CSC 411: Lecture 05: Nearest Neighbors

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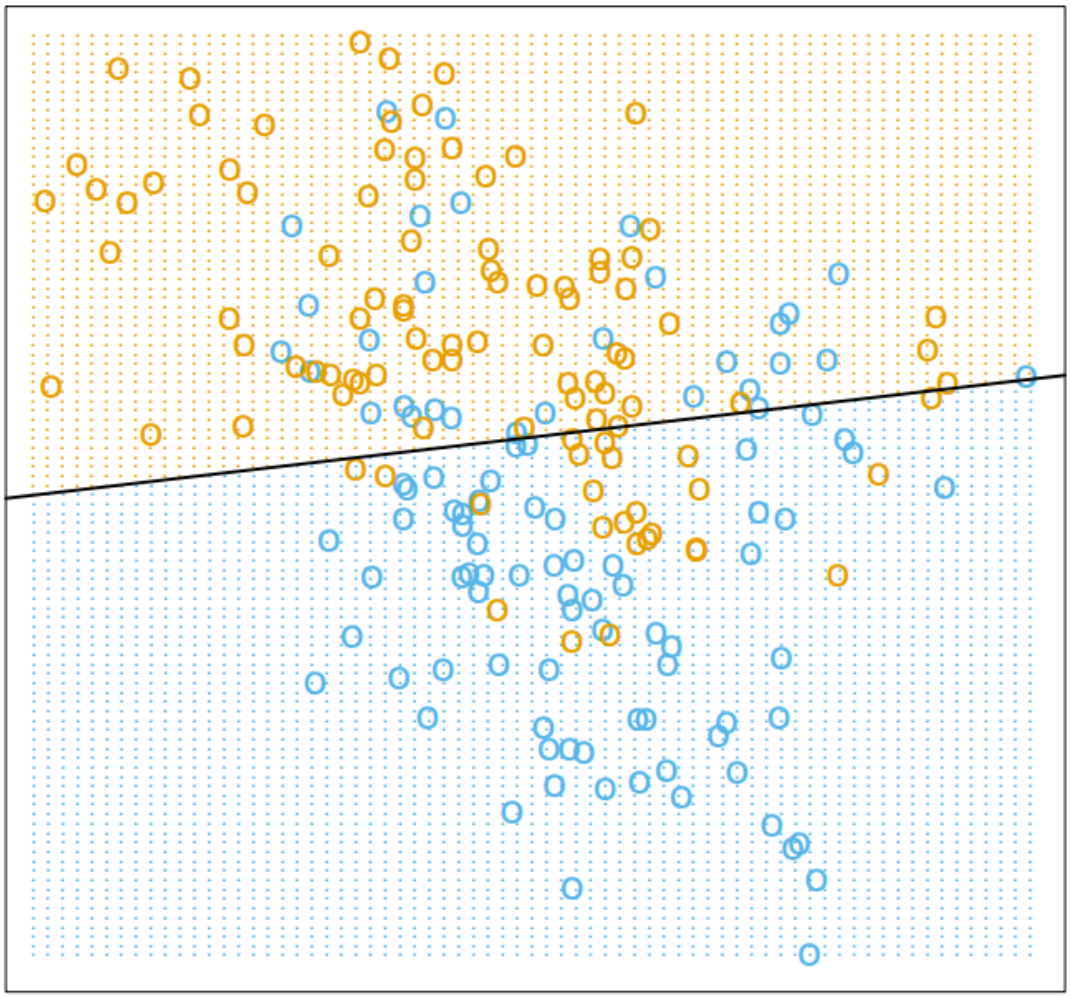
Today

- 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

Nonlinear Classification

We can construct a linear decision boundary $y = sign(w_0 + w_1 x_1 + w_2 x_2)$



[Image credit: "The Elements of Statistical Learning"]

What is the meaning of "linear" classification

- Linear classification means that the decision boundary is linear

$$\mathbf{w}^T\mathbf{x} = 0$$

- Most problems are not linear
  - "Classification of mathematical problems as linear and nonlinear is like classification of the Universe as bananas and non-bananas."
- This can be solved with good features but... how do you find good features? (hint: Deep learning)

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)
- NN Learning amounts to simply memorizing 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

Parametric vs. Non-parametric Models

- **Parametric**
  - Fixed Number of parameters
- **Non-parametric**
  - No fixed number of parameters
  - Parameters grow with the number of training data points

Non-parametric does not mean no parameters!

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:

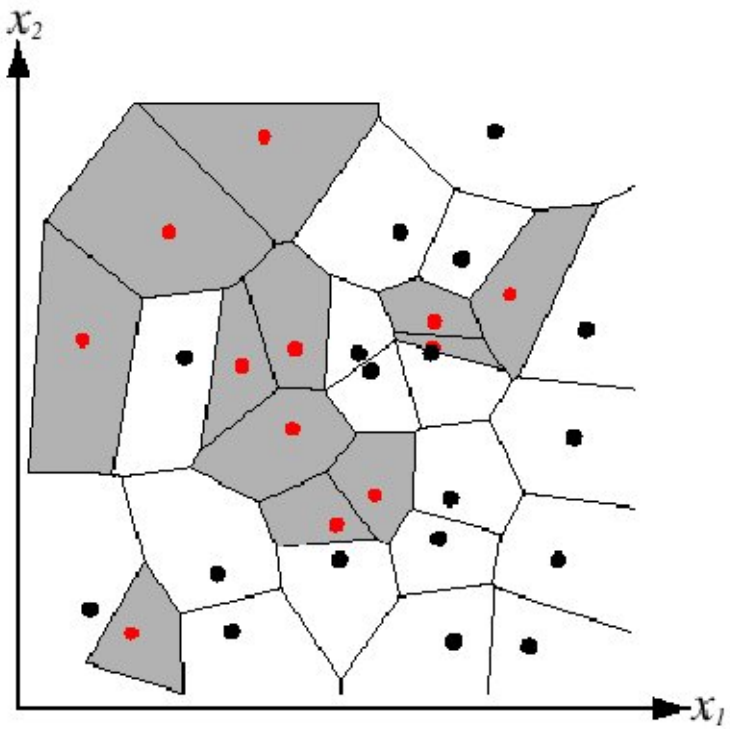
$$\mathbf{x}^* = \underset{\mathbf{x}^{(i)} \in \text{train. set}}{\text{argmin}} \ \text{distance}(\mathbf{x}^{(i)}, \mathbf{x})$$

2. Output $y = t^*$

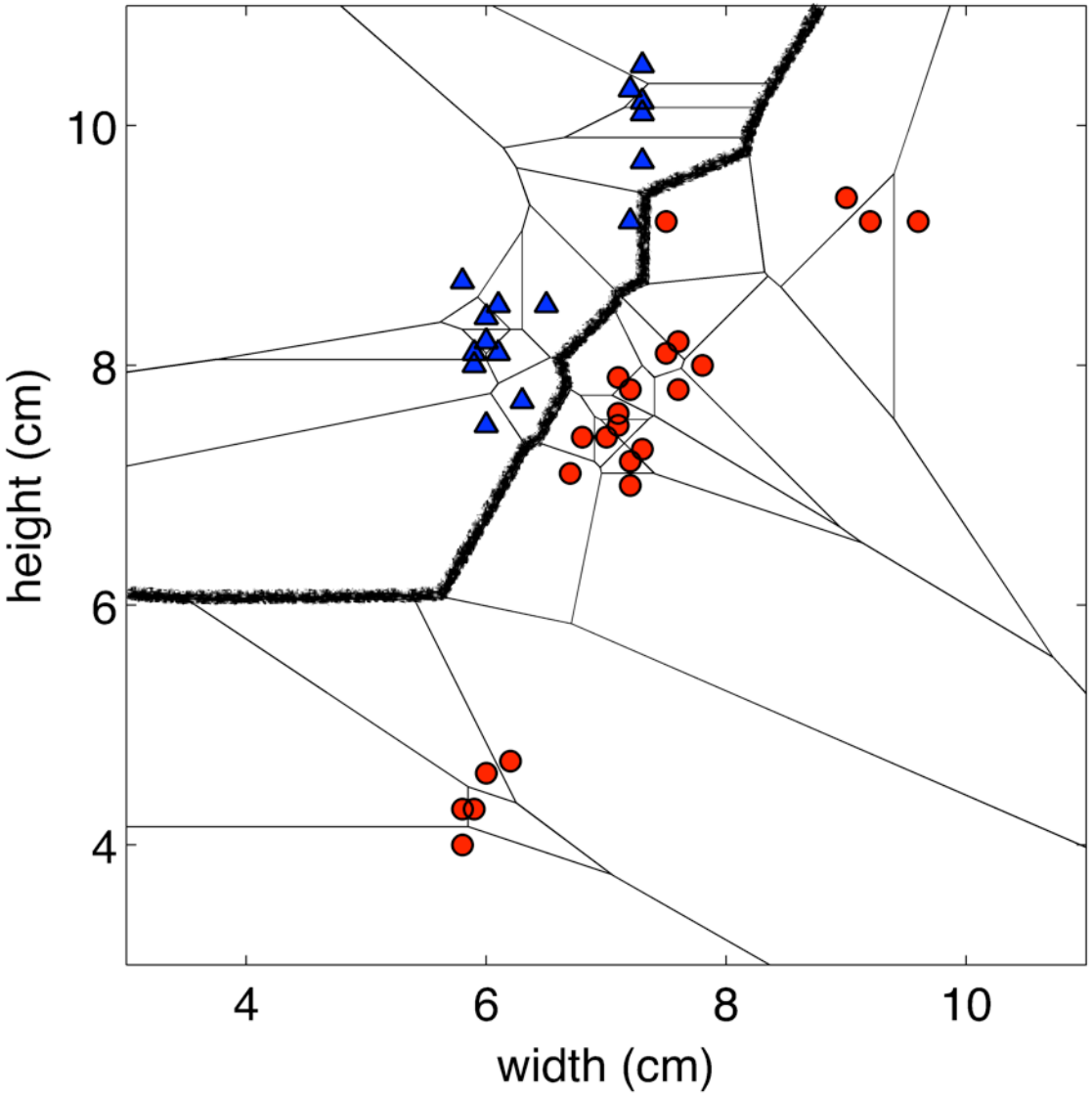
- Note: we don't really need to compute the square root. Why?

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

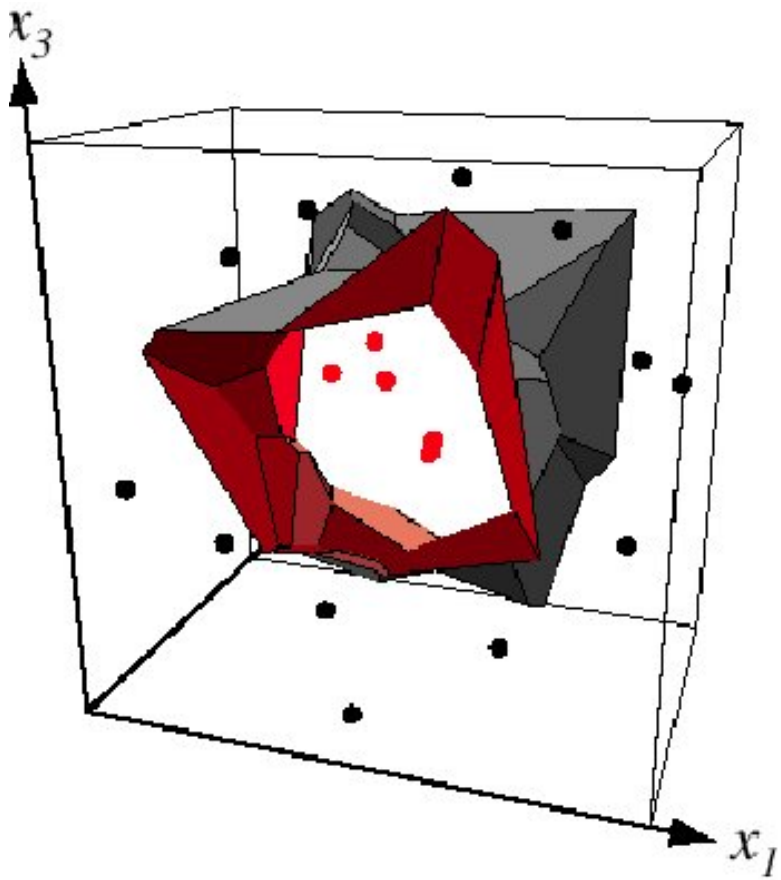


Nearest Neighbors: Decision Boundaries



Example: 2D decision boundary

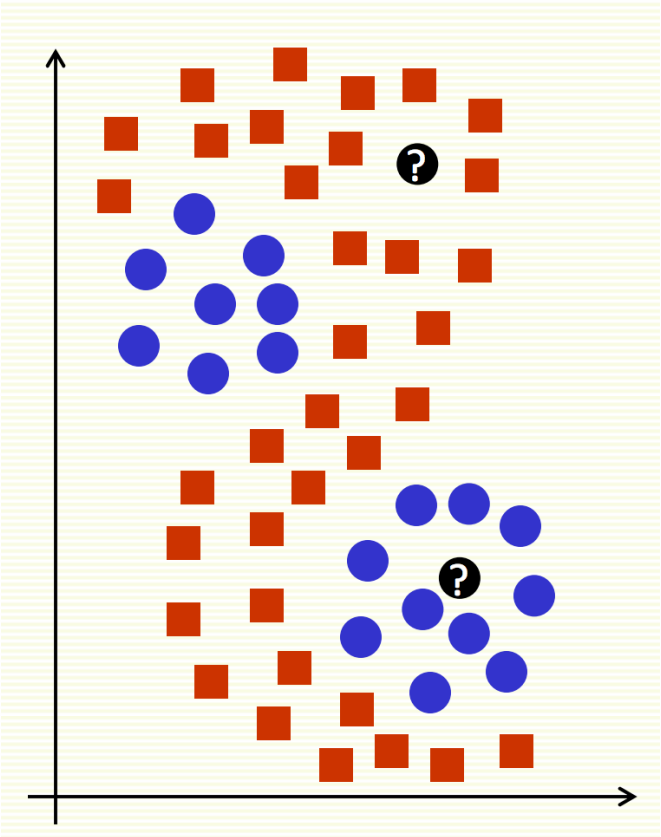
Nearest Neighbors: Decision Boundaries



Example: 3D decision boundary

Nearest Neighbors: Multi-modal Data

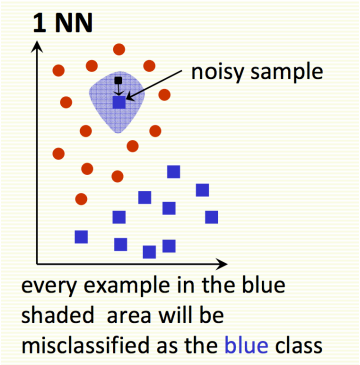
- Nearest Neighbor approaches can work with multi-modal data

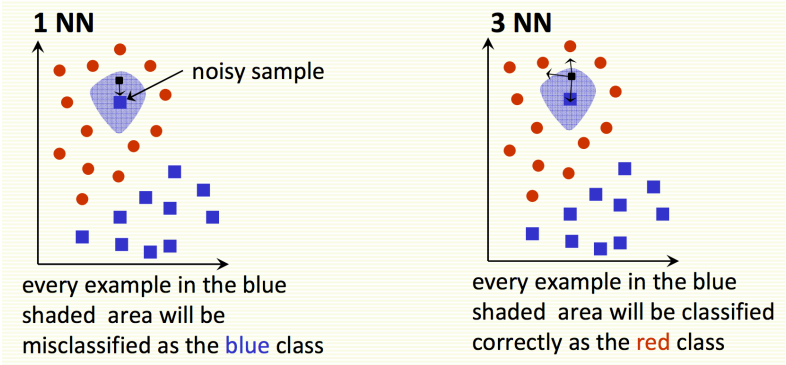


[Slide credit: O. Veksler]

k-Nearest Neighbors

[Pic by Olga Veksler]





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

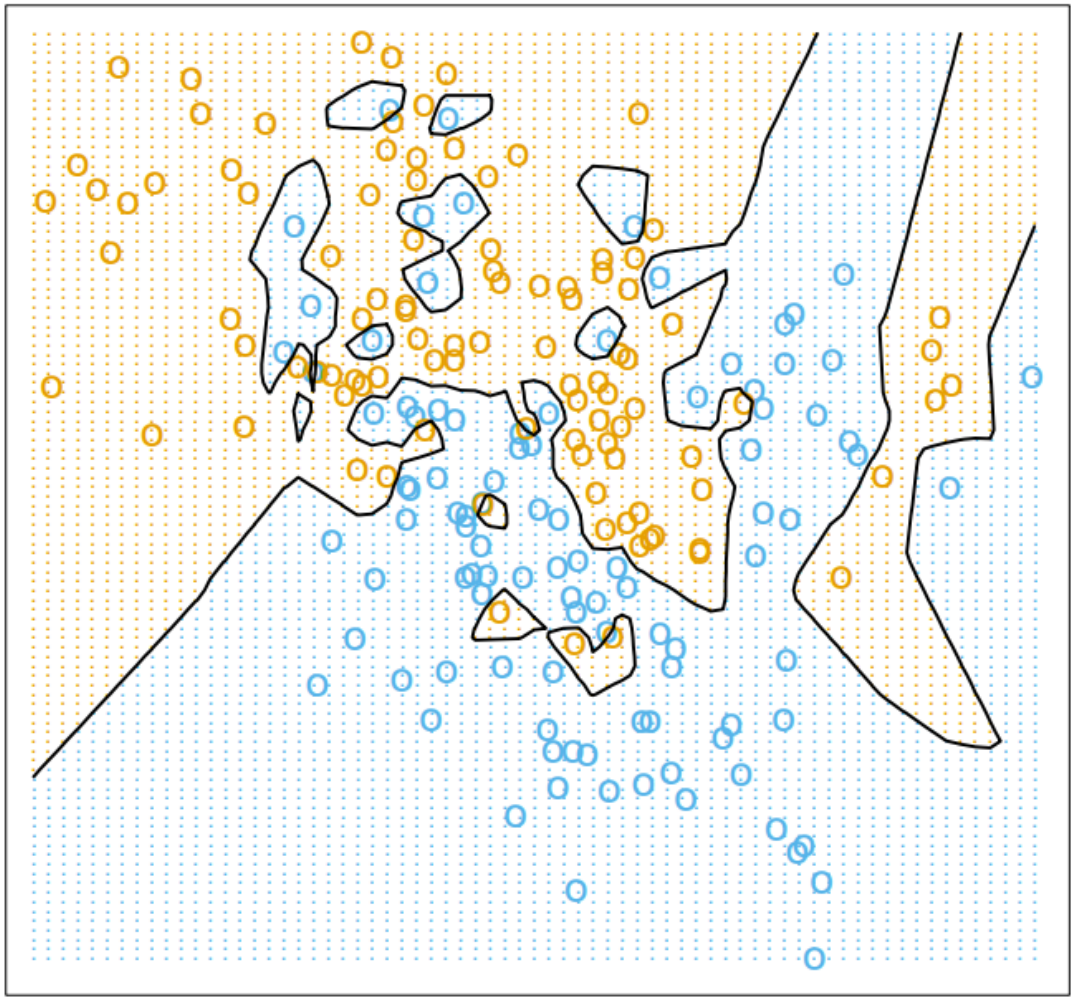
Algorithm (kNN):

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

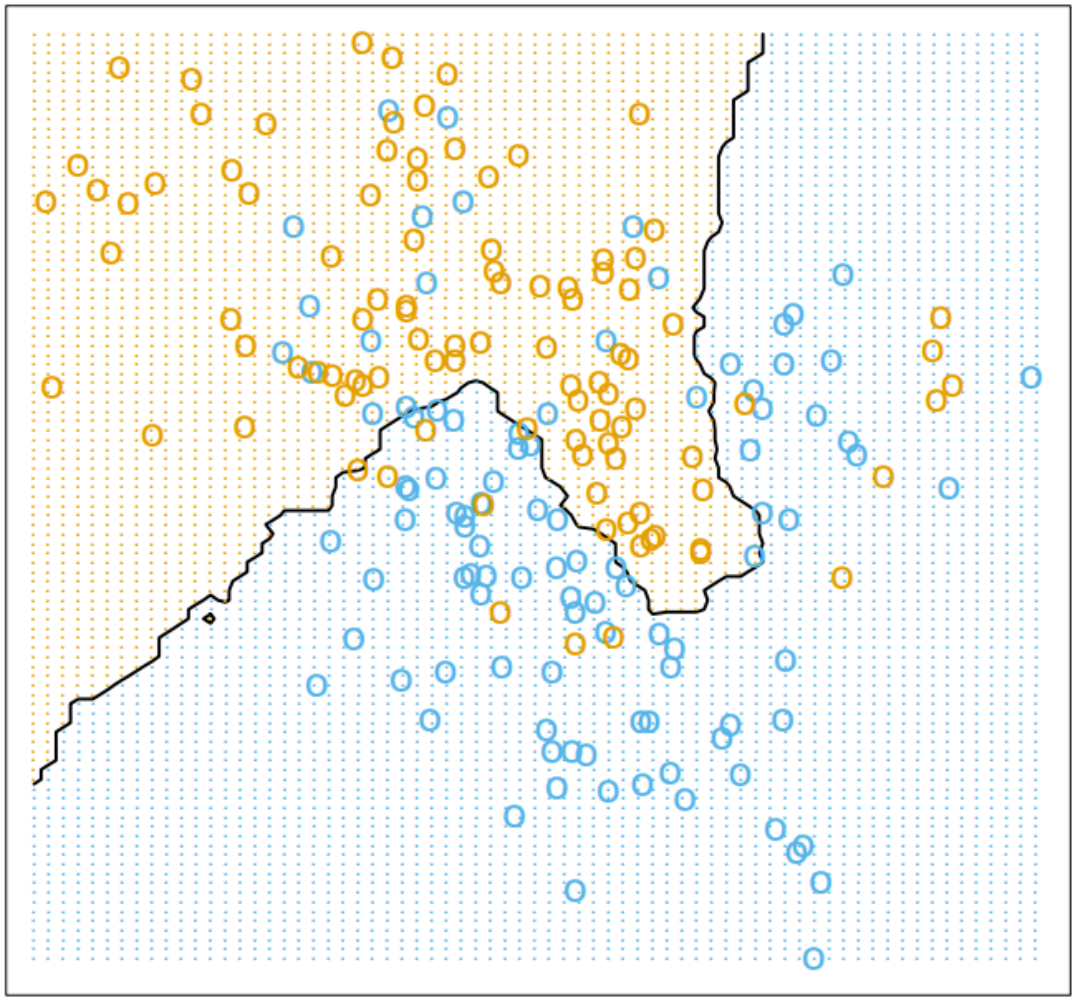
k=1



[Image credit: "The Elements of Statistical Learning"]

K-Nearest neighbors

k=15



[Image credit: "The Elements of Statistical Learning"]

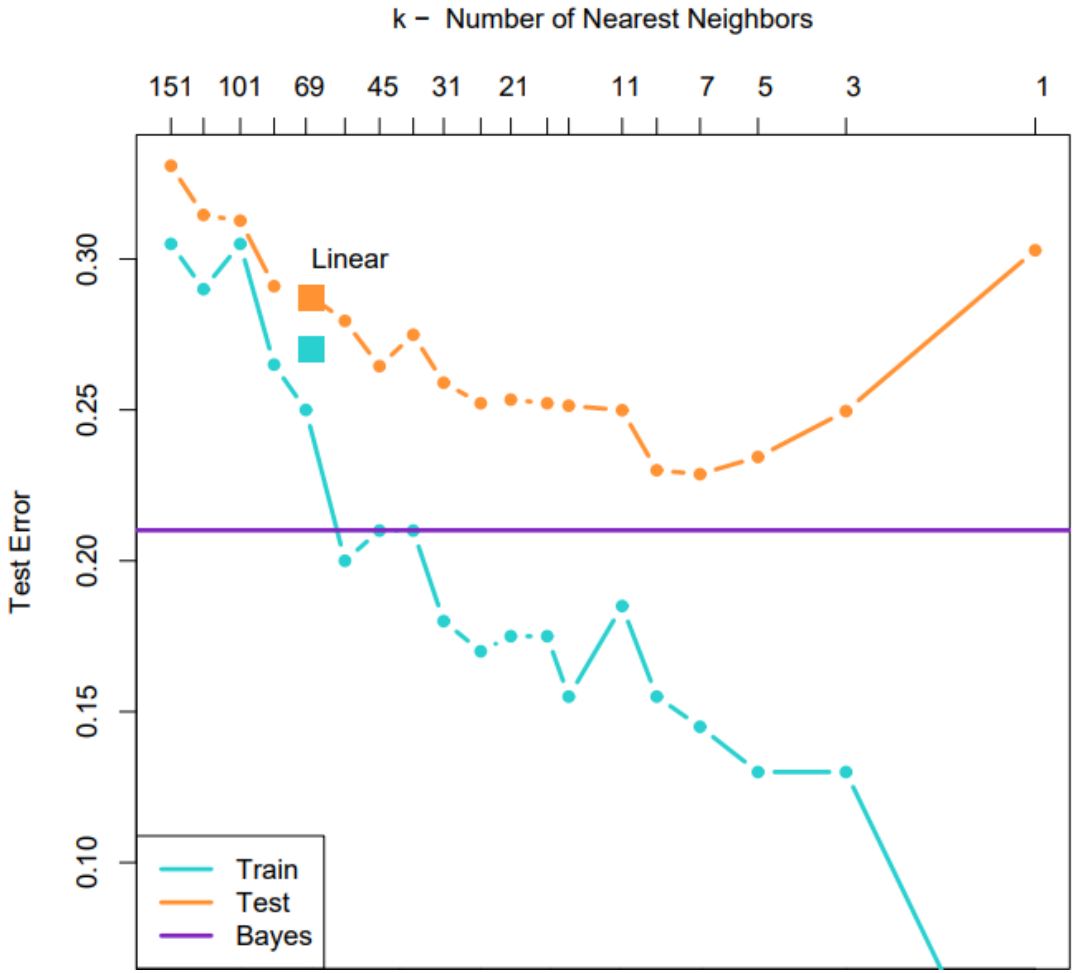
k-Nearest Neighbors

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 validation set / 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



[Image credit: "The Elements of Statistical Learning"]

NN Theory in a nutshell *

- Can we generalize just by memorizing?
- Assumptions:
  - NN assumes smoothness - we will assume $p(y = 1|x)$ is c-Lipschitz.
  - The inputs are in unit cube $x \in [0, 1]^d$
- Definition:
  - The Bayes-optimal classifier is (for binary prediction)

$$h^*(x) = \begin{cases} 1 & \text{if } p(y = 1|x) \geq 0.5 \\ -1 & \text{if } p(y = 1|x) < 0.5 \end{cases}$$

  - Given a sample S of size m, h_S is the 1-NN classifier.

Theorem::

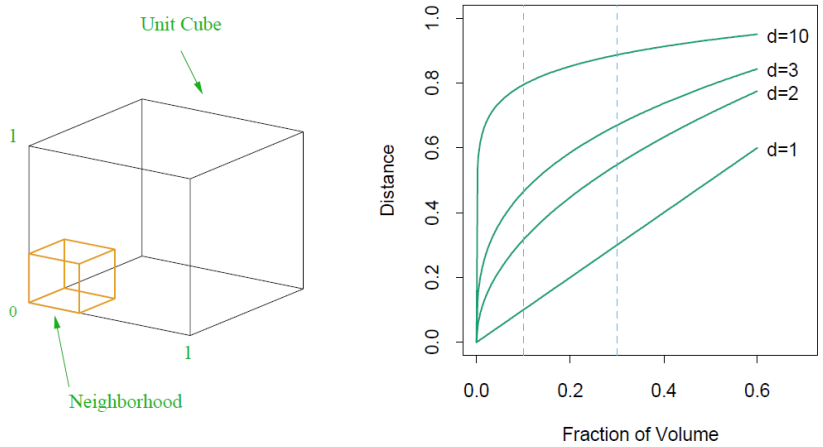
Under these assumptions

$$\mathbb{E}_S[L_{\mathcal{D}}(h_S)] \leq 2 \cdot L_{\mathcal{D}}(h^*) + \frac{4c\sqrt{d}}{m^{1/(d+1)}}$$

Converges to twice the optimal loss but exponentially slow in d.

The curse of dimensionality

- If we want the nearest neighbor to be closer then ϵ, how many points do we need to guarantee it?
- The volume of a single ball of radius ϵ is $\mathcal{O}(\epsilon^d)$
- The total volume of $[0,1]^d$ is 1.
- Therefore $\mathcal{O}\left((\frac{1}{\epsilon})^d\right)$ balls are needed to cover the volume.



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k-Nearest Neighbors: 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
- 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
- High Dimensional Data: "Curse of Dimensionality"
  - Required amount of training data increases exponentially with dimension
  - Computational cost also increases

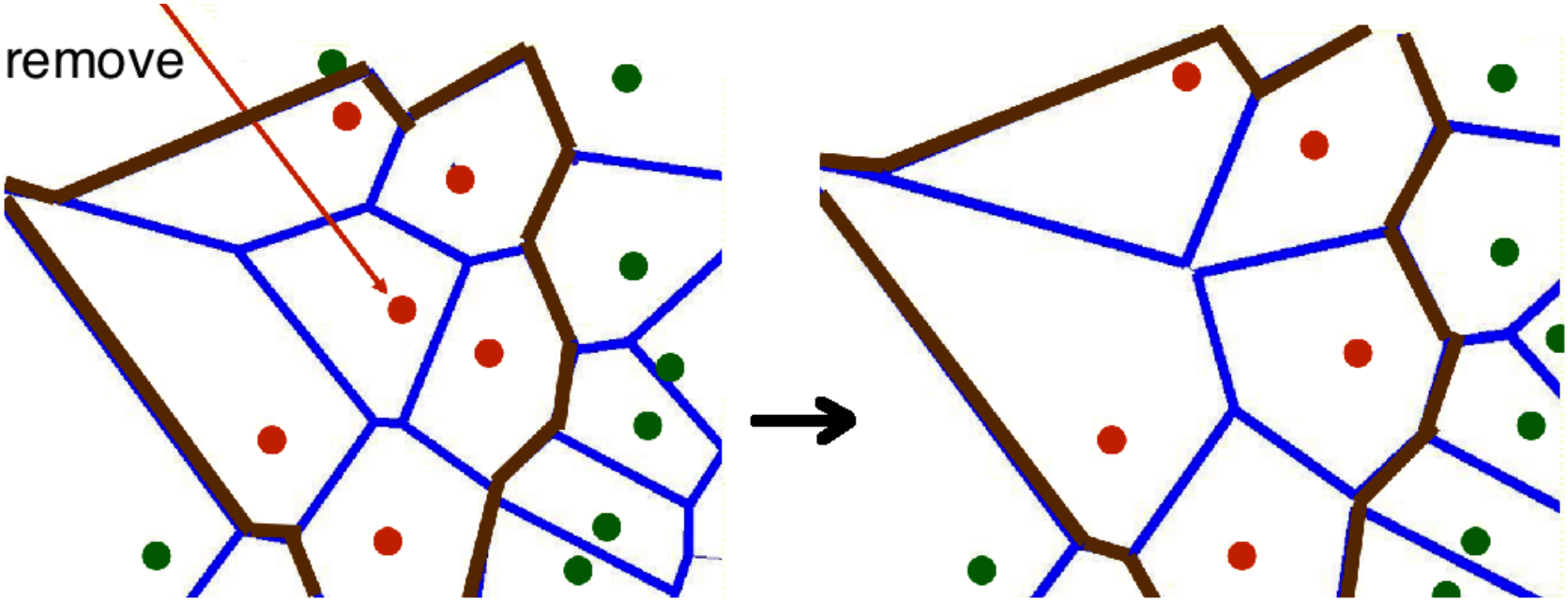
k-Nearest Neighbors: Issues (Complexity) & Remedies

- 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

[Slide credit: David Claus]

k-Nearest Neighbors Remedies: Remove Redundancy

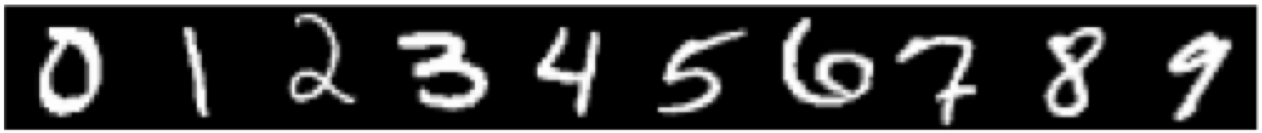
- If all Voronoi neighbors have the same class, a sample is useless, remove it



[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?

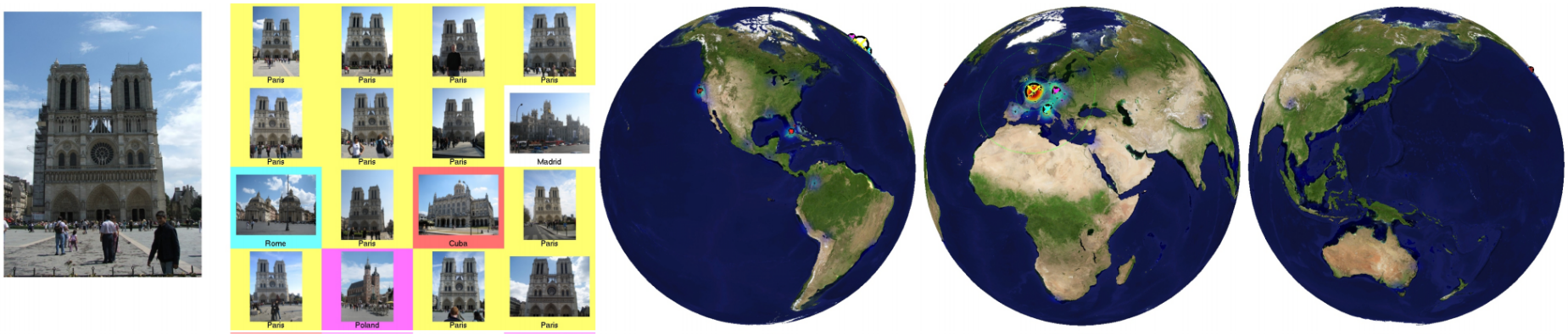
- Problem: Where (e.g., which country or GPS location) was this picture taken?



[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/]

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!



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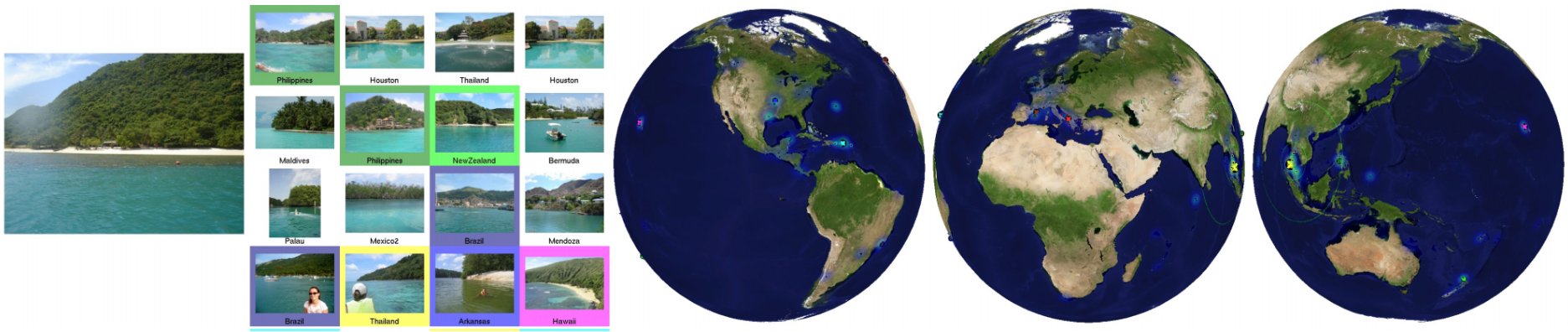
- Problem: Where (eg, which country or GPS location) was this picture taken?
  - Get 6M images from Flickr with gps info (dense sampling across world)
  - Represent each image with meaningful features
  - Do kNN (large k better, they use $k = 120$)!



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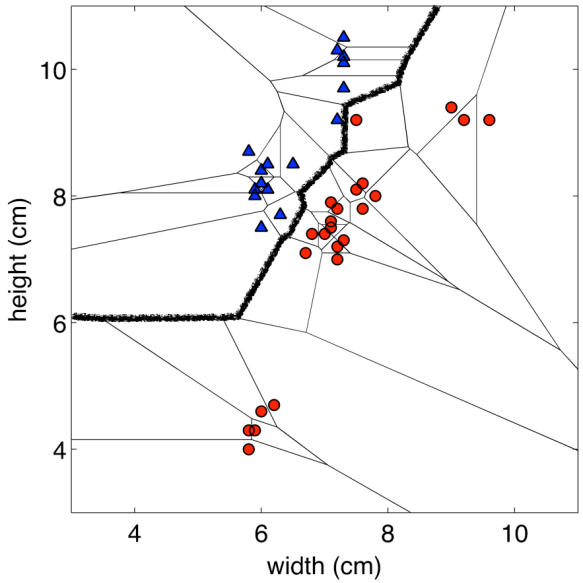
K-NN Summary



- 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
  - Expensive at run time.
- Inductive Bias: What kind of decision boundaries do we expect to find?