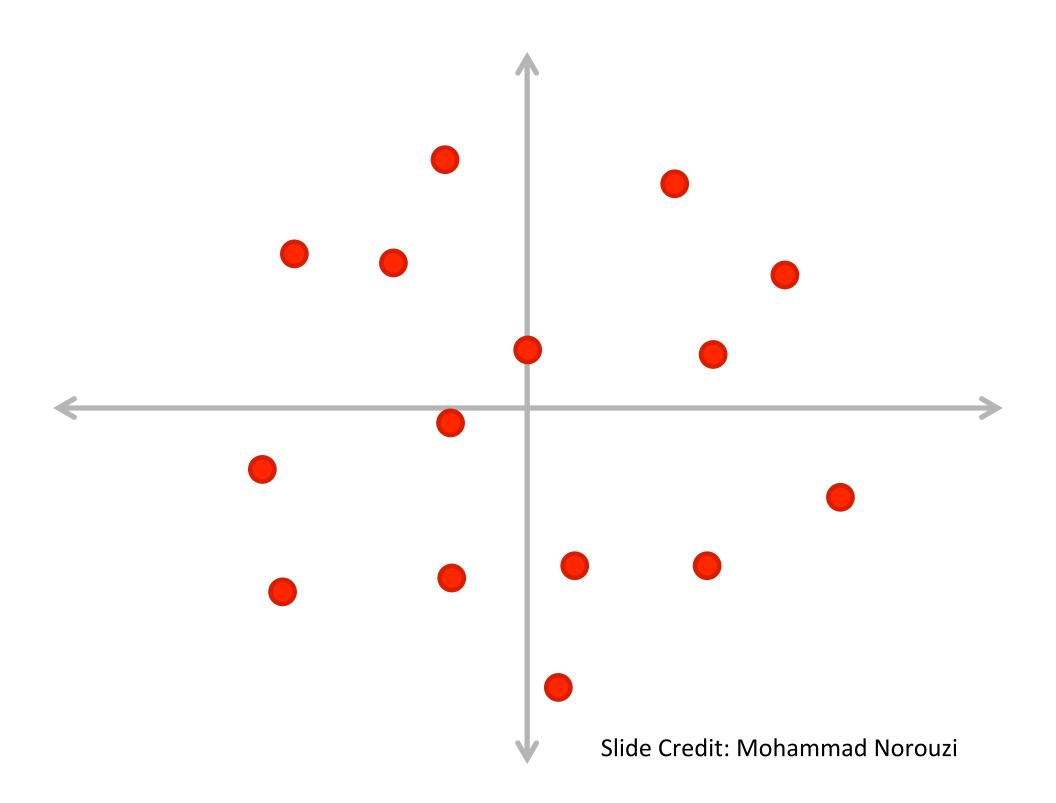
- 1. find example  $(\mathbf{x}^*, t^*)$  closest to the test instance  $\mathbf{x}^{(q)}$
- 2. output  $y^{(q)} = t^*$

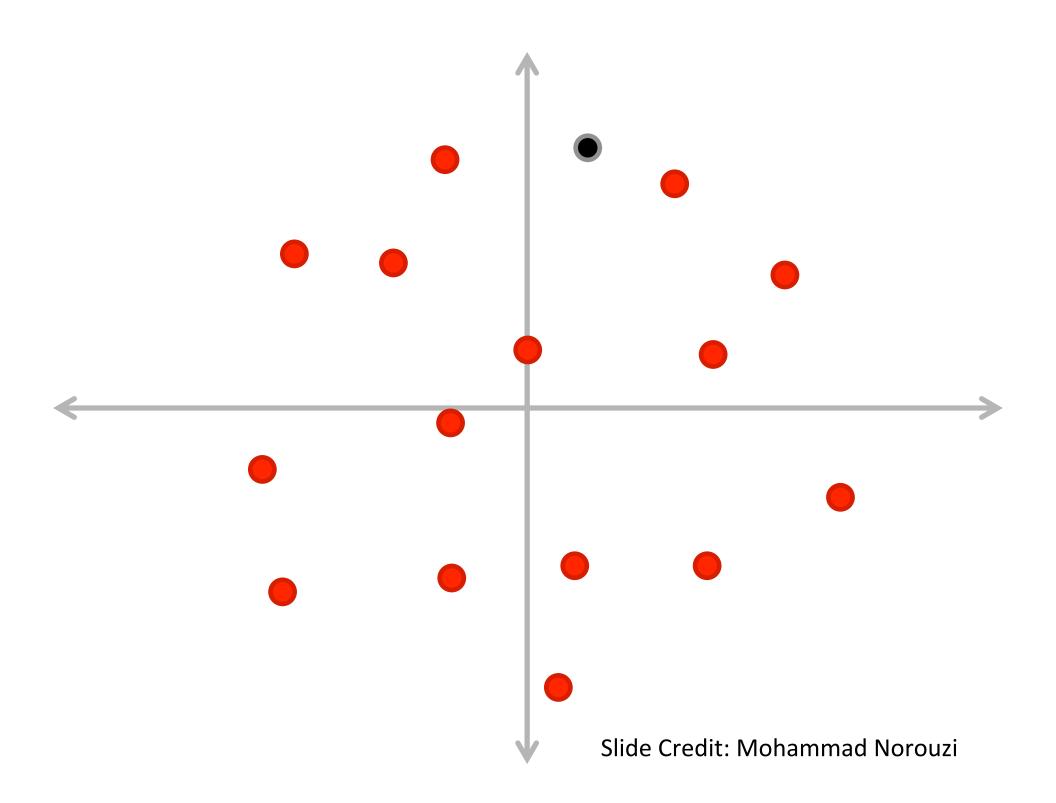
- Assume training examples correspond to points in d-dimensional Euclidean space
- Target function value for new query estimated from known value of nearest training example(s)
- Distance typically defined to be Euclidean:

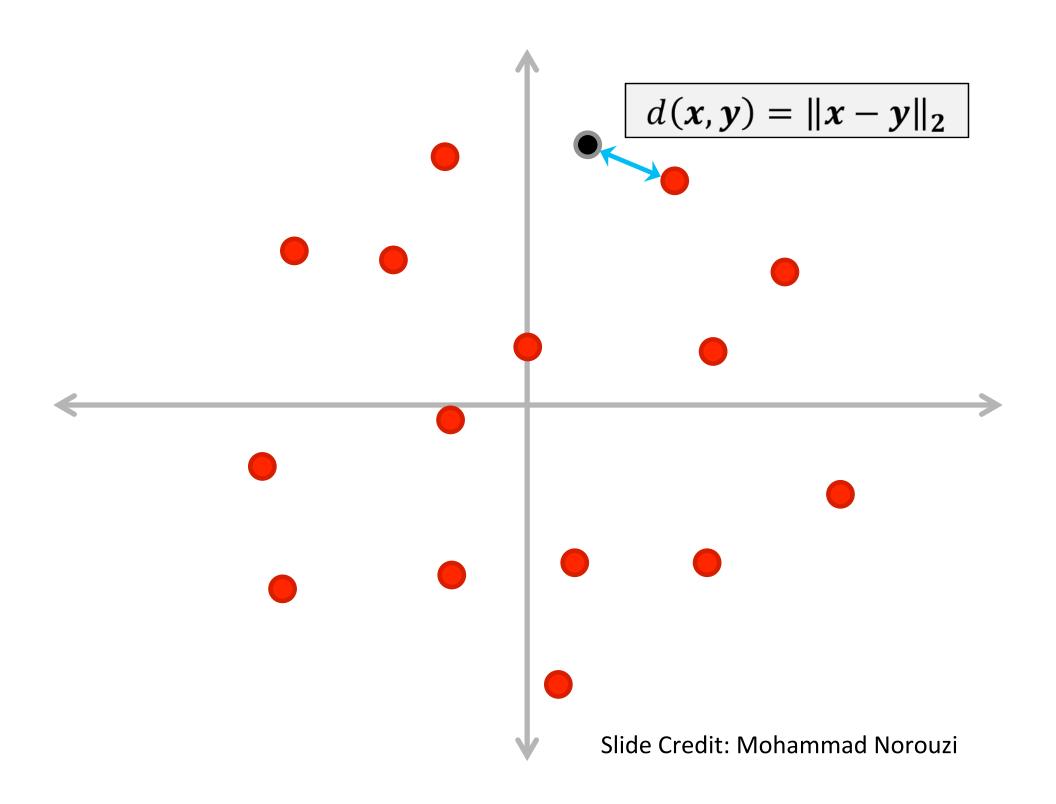
$$||\mathbf{x}^{(a)} - \mathbf{x}^{(b)}||_2 = \sqrt{\sum_{j=1}^d (x_j^{(a)} - x_j^{(b)})^2}$$

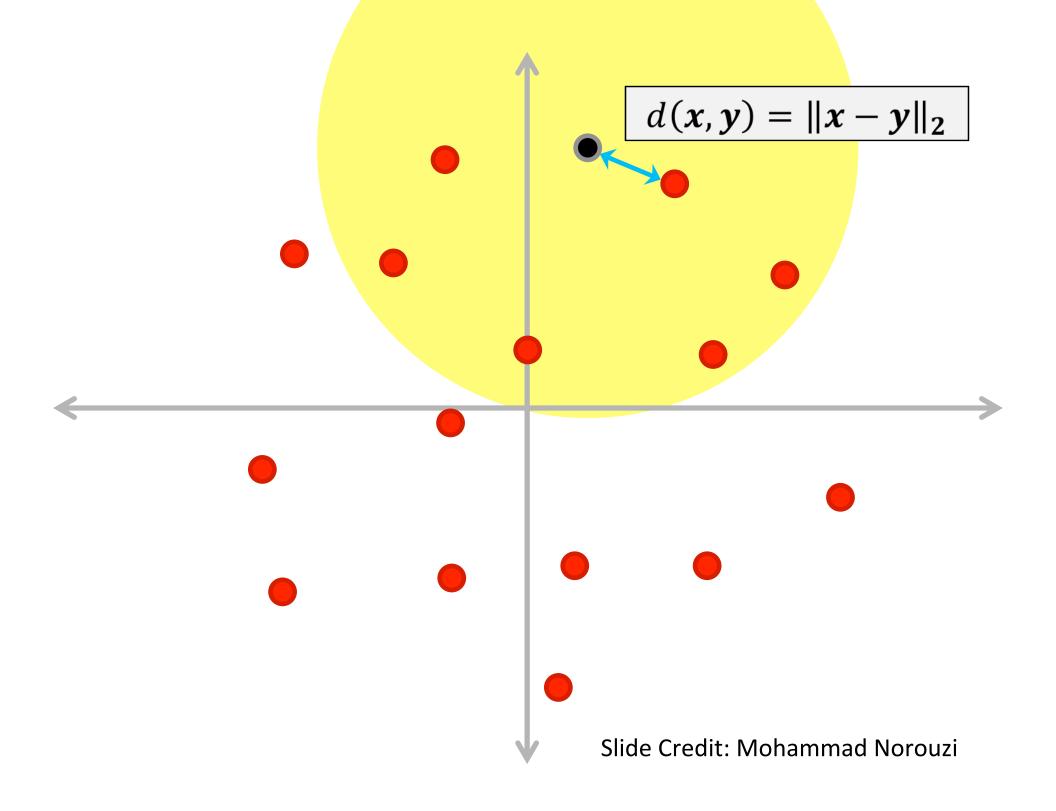
Algorithm

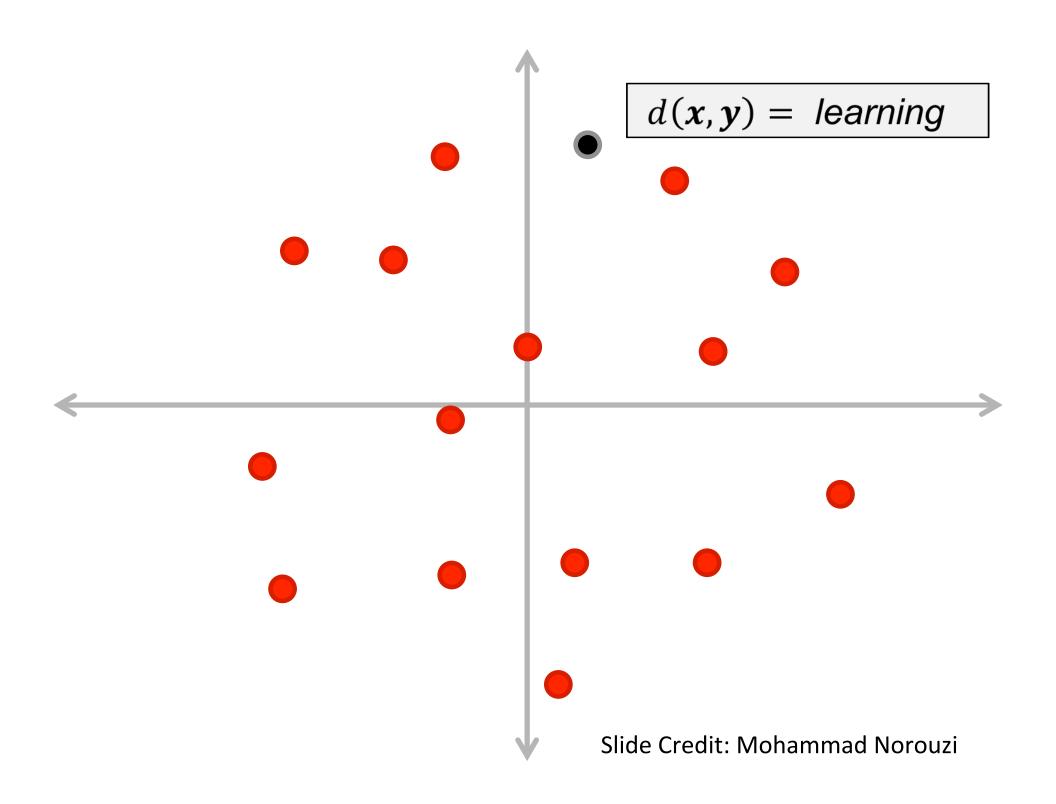
- 1. find example  $(\mathbf{x}^*, t^*)$  closest to the test instance  $\mathbf{x}^{(q)}$
- 2. output  $y^{(q)} = t^*$
- Note: we don't need to compute the square root. Why?

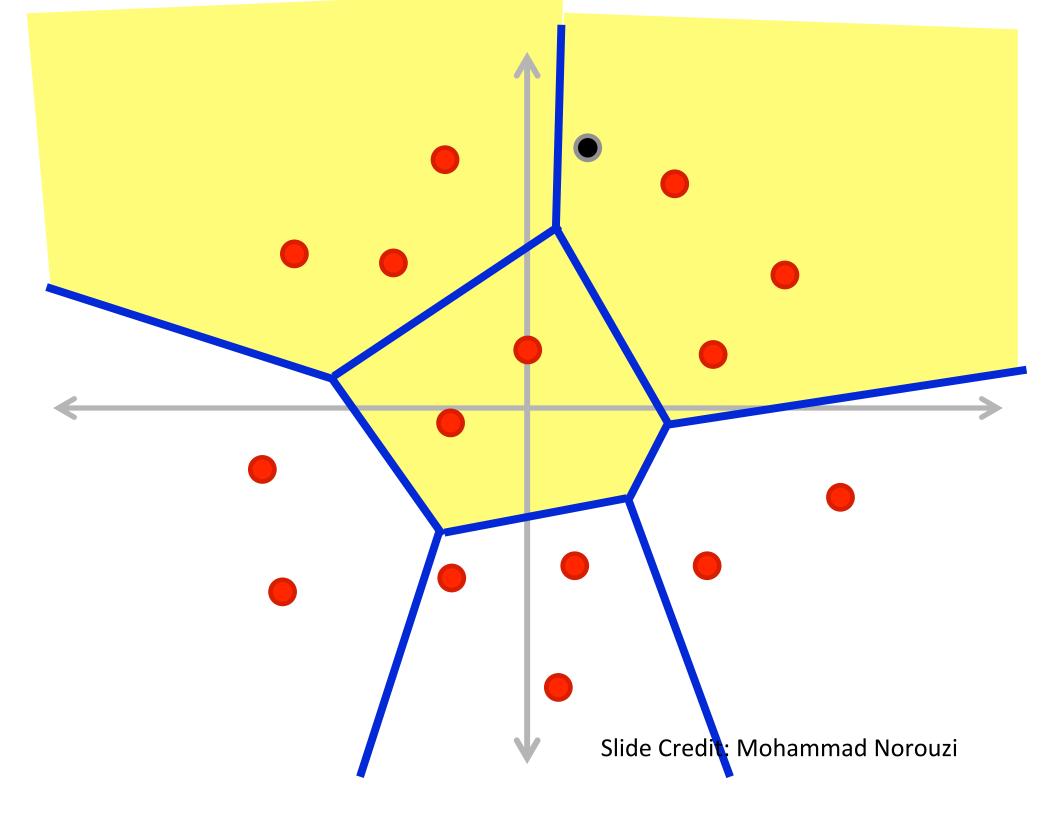






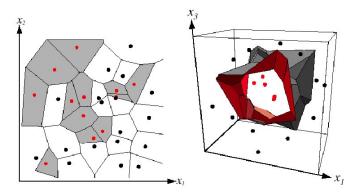






## Nearest Neighbors Decision Boundaries

- Nearest neighbor algorithm does not explicitly compute decision boundaries, but these can be inferred
- Decision boundaries: Voronoi diagram visualization
  - show how input space divided into classes
  - each line segment is equidistant between two points of opposite classes



 $\bullet$  Nearest neighbors sensitive to mis-labeled data ("class noise" )  $\to$  smooth by having k nearest neighbors vote

- $\bullet$  Nearest neighbors sensitive to mis-labeled data ("class noise")  $\to$  smooth by having k nearest neighbors vote
- Algorithm:
  - 1. find k examples  $\{\mathbf{x}^{(i)}, t^{(i)}\}$  closest to the test instance **x**
  - 2. classification output is majority class

$$y = \arg \max_{t^{(z)}} \sum_{r=1}^k \delta(t^{(z)}, t^{(r)})$$

• Some attributes have larger ranges, so are treated as more important

- Some attributes have larger ranges, so are treated as more important
  - normalize scale

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)
  - Hamming distance

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)
  - Hamming distance
- Brute-force approach: calculate Euclidean distance to test point from each stored point, keep closest:  $O(dn^2)$ . We need to reduce computational burden:
  - 1. Use subset of dimensions
  - 2. Use subset of examples

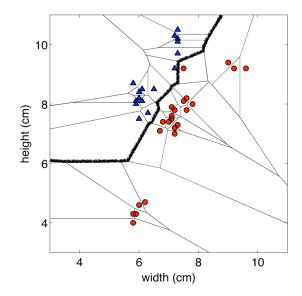
#### k Nearest Neighbors: Issues & Remedies

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)
  - Hamming distance
- Brute-force approach: calculate Euclidean distance to test point from each stored point, keep closest:  $O(dn^2)$ . We need to reduce computational burden:
  - 1. Use subset of dimensions
  - 2. Use subset of examples
    - Remove examples that lie within Voronoi region

### k Nearest Neighbors: Issues & Remedies

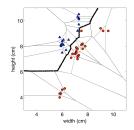
- Some attributes have larger ranges, so are treated as more important
  - normalize scale
- Irrelevant, correlated attributes add noise to distance measure
  - eliminate some attributes
  - or vary and possibly adapt weight of attributes
- Non-metric attributes (symbols)
  - Hamming distance
- Brute-force approach: calculate Euclidean distance to test point from each stored point, keep closest:  $O(dn^2)$ . We need to reduce computational burden:
  - 1. Use subset of dimensions
  - 2. Use subset of examples
    - Remove examples that lie within Voronoi region
    - ▶ Form efficient search tree (kd-tree), use Hashing (LSH), etc

### Decision Boundary K-NN

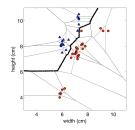


Urtasun & Zemel (UofT)

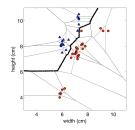
Sep 28, 2015 12 / 13



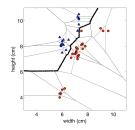
 $\bullet~$  Single parameter (k)  $\rightarrow~$  how do we set it?



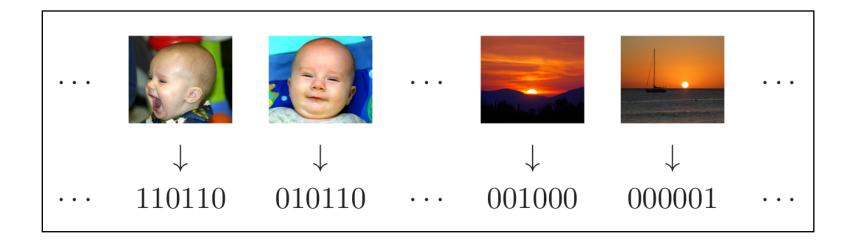
- Single parameter (k)  $\rightarrow$  how do we set it?
- Naturally forms complex decision boundaries; adapts to data density



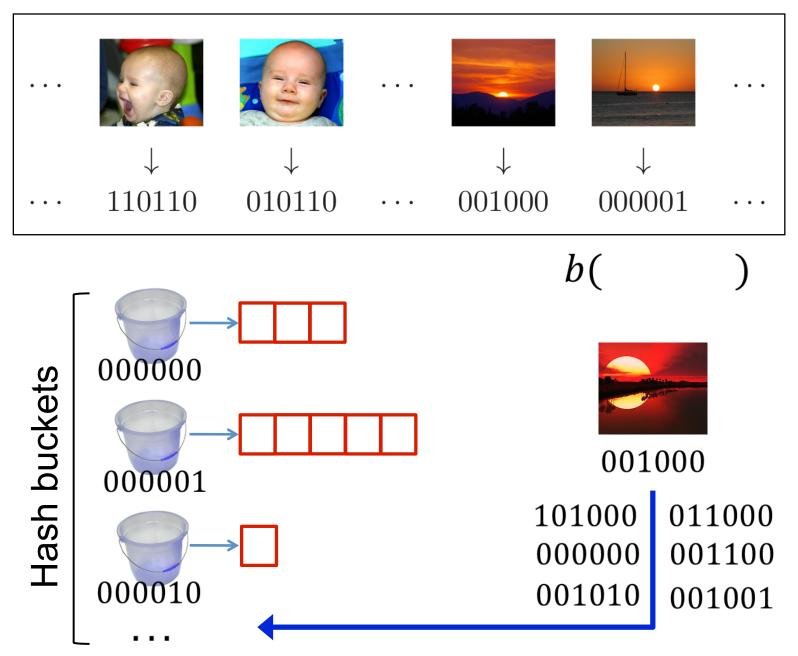
- Single parameter  $(k) \rightarrow how do we set it?$
- Naturally forms complex decision boundaries; adapts to data density
- Problems:
  - Sensitive to class noise.
  - Sensitive to dimensional scales.
  - Distances are less meaningful in high dimensions
  - Scales with number of examples



- Single parameter  $(k) \rightarrow how do we set it?$
- Naturally forms complex decision boundaries; adapts to data density
- Problems:
  - Sensitive to class noise.
  - Sensitive to dimensional scales.
  - Distances are less meaningful in high dimensions
  - Scales with number of examples
- Inductive Bias: What kind of decision boundaries do we expect to find?

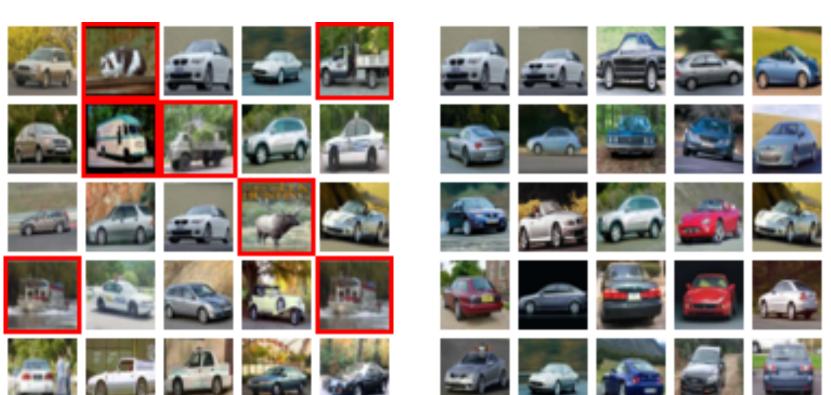


- Similar data points map to nearby codes
- Dissimilar data points map to distant codes





## Query



## **Euclidean NNs**

## Hamming NNs



## Query



## **Euclidean NNs**

# Hamming NNs



## Query



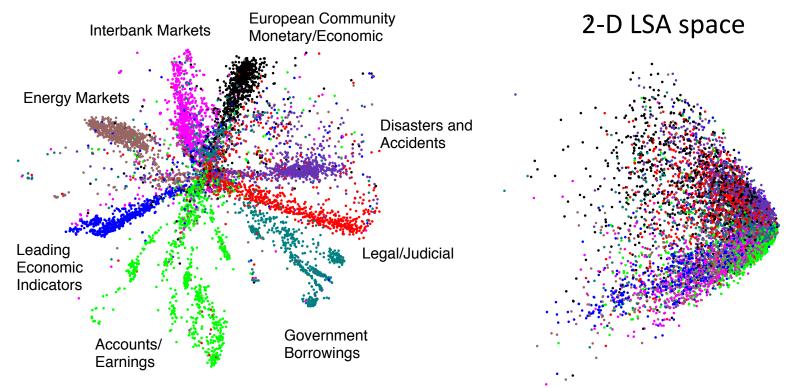
## **Euclidean NNs**



## Hamming NNs

Examples of using Nearest Neighbor Approaches

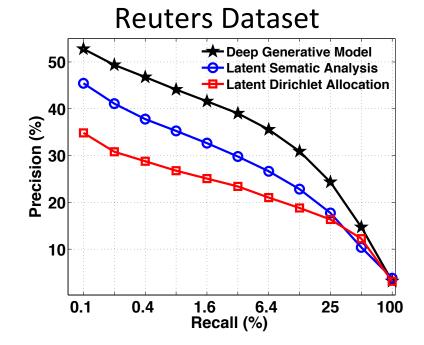
# Information Retrieval using NN



• The Reuters Corpus Volume II contains 804,414 newswire stories (randomly split into **402,207 training** and **402,207 test)**.

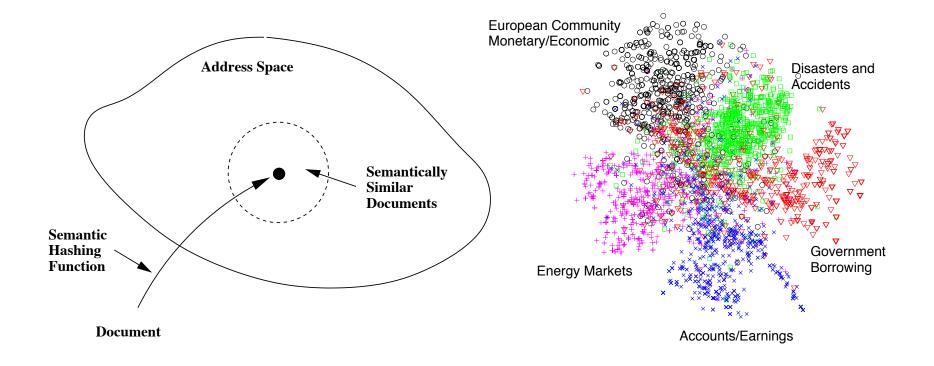
• "Bag-of-words" representation: each article is represented as a vector containing the counts of the most frequently used 2000 words in the training set.

# **Information Retrieval**



Reuters dataset: 804,414 newswire stories.

# Semantic Hashing (using Hamming Distance)

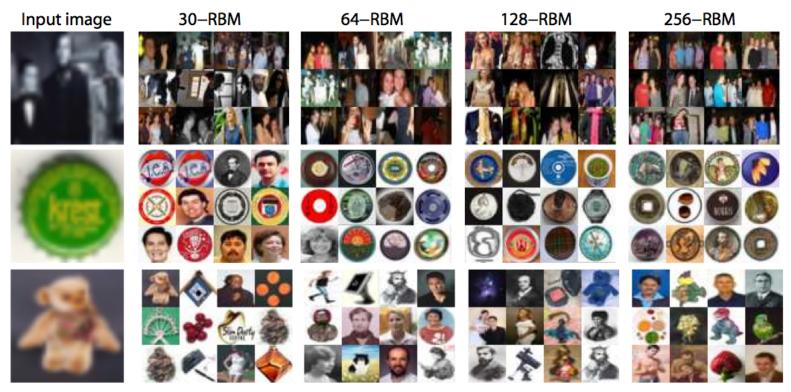


- Learn to map documents into semantic 20-D binary codes.
- Retrieve similar documents stored at the nearby addresses with no search at all.

(Salakhutdinov and Hinton, SIGIR 2007)

# Searching Large Image Database using Binary Codes

• Map images into binary codes for fast retrieval.



- Small Codes, Torralba, Fergus, Weiss, CVPR 2008
- Spectral Hashing, Y. Weiss, A. Torralba, R. Fergus, NIPS 2008
- Kulis and Darrell, NIPS 2009, Gong and Lazebnik, CVPR 20111
- Norouzi and Fleet, ICML 2011,

# **Retrieval using Nearest Neighbors**

fluffy

delicious



# **Retrieving Sentences using 1-NN**



The dogs are in the snow in front of a fence .



Four men playing basketball , two from each team .



A boy skateboarding



Two men and a woman smile at the camera .



Women participate in a skit onstage .



A man is doing tricks on a bicycle on ramps in front of a crowd .

# Tagging and Retrieval using NN



mosque, tower, building, cathedral, dome, castle



ski, skiing, skiers, skiiers, snowmobile



kitchen, stove, oven, refrigerator, microwave



bowl, cup, soup, cups, coffee



beach

snow