CS 188: Artificial Intelligence
Fall 2007

Lecture 26: Kernels
11/29/2007

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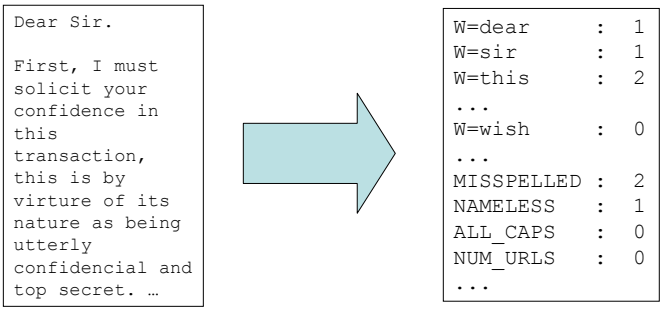
Feature Extractors

- A feature extractor maps inputs to feature vectors



- Many classifiers take feature vectors as inputs
- Feature vectors usually very sparse, use sparse encodings (i.e. only represent non-zero keys)

The Perceptron Update Rule

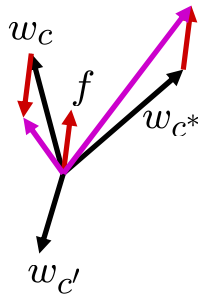
- Start with zero weights
- Pick up training instances one by one
- Try to classify

$$c = \arg\max_c \; w_c \cdot f(x)$$
$$= \arg\max_c \; \sum_i w_{c,i} \cdot f_i(x)$$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

$$w_c = w_c - f(x)$$

$$w_{c^*} = w_{c^*} + f(x)$$



Nearest-Neighbor Classification

- Nearest neighbor for digits:
  - Take new image
  - Compare to all training images
  - Assign based on closest example

- Encoding: image is vector of intensities:

 $= \langle 0.0 \;\; 0.0 \;\; 0.3 \;\; 0.8 \;\; 0.7 \;\; 0.1 \ldots 0.0 \rangle$

- What's the similarity function?
  - Dot product of two images vectors?

$$\text{sim}(x, y) = x \cdot y = \sum_i x_i y_i$$

  - Usually normalize vectors so ||x|| = 1
  - min = 0 (when?), max = 1 (when?)

Basic Similarity

- Many similarities based on feature dot products:

$$\text{sim}(x, y) = f(x) \cdot f(y) = \sum_i f_i(x) f_i(y)$$

- If features are just the pixels:

$$\text{sim}(x, y) = x \cdot y = \sum_i x_i y_i$$

- Note: not all similarities are of this form

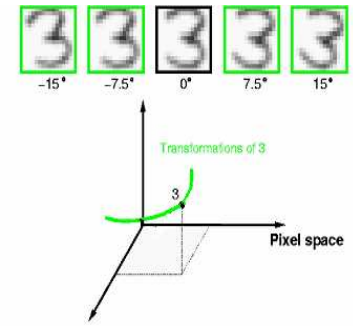
Invariant Metrics

- Better distances use knowledge about vision
- Invariant metrics:
  - Similarities are invariant under certain transformations
  - Rotation, scaling, translation, stroke-thickness…
  - E.g:


    - 16 x 16 = 256 pixels; a point in 256-dim space
    - Small similarity in R^{256} (why?)
  - How to incorporate invariance into similarities?

This and next few slides adapted from Xiao Hu, UIUC

Rotation Invariant Metrics



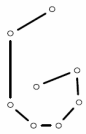
- Each example is now a curve in R^{256}
- Rotation invariant similarity:

s'=max s(r(), r())

- E.g. highest similarity between images' rotation lines

Template Deformation

- Deformable templates:
  - An "ideal" version of each category
  - Best-fit to image using min variance
  - Cost for high distortion of template
  - Cost for image points being far from distorted template
- Used in many commercial digit recognizers



Examples from [Hastie 94]

A Tale of Two Approaches…

- Nearest neighbor-like approaches
  - Can use fancy kernels (similarity functions)
  - Don't actually get to do explicit learning
- Perceptron-like approaches
  - Explicit training to reduce empirical error
  - Can't use fancy kernels (why not?)
  - Or can you? Let's find out!

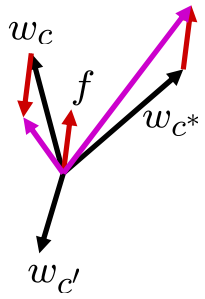
The Perceptron, Again

- Start with zero weights
- Pick up training instances one by one
- Try to classify

$$c = \arg\max_c \; w_c \cdot f(x)$$
$$= \arg\max_c \; \sum_i w_{c,i} \cdot f_i(x)$$

- If correct, no change!
- If wrong: lower score of wrong answer, raise score of right answer

$$w_c = w_c - f(x)$$
$$w_{c^*} = w_{c^*} + f(x)$$



Perceptron Weights

- What is the final value of a weight w_c?
  - Can it be any real vector?
  - No! It's built by adding up inputs.

$$w_c = 0 + f(x_1) - f(x_5) + \dots$$

$$w_c = \sum_i \alpha_{i,c} f(x_i)$$

- Can reconstruct weight vectors (the primal representation) from update counts (the dual representation)

$$\alpha_c = \langle \alpha_{1,c} \;\; \alpha_{2,c} \;\; \dots \;\; \alpha_{n,c} \rangle$$

Dual Perceptron

- How to classify a new example x?

$$\begin{aligned} \text{score}(c, x) &= w_c \cdot f(x) \\ &= \left(\sum_i \alpha_{i,c} f(x_i) \right) \cdot f(x) \\ &= \sum_i \alpha_{i,c} \left(f(x_i) \cdot f(x) \right) \\ &= \sum_i \alpha_{i,c} \; K(x_i, x) \end{aligned}$$

- If someone tells us the value of K for each pair of examples, never need to build the weight vectors!

Dual Perceptron

- Start with zero counts (alpha)
- Pick up training instances one by one
- Try to classify x_n,

$$c = \arg\max_c \sum_i \alpha_{i,c} K(x_i, x)$$

- If correct, no change!
- If wrong: lower count of wrong class (for this instance), raise score of right class (for this instance)

$$\alpha_{c,n} = \alpha_{c,n} - 1 \qquad w_c = w_c - f(x)$$

$$\alpha_{c^*,n} = \alpha_{c^*,n} + 1 \qquad w_{c^*} = w_{c^*} + f(x)$$

Kernelized Perceptron

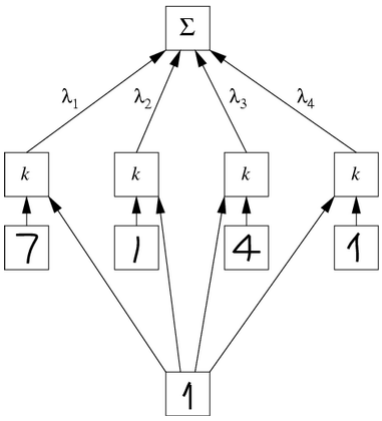
- If we had a black box (kernel) which told us the dot product of two examples x and y:
  - Could work entirely with the dual representation
  - No need to ever take dot products ("kernel trick")

$$\text{score}(c, x) = w_c \cdot f(x)$$

$$= \sum_i \alpha_{i,c} K(x_i, x)$$

- Like nearest neighbor – work with black-box similarities
- Downside: slow if many examples get nonzero alpha

Kernelized Perceptron Structure



$$\sum = \text{score}(c, x)$$

$$\lambda_i = \alpha_{c,i}$$

Kernels: Who Cares?

- So far: a very strange way of doing a very simple calculation
- "Kernel trick": we can substitute any* similarity function in place of the dot product
- Lets us learn new kinds of hypothesis

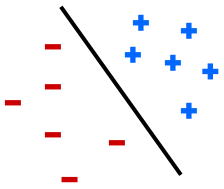
* Fine print: if your kernel doesn't satisfy certain technical requirements, lots of proofs break. E.g. convergence, mistake bounds. In practice, illegal kernels *sometimes* work (but not always).

Properties of Perceptrons

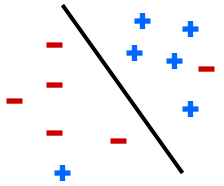
- Separability: some parameters get the training set perfectly correct
- Convergence: if the training is separable, perceptron will eventually converge (binary case)
- Mistake Bound: the maximum number of mistakes (binary case) related to the *margin* or degree of separability

$$\text{mistakes} < \frac{1}{\delta^2}$$

Separable

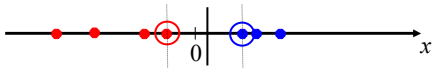


Non-Separable

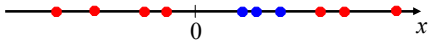


Non-Linear Separators

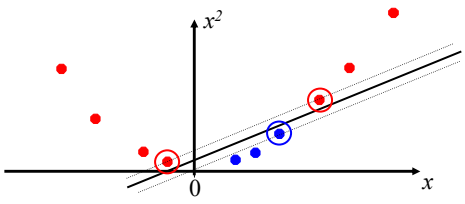
- Data that is linearly separable (with some noise) works out great:



- But what are we going to do if the dataset is just too hard?



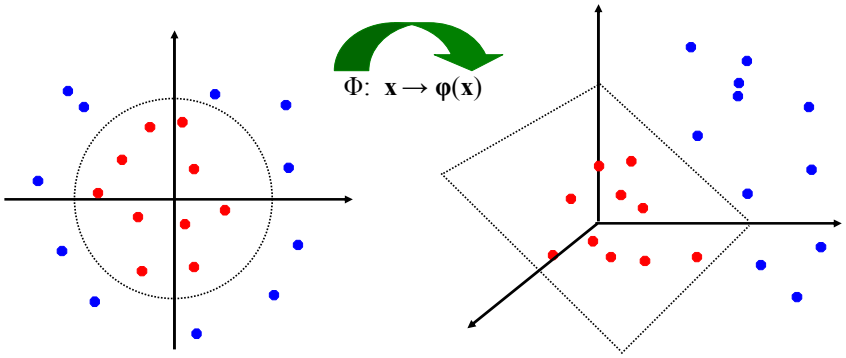
- How about… mapping data to a higher-dimensional space:



This and next few slides adapted from Ray Mooney, UT

Non-Linear Separators

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



Some Kernels

- Kernels implicitly map original vectors to higher dimensional spaces, take the dot product there, and hand the result back
- Linear kernel: $K(x, x') = x' \cdot x' = \sum_i x_i x'_i$
- Quadratic kernel: $K(x, x') = (x \cdot x' + 1)^2$

$$= \sum_{i,j} x_i x_j x'_i x'_j + 2 \sum_i x_i x'_i + 1$$

- RBF: infinite dimensional representation

$$K(x, x') = \exp(-||x - x'||^2)$$

- Discrete kernels: e.g. string kernels

Recap: Classification

- Classification systems:
  - Supervised learning
  - Make a rational prediction given evidence
  - We've seen several methods for this
  - Useful when you have labeled data (or can get it)

Clustering

- Clustering systems:
  - Unsupervised learning
  - Detect patterns in unlabeled data
    - E.g. group emails or search results
    - E.g. find categories of customers
    - E.g. detect anomalous program executions
  - Useful when don't know what you're looking for
  - Requires data, but no labels
  - Often get gibberish

Clustering

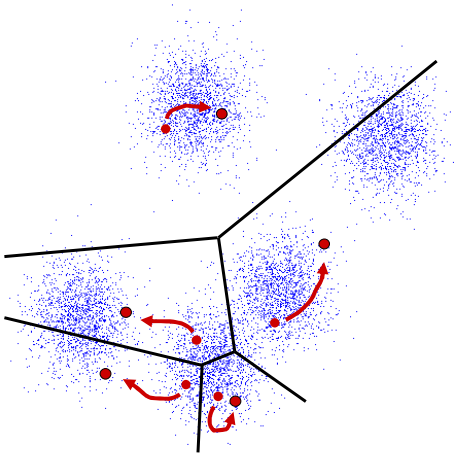
- Basic idea: group together similar instances
- Example: 2D point patterns

- What could "similar" mean?
  - One option: small (squared) Euclidean distance

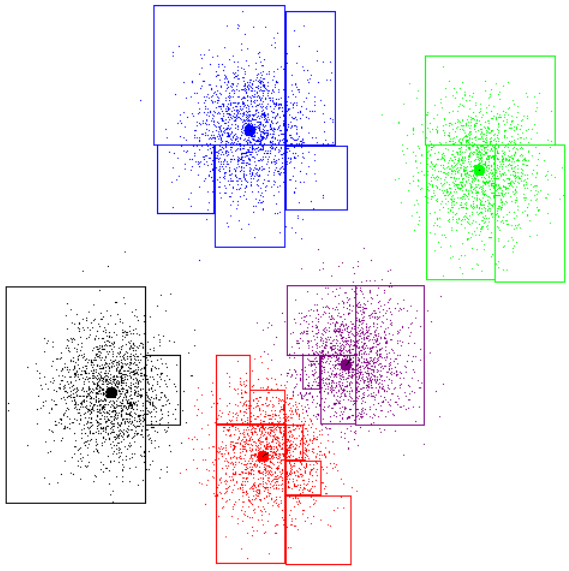
$$\text{dist}(x, y) = (x - y)^{\top}(x - y) = \sum_i (x_i - y_i)^2$$

K-Means

- An iterative clustering algorithm
  - Pick K random points as cluster centers (means)
  - Alternate:
    - Assign data instances to closest mean
    - Assign each mean to the average of its assigned points
  - Stop when no points' assignments change



K-Means Example



K-Means as Optimization

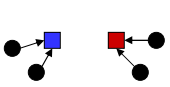
- Consider the total distance to the means:

$$\phi(\{x_i\},\{a_i\},\{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

points assignments means

- Each iteration reduces phi

- Two stages each iteration:
  - Update assignments: fix means c, change assignments a
  - Update means: fix assignments a, change means c



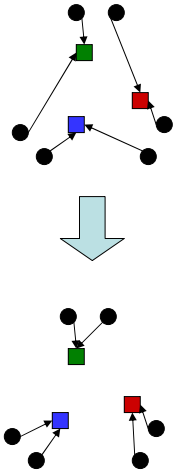
Phase I: Update Assignments

- For each point, re-assign to closest mean:

$$a_i = \underset{k}{\text{argmin}}\, \text{dist}(x_i, c_k)$$

- Can only decrease total distance phi!

$$\phi(\{x_i\}, \{a_i\}, \{c_k\}) = \sum_i \text{dist}(x_i, c_{a_i})$$

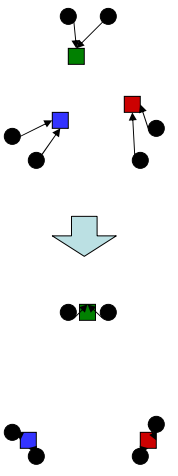


Phase II: Update Means

- Move each mean to the average of its assigned points:

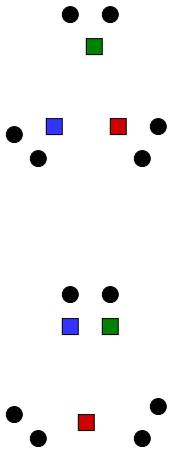
$$c_k = \frac{1}{|\{i : a_i = k\}|} \sum_{i:a_i=k} x_i$$

- Also can only decrease total distance… (Why?)
- Fun fact: the point y with minimum squared Euclidean distance to a set of points {x} is their mean



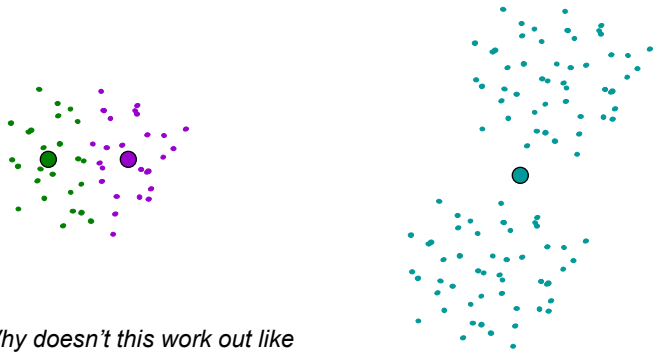
Initialization

- K-means is non-deterministic
  - Requires initial means
  - It does matter what you pick!
  - What can go wrong?
  - Various schemes for preventing this kind of thing: variance-based split / merge, initialization heuristics



K-Means Getting Stuck

- A local optimum:



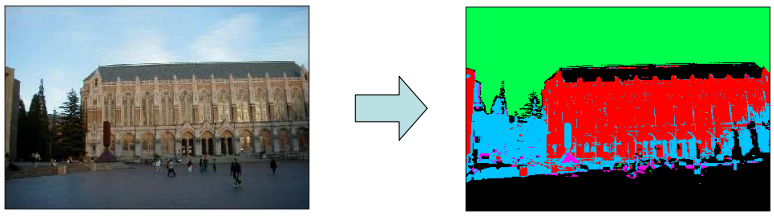
Why doesn't this work out like the earlier example, with the purple taking over half the blue?

K-Means Questions

- Will K-means converge?
  - To a global optimum?
- Will it always find the true patterns in the data?
  - If the patterns are very very clear?
- Will it find something interesting?
- Do people ever use it?
- How many clusters to pick?

Clustering for Segmentation

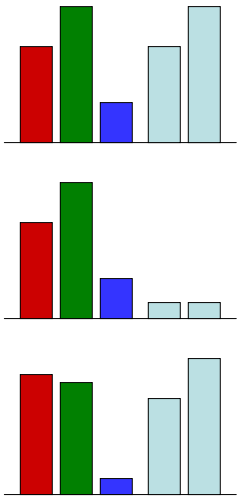
- Quick taste of a simple vision algorithm
- Idea: break images into manageable regions for visual processing (object recognition, activity detection, etc.)



http://www.cs.washington.edu/research/imagedatabase/demo/kmcluster/

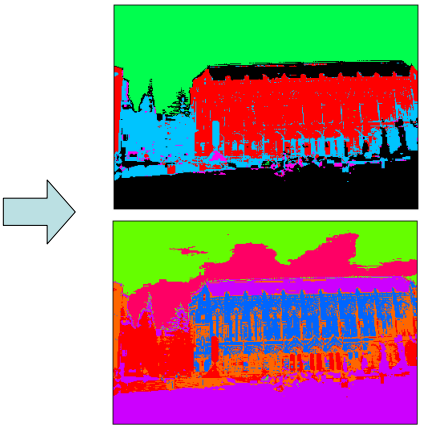
Representing Pixels

- Basic representation of pixels:
  - 3 dimensional color vector <r, g, b>
  - Ranges: r, g, b in [0, 1]
  - What will happen if we cluster the pixels in an image using this representation?
- Improved representation for segmentation:
  - 5 dimensional vector <r, g, b, x, y>
  - Ranges: x in [0, M], y in [0, N]
  - Bigger M, N makes position more important
  - How does this change the similarities?
- Note: real vision systems use more sophisticated encodings which can capture intensity, texture, shape, and so on.



K-Means Segmentation

- Results depend on initialization!
  - Why?



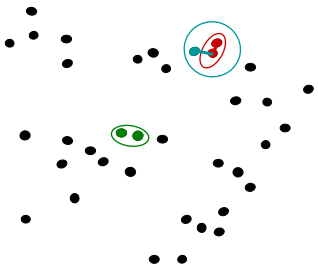
- Note: best systems use graph segmentation algorithms

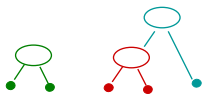
Other Uses of K-Means

- Speech recognition: can use to quantize wave slices into a small number of types (SOTA: work with multivariate continuous features)
- Document clustering: detect similar documents on the basis of shared words (SOTA: use probabilistic models which operate on topics rather than words)

Agglomerative Clustering

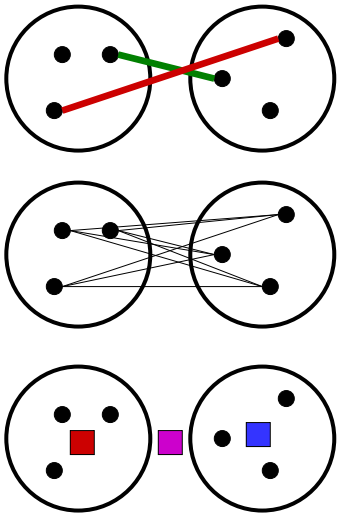
- Agglomerative clustering:
  - First merge very similar instances
  - Incrementally build larger clusters out of smaller clusters
- Algorithm:
  - Maintain a set of clusters
  - Initially, each instance in its own cluster
  - Repeat:
    - Pick the two closest clusters
    - Merge them into a new cluster
    - Stop when there's only one cluster left
- Produces not one clustering, but a family of clusterings represented by a dendrogram





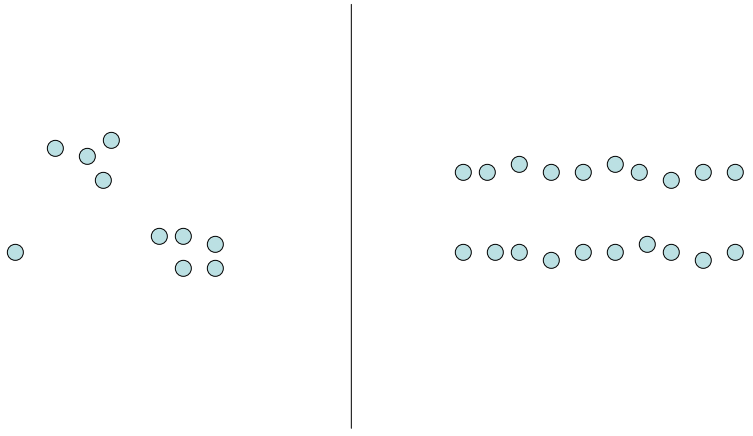
Agglomerative Clustering

- How should we define "closest" for clusters with multiple elements?
- Many options
  - Closest pair (single-link clustering)
  - Farthest pair (complete-link clustering)
  - Average of all pairs
  - Distance between centroids (broken)
  - Ward's method (my pick, like k-means)
- Different choices create different clustering behaviors



Agglomerative Clustering

- Complete Link (farthest) vs. Single Link (closest)



Back to Similarity

- K-means naturally operates in Euclidean space (why?)
- Agglomerative clustering didn't require any mention of averaging
  - Can use any function which takes two instances and returns a similarity
  - Kernelized clustering: if your similarity function has the right properties, can adapt k-means too
- Kinds of similarity functions:
  - Euclidian (dot product)
  - Weighted Euclidian
  - Edit distance between strings
  - Anything else?

Collaborative Filtering

- Ever wonder how online merchants decide what products to recommend to you?
- Simplest idea: recommend the most popular items to everyone
  - Not entirely crazy! (Why)
  - Can do better if you know something about the customer (e.g. what they've bought)
- Better idea: recommend items that similar customers bought
  - A popular technique: collaborative filtering
  - Define a similarity function over customers (how?)
  - Look at purchases made by people with high similarity
  - Trade-off: relevance of comparison set vs confidence in predictions
  - How can this go wrong?