CSC 411: Lecture 05: Nearest Neighbors

Class based on Raquel Urtasun & Rich Zemel's lectures

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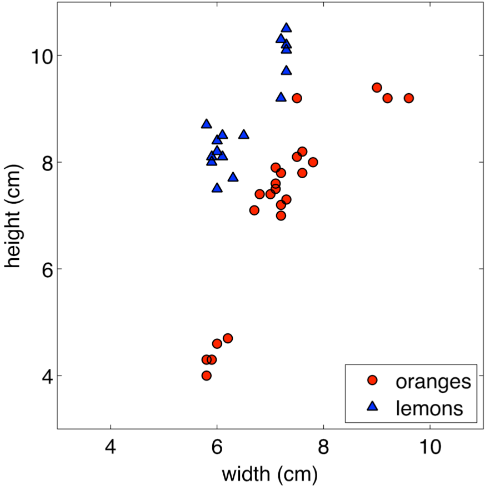
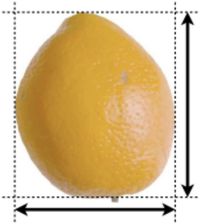
Today

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

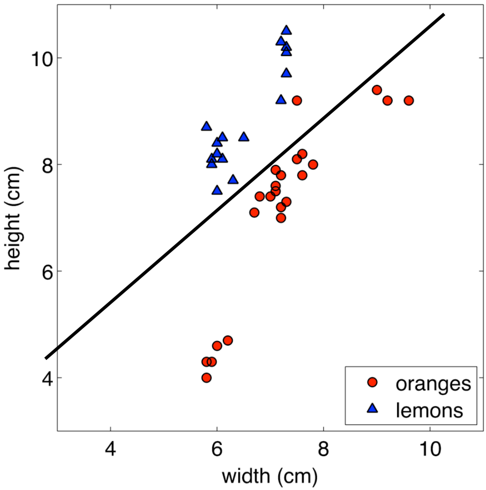
Note: We will mainly use today's method for classification, but it can also be used for regression

Classification: Oranges and Lemons



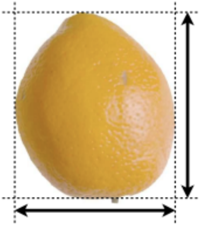


Classification: Oranges and Lemons



Can construct simple linear decision boundary:

$$y = \text{sign}(w_0 + w_1 x_1 + w_2 x_2)$$



What is the meaning of "linear" classification

- 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)

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

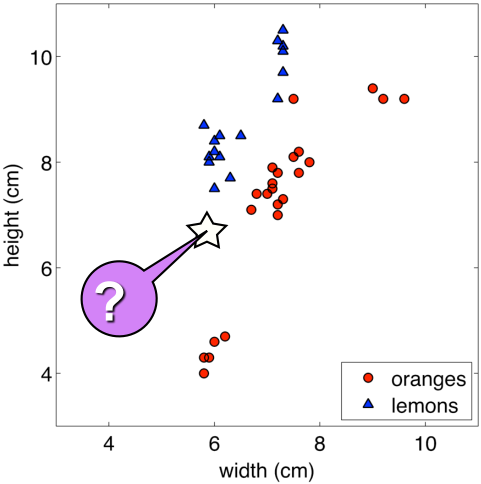
  with adaptive $\mathbf{w}$, w_0

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

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

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

Classification as Induction



Instance-based Learning

- Alternative to parametric models are non-parametric models
- These are typically simple methods for approximating discrete-valued or real-valued target functions (they work for 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

Nearest Neighbors

- Assume training examples correspond to points in d-dim Euclidean space
- **Idea**: The value of the target function for a new query is estimated from the known value(s) of the 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 $(\mathbf{x}^*, t^*)$ (from the stored training set) closest to the test instance $\mathbf{x}$. That is:

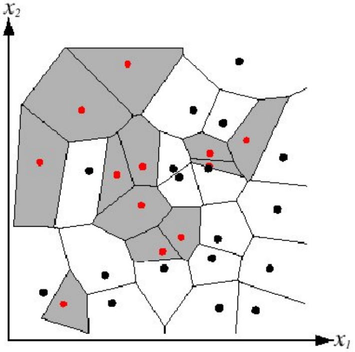
$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\text{argmin}} \ \text{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

2. Output $y = t^*$

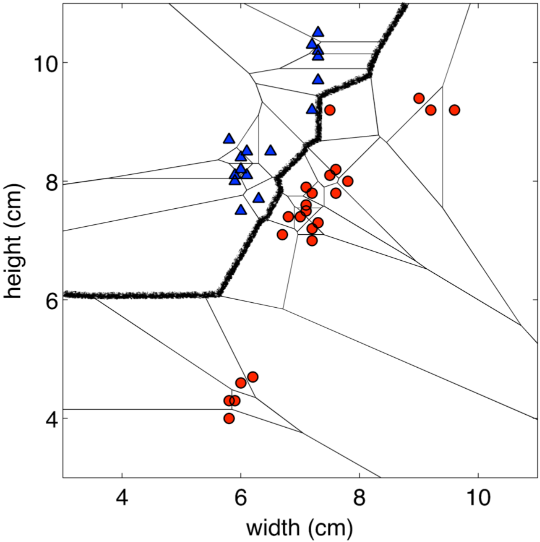
- Note: we don't really need to compute the square root. Why?

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

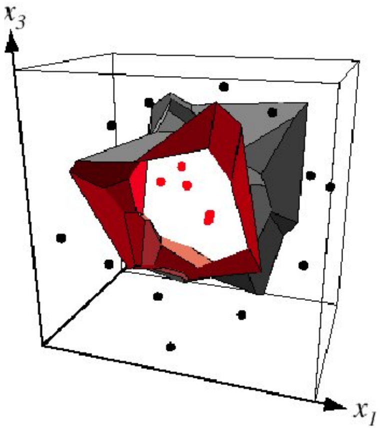


Nearest Neighbors: Decision Boundaries



Example: 2D decision boundary

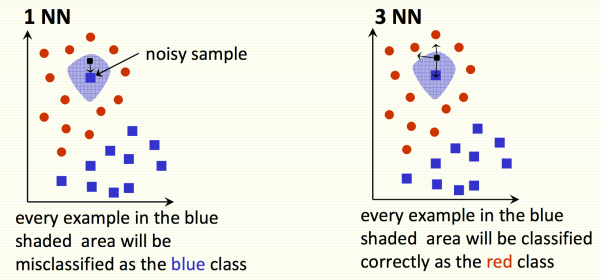
Nearest Neighbors: Decision Boundaries



Example: 3D decision boundary

k-Nearest Neighbors

[Pic by Olga Veksler]



- Nearest neighbors sensitive to mis-labeled data ("class noise"). Solution?
- Smooth by having k nearest neighbors vote

Algorithm (kNN):

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

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

k-Nearest Neighbors

How do we choose k?

- Larger k may lead to better performance
- But if we set k too large we may end up looking at samples that are not neighbors (are far away from the query)
- We can use cross-validation to find k
- Rule of thumb is $k < sqrt(n)$, where n is the number of training examples

[Slide credit: O. Veksler]

k-Nearest Neighbors: Issues & Remedies

- Some attributes have larger ranges, so are treated as more important
  - normalize scale
    - Simple option: Linearly scale the range of each feature to be, eg, in range [0,1]
    - Linearly scale each dimension to have 0 mean and variance 1 (compute mean μ and variance σ^2 for an attribute x_j and scale: $(x_j - m)/\sigma$)
  - be careful: sometimes scale matters
- 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

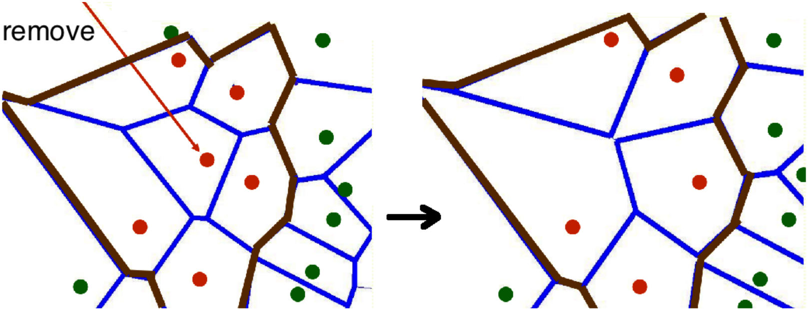
k-Nearest Neighbors: Issues (Complexity) & Remedies

- **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 (kd-trees)
  - Compute only an approximate distance (LSH)
  - Remove redundant data (condensing)
- **Storage Requirements:** Must store all training data
  - Remove redundant data (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 dramatically

[Slide credit: David Claus]

k-Nearest Neighbors Remedies: Remove Redundancy

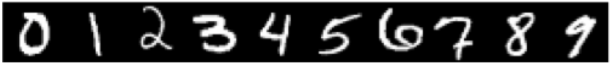
- If all Voronoi neighbors have the same class, a sample is useless, remove it



[Slide credit: O. Veksler]

Example: Digit Classification

- Decent performance when lots of data



- 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

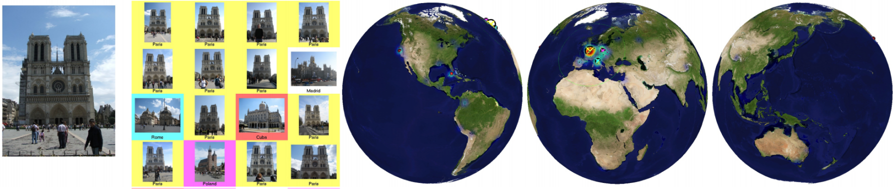
Fun Example: Where on Earth is this Photo From?

- Problem: Where (eg, 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/]

Fun Example: Where on Earth is this Photo From?

- 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!



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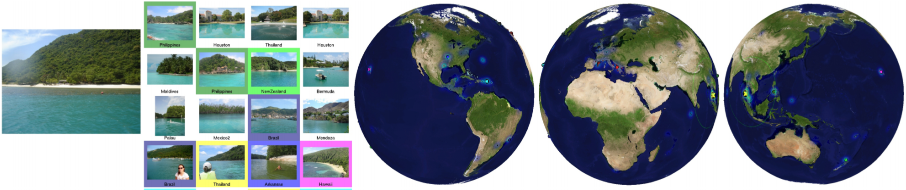
  - Do kNN (large k better, they use $k = 120$)!



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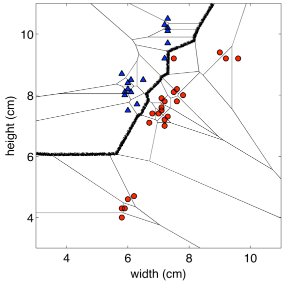
K-NN Summary



- Naturally forms complex decision boundaries; adapts to data density
- If we have lots of samples, kNN typically works well
- Problems:
  - Sensitive to class noise.
  - Sensitive to scales of attributes.
  - Distances are less meaningful in high dimensions
  - Scales linearly with number of examples
- Inductive Bias: What kind of decision boundaries do we expect to find?