## CSC 411: Lecture 05: Nearest Neighbors

Rich Zemel, Raquel Urtasun and Sanja Fidler

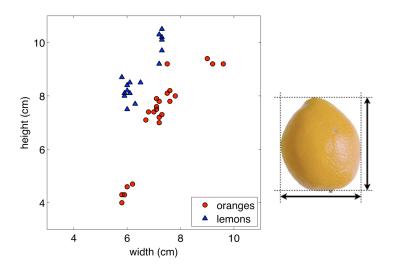
University of Toronto

## **Today**

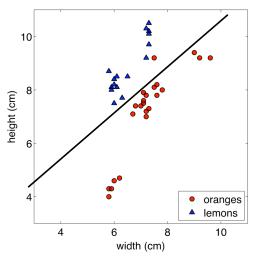
- Non-parametric models
  - distance
  - non-linear decision boundaries

Note: We will mainly use today's method for classification, but it can also be used for regression

## Classification: Oranges and Lemons

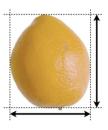


## Classification: Oranges and Lemons



Can construct simple linear decision boundary:

$$y = sign(w_0 + w_1x_1 + w_2x_2)$$



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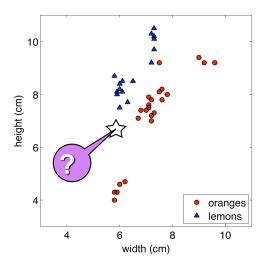
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• What functions f() have we seen so far in class?

## Classification as Induction



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- These are typically simple methods for approximating discrete-valued or real-valued target functions (they work for classification or regression problems)
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- 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

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#### Algorithm:

1. Find example  $(\mathbf{x}^*, t^*)$  (from the stored training set) closest to the test instance  $\mathbf{x}$ . That is:

$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\operatorname{argmin}} \operatorname{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

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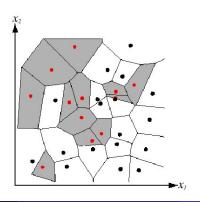
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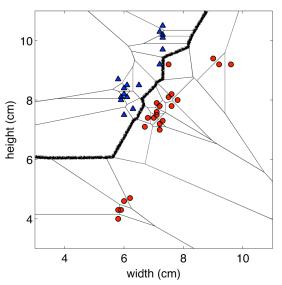
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- Note: we don't really need to compute the square root. Why?

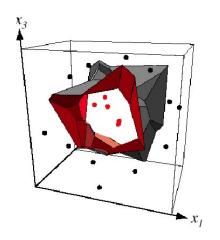
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- Decision boundaries: Voronoi diagram visualization
  - show how input space divided into classes
  - each line segment is equidistant between two points of opposite classes





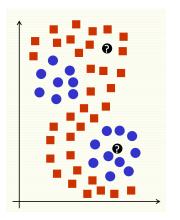
Example: 2D decision boundary



Example: 3D decision boundary

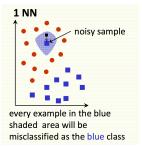
## Nearest Neighbors: Multi-modal Data

Nearest Neighbor approaches can work with multi-modal data

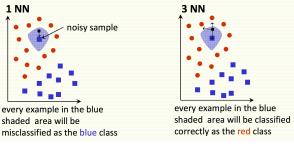


[Slide credit: O. Veksler]

[Pic by Olga Veksler]



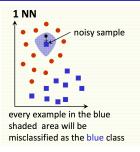
• Nearest neighbors sensitive to mis-labeled data ("class noise"). Solution?

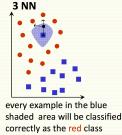


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#### Algorithm (kNN):

- 1. Find k examples  $\{\mathbf{x}^{(i)},t^{(i)}\}$  closest to the test instance  $\mathbf{x}$
- 2. Classification output is majority class

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

#### How do we choose k?

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- We can use cross-validation to find k
- Rule of thumb is k < sqrt(n), where n is the number of training examples

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    - Simple option: Linearly scale the range of each feature to be, e.g., in range [0,1]
    - Linearly scale each dimension to have 0 mean and variance 1 (compute mean  $\mu$  and variance  $\sigma^2$  for an attribute  $x_i$  and scale:  $(x_i m)/\sigma$ )
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- Non-metric attributes (symbols)
  - ► Hamming distance

## k-Nearest Neighbors: Issues (Complexity) & Remedies

- Expensive at test time: To find one nearest neighbor of a query point  $\mathbf{x}$ , we must compute the distance to all N training examples. Complexity: O(kdN) for kNN
  - Use subset of dimensions

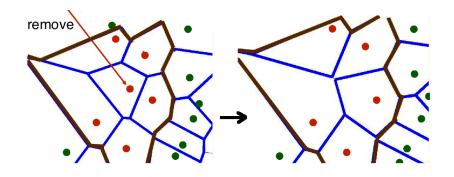


- Pre-sort training examples into fast data structures (e.g., kd-trees)
- Compute only an approximate distance (e.g., LSH)
- Remove redundant data (e.g., condensing)
- Storage Requirements: Must store all training data
  - Remove redundant data (e.g., condensing)
  - Pre-sorting often increases the storage requirements
- High Dimensional Data: "Curse of Dimensionality"
  - Required amount of training data increases exponentially with dimension
  - Computational cost also increases

[Slide credit: David Claus]

## k-Nearest Neighbors Remedies: Remove Redundancy

• If all Voronoi neighbors have the same class, a sample is useless, remove it



[Slide credit: O. Veksler]

## Example: Digit Classification

Decent performance when lots of data

# 0123456789

- Yann LeCunn MNIST Digit Recognition
  - Handwritten digits
  - 28x28 pixel images: d = 784
  - 60,000 training samples
  - 10,000 test samples
- Nearest neighbour is competitive

	Test Error Rate (%)
Linear classifier (1-layer NN)	12.0
K-nearest-neighbors, Euclidean	5.0
K-nearest-neighbors, Euclidean,	deskewed 2.4
K-NN, Tangent Distance, 16x16	1.1
K-NN, shape context matching	0.67
1000 RBF + linear classifier	3.6
SVM deg 4 polynomial	1.1
2-layer NN, 300 hidden units	4.7
2-layer NN, 300 HU, [deskewing]	1.6
LeNet-5, [distortions]	0.8
Boosted LeNet-4, [distortions]	0.7

## Fun Example: Where on Earth is this Photo From?

 Problem: Where (e.g., which country or GPS location) was this picture taken?



[Paper: James Hays, Alexei A. Efros. im2gps: estimating geographic information from a single image. CVPR'08. Project page: http://graphics.cs.cmu.edu/projects/im2gps/]

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- Problem: Where (e.g., which country or GPS location) was this picture taken?
  - ► Get 6M images from Flickr with GPs info (dense sampling across world)
  - ▶ Represent each image with meaningful features
  - ► Do kNN!



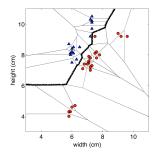
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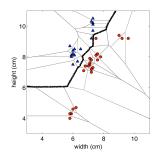
- Problem: Where (eg, which country or GPS location) was this picture taken?
  - ► Get 6M images from Flickr with gps info (dense sampling across world)
  - Represent each image with meaningful features
  - ▶ Do kNN (large k better, they use k = 120)!



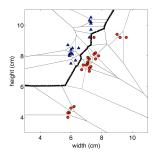
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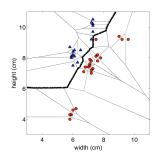
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- Problems:
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- Inductive Bias: What kind of decision boundaries do we expect to find?