ITCS 6156/8156 Fall 2024
Machine Learning

K-Nearest Neighbors

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Class Meeting: Tue & Thu, 4:00 PM – 5:15 PM, WWH 130

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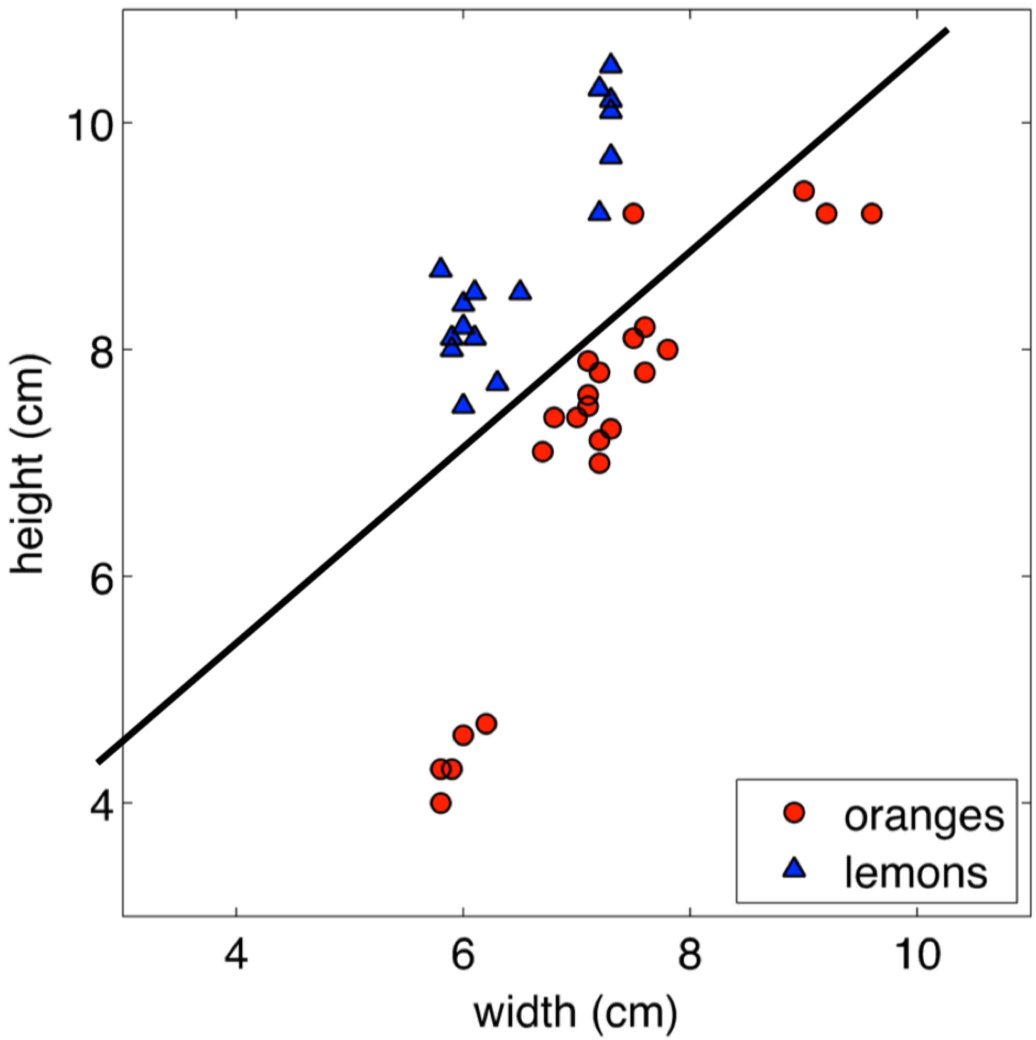
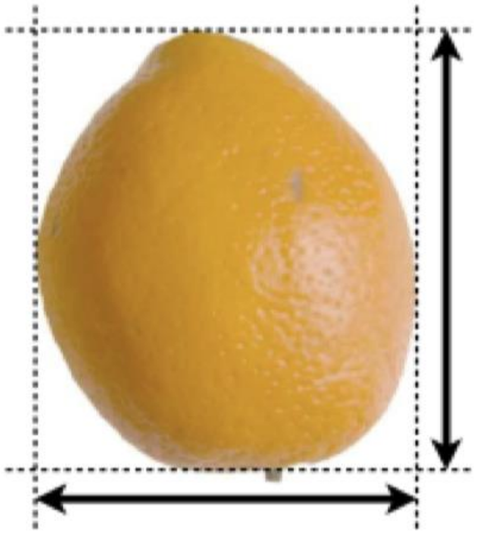
Some content in the slides is based on Dr. Raquel Urtasun's lecture

Classification: Oranges and Lemons





Can construct simple linear decision boundary:

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

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)

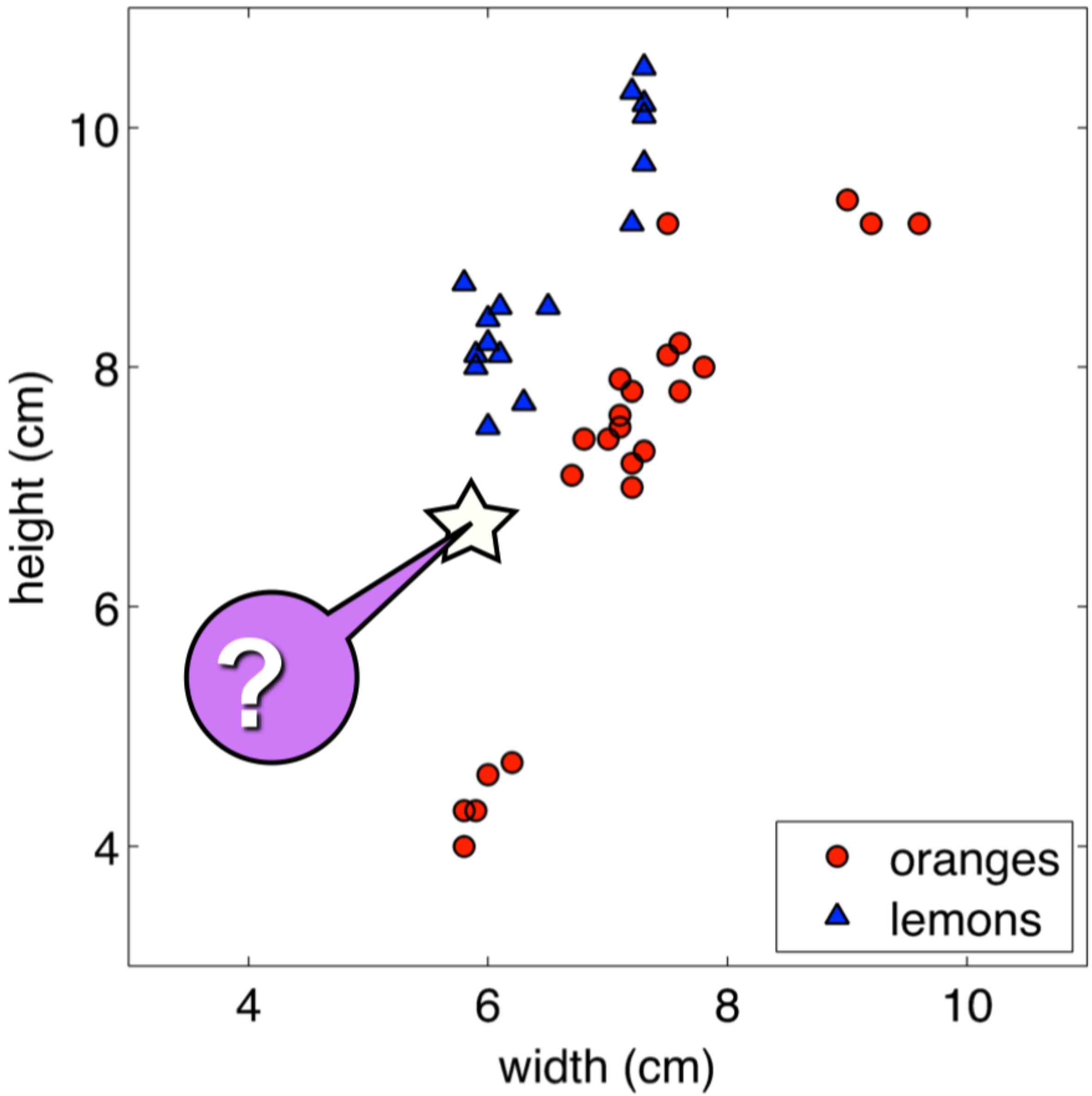
$$z(x) = \mathbf{w}^T\mathbf{x} + w_0$$

  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

- Training example in Euclidean space: $\mathbf{x} \in \Re^d$
- 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:

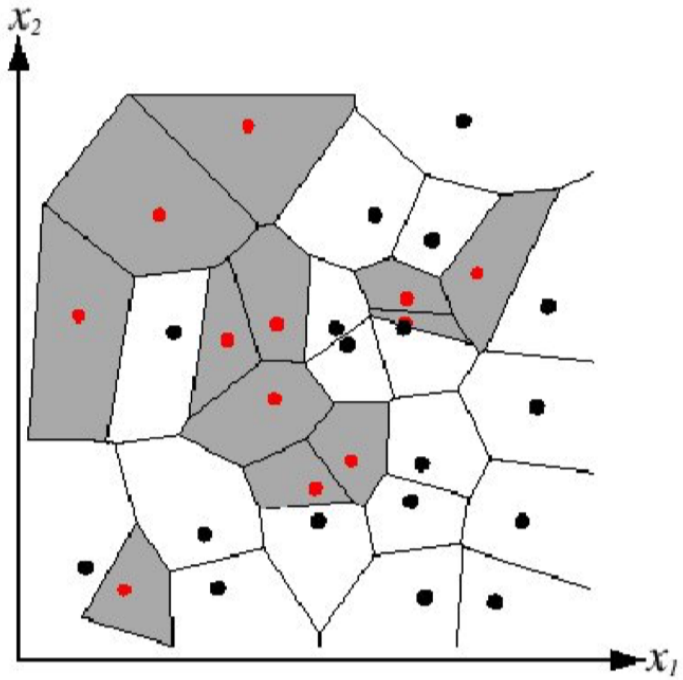
$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\operatorname{argmin}} \; \text{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

2. Output $y = t^*$

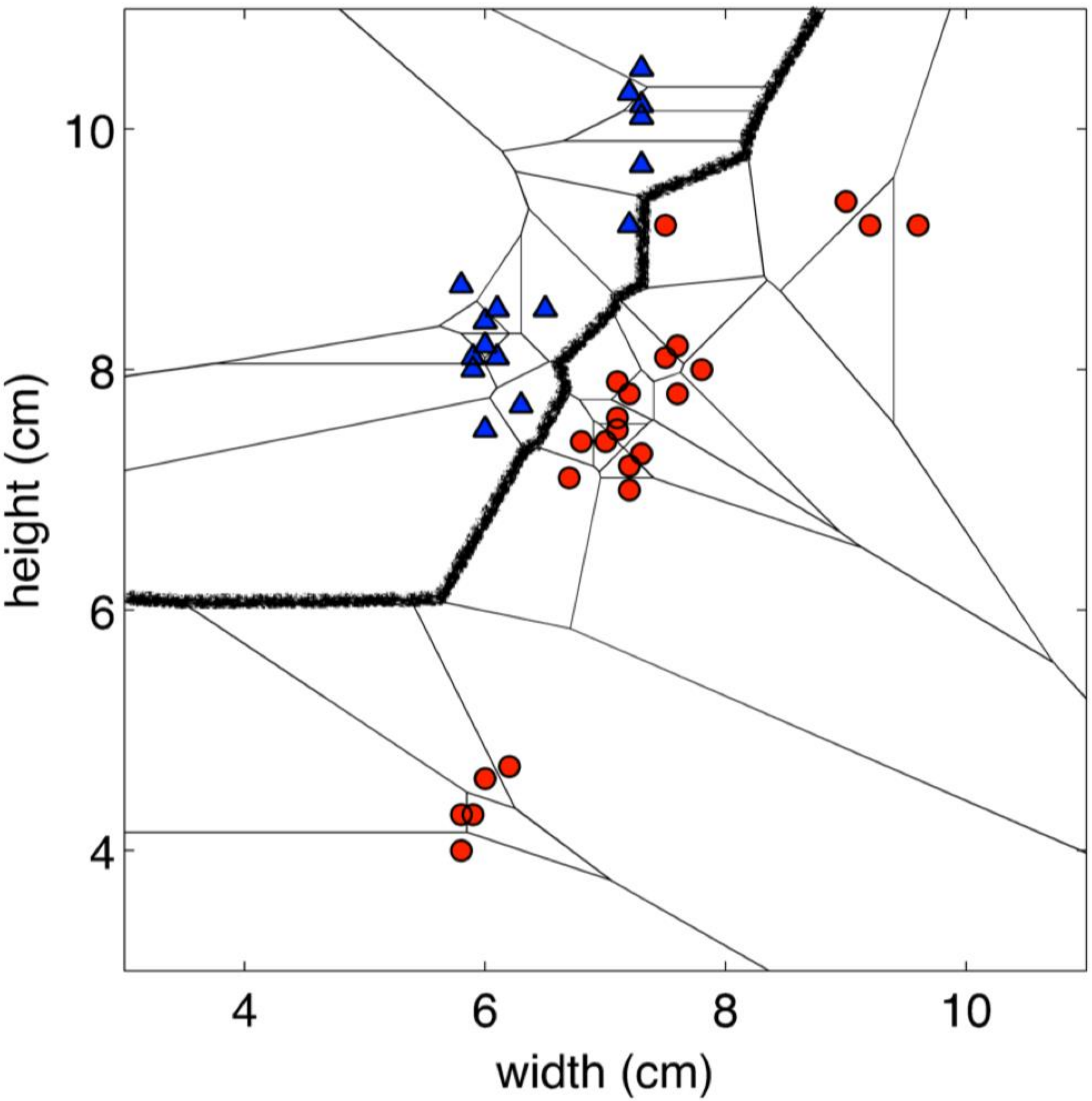
- Note: we don't really need to compute the square root. Why?

Nearest Neighbors: Decision Boundaries

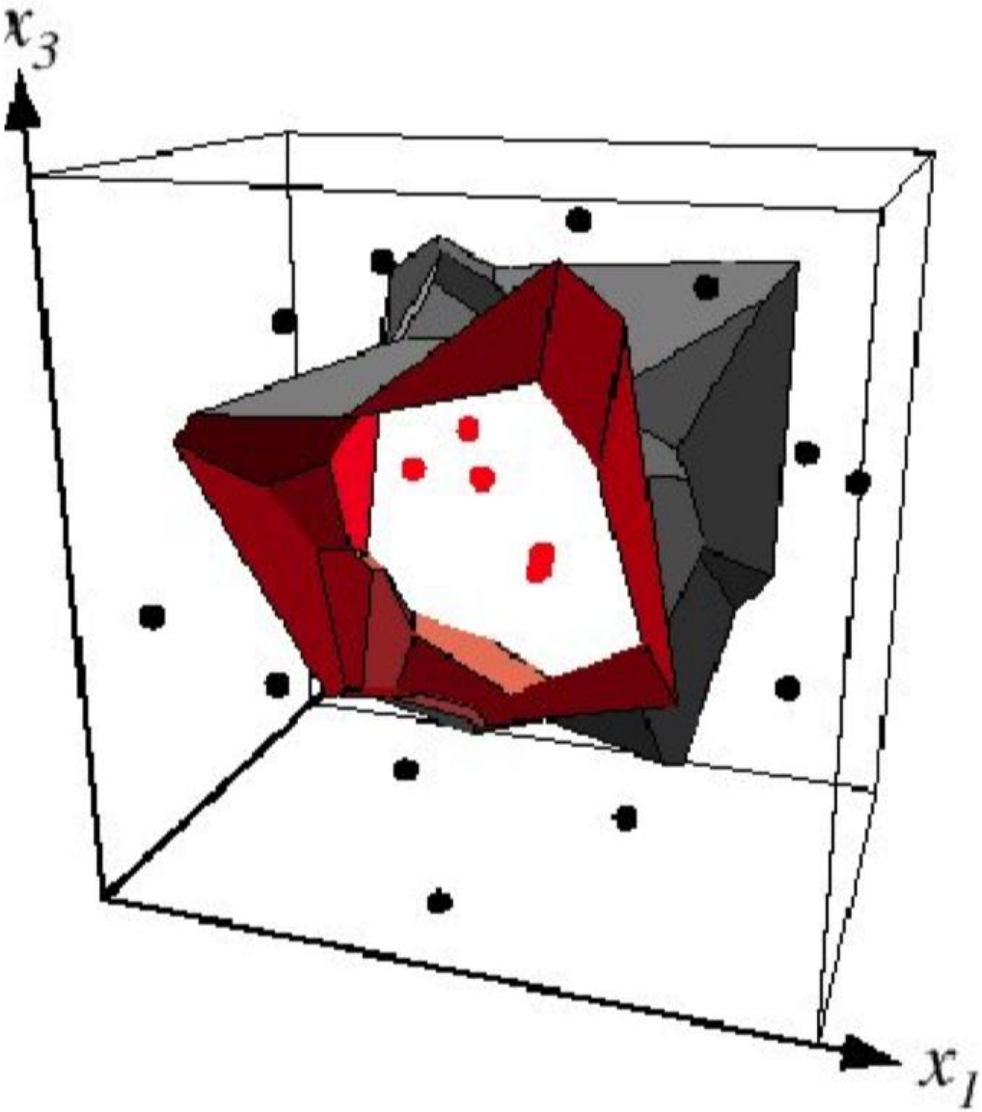
- Nearest neighbor algorithm does not explicitly compute decision boundaries, but these can be inferred
- Decision boundaries: Voronoi diagram visualization
  - show how input space divided into classes
  - each line segment is equidistant between two points of opposite classes



2D Decision Boundaries

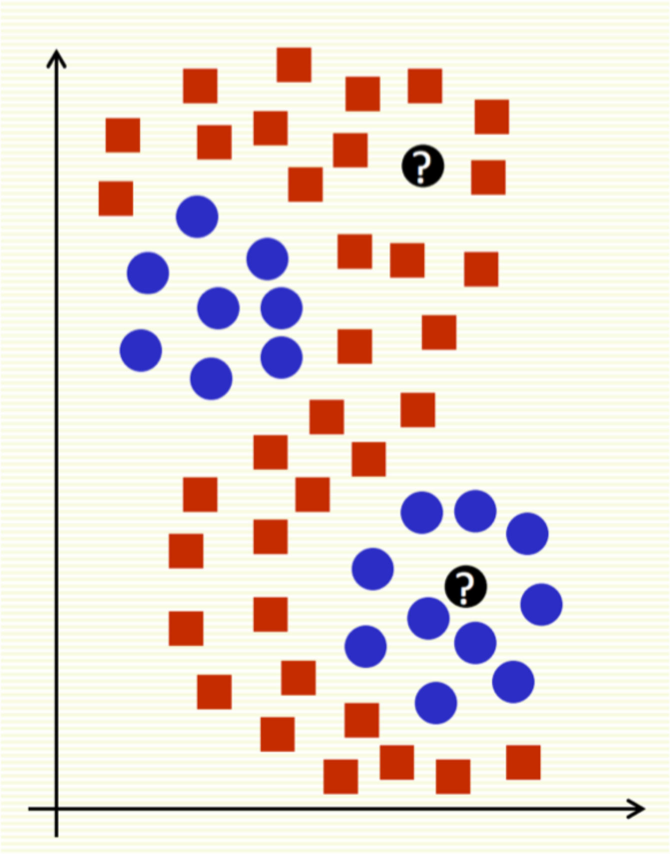


3D Decision Boundaries

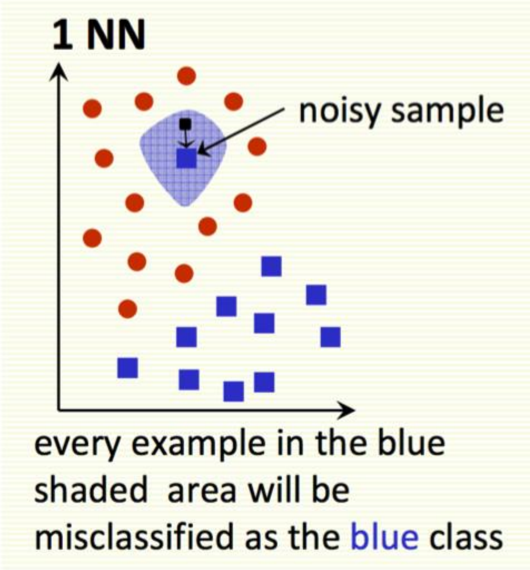


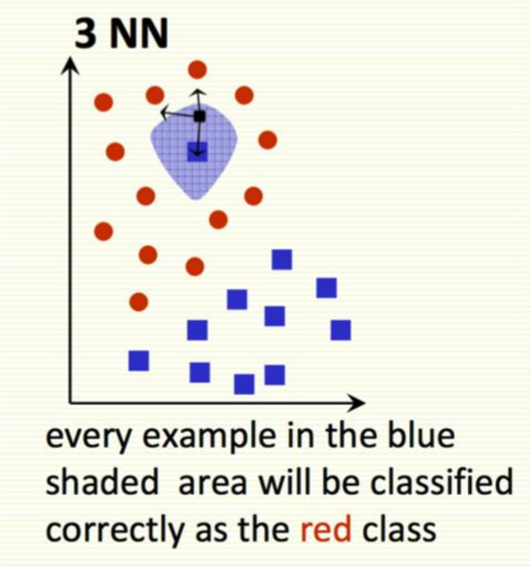
Multi-modal Data

- Nearest Neighbor approaches can work with multi-modal data



k-Nearest Neighbors





- 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

k-Nearest Neighbors

How do we choose k?

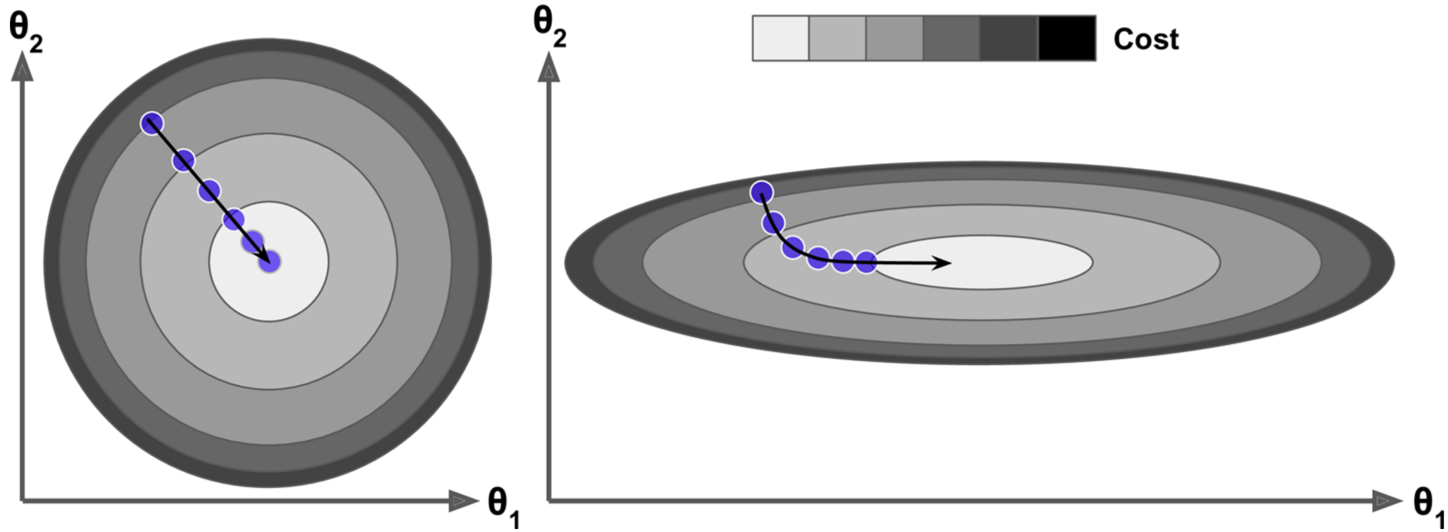
- Larger k may lead to better performance
- But if we set k too large we may end up looking at samples that are not neighbors (are far away from the query)
- We can use cross-validation to find k
- Rule of thumb is $k < sqrt(n)$, where n is the number of training examples

Issues & Remedies

- If some attributes (coordinates of $\mathbf{x}$) have larger ranges, they are treated as more important
  - normalize scale
    - 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 μ and variance σ^2 for an attribute x_j and scale: $(x_j - m)/\sigma$)
  - be careful: sometimes scale matters

Pre-processing Features

- Features may have very different scales, e.g. x_1 = rooms vs. x_2 = size in sq ft.
  - Right (*different scales*): GD goes first towards the bottom of the bowl, then slowly along an almost flat valley.
  - Left (*scaled features*): GD goes straight towards the minimum.



Feature Scaling

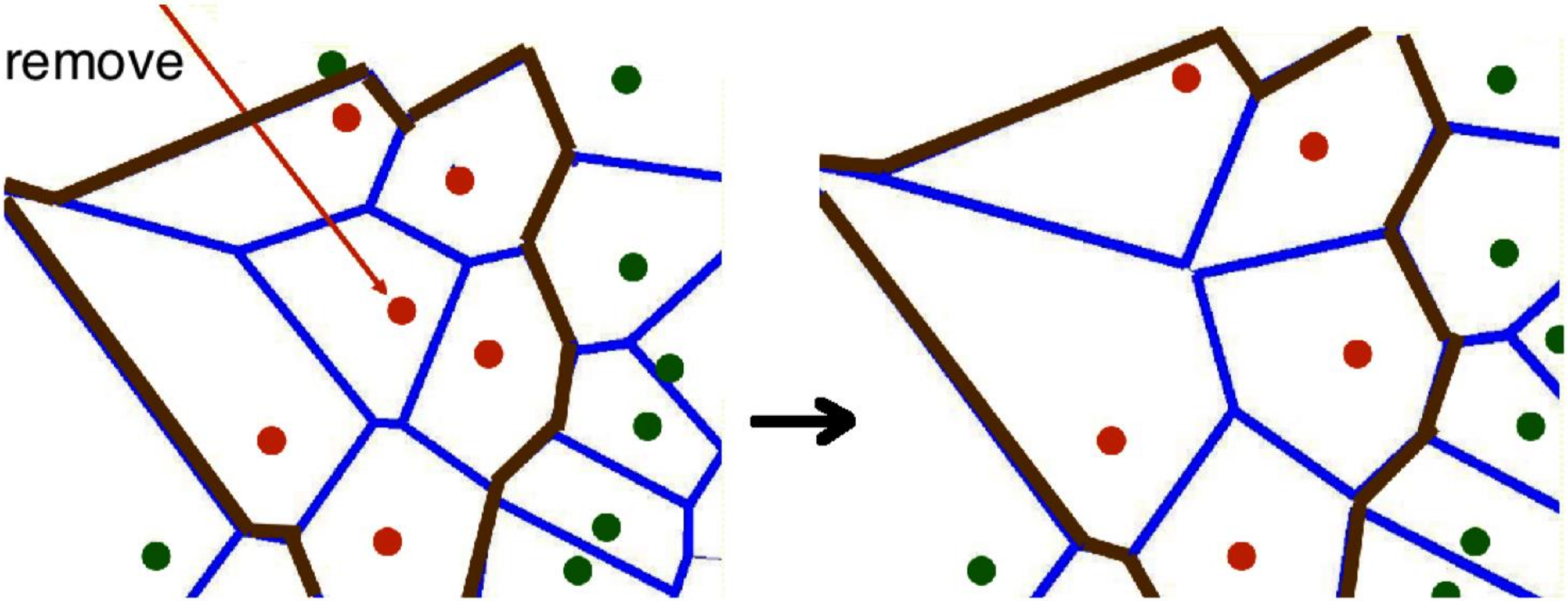
- Scaling between [0, 1] or [−1, +1]:
  - For each feature x_j, compute min_j and max_j **over the training examples**.
  - Scale x_j as follows: $\hat{x}_j = \frac{x_j - min_j}{max_j - min_j}$
- Scaling to standard normal distribution:
  - For each feature x_j, compute sample μ_j and sample σ_j **over the training examples**.
  - Scale x_j as follows: $\hat{x}_j = \frac{x_j - \mu_j}{\sigma_j}$
- **Use the same scaling factors at test time**:
  - Clip to min_j and max_j.

Issues & 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

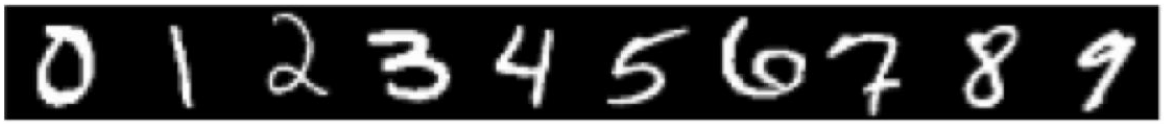
Remove Redundancy

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



Example: Digit Classification

- Decent performance when lots of data

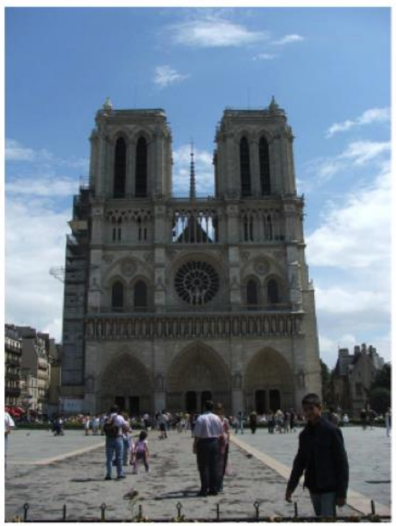


- Yann LeCunn – MNIST Digit Recognition
  - Handwritten digits
  - 28x28 pixel images: d = 784
  - 60,000 training samples
  - 10,000 test samples
- Nearest neighbour is competitive

	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

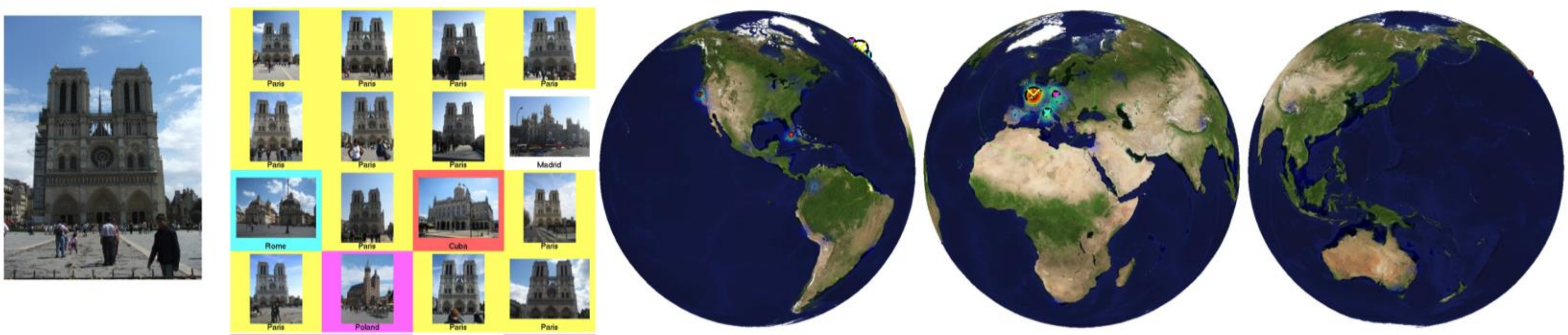
Fun Example: Where on Earth is this Photo From?

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



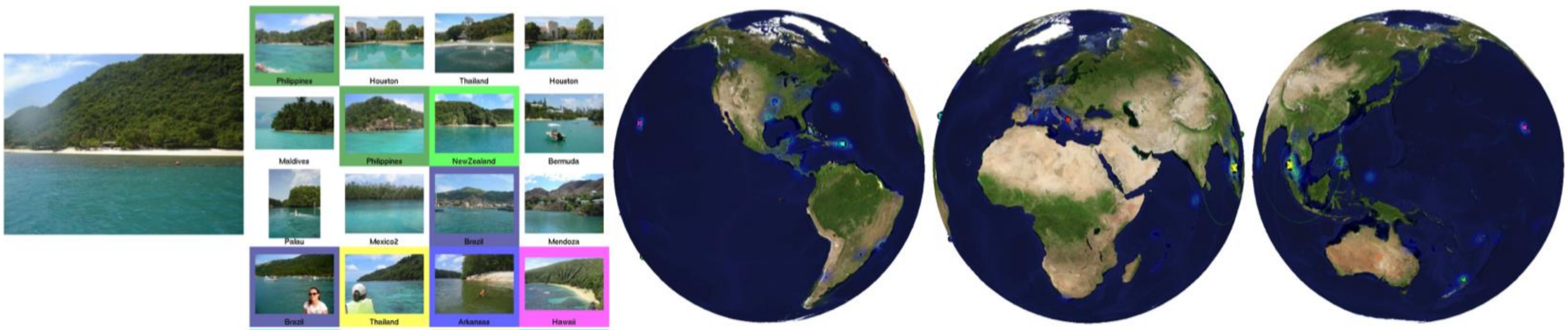
Fun Example: Where on Earth is this Photo From?

- 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!

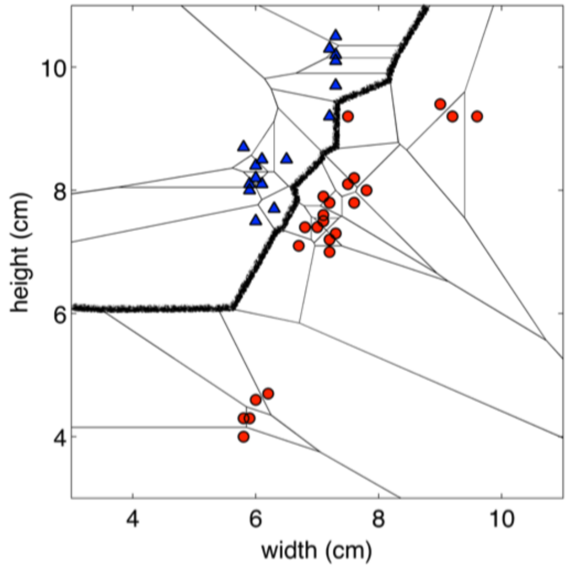


Fun Example: Where on Earth is this Photo From?

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



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

Questions?

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