Machine Learning Crash Course



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Photo: CMU Machine Learning Department protests G20

Machine Learning Problems

Supervised Learning

Unsupervised Learning

classification or categorization

clustering

regression

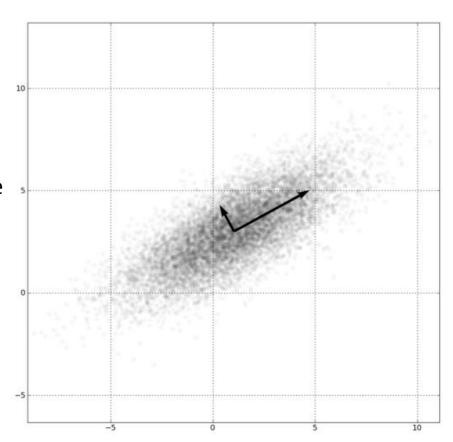
dimensionality reduction

Discrete

Continuous

Dimensionality Reduction

- PCA, ICA, LLE, Isomap,
 Autoencoder
- PCA is the most important technique to know. It takes advantage of correlations in data dimensions to produce the best possible lower dimensional representation based on linear projections (minimizes reconstruction error).
- PCA should be used for dimensionality reduction, not for discovering patterns or making predictions. Don't try to assign semantic meaning to the bases.



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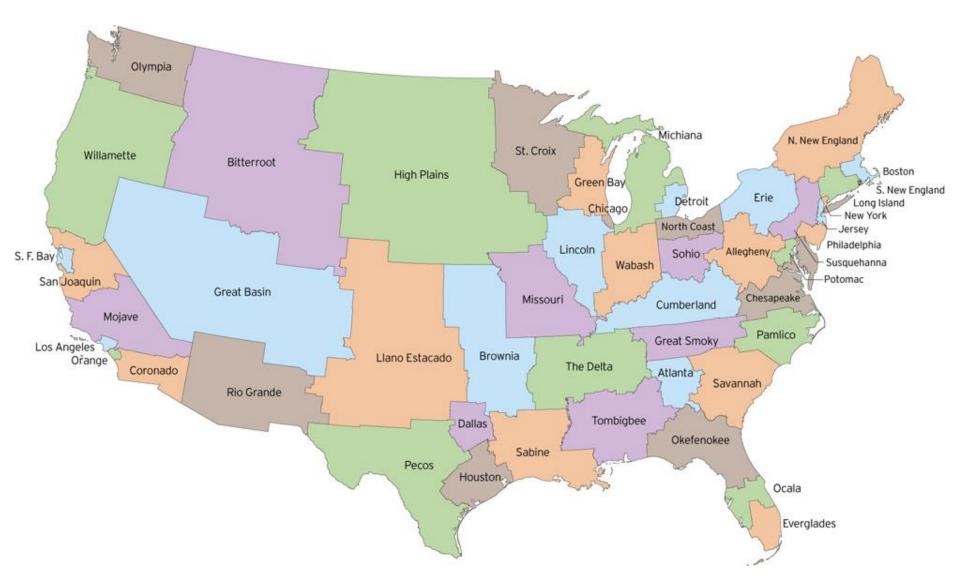
regression

dimensionality reduction

Discrete

Continuous





http://fakeisthenewreal.org/reform/

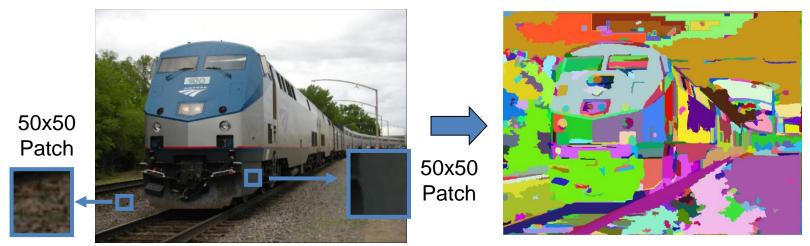
The United States redrawn as Fifty States with Equal Population Seattle RAINIER & Spokane Portland # Billings ⊕ MESAB MENOMINEE SHASTA ADIRONDACK SALT LAKE OGALLALA **⊗** Sioux Falls MENDOCINO ○ Cedar Rapids Salt Lake City Des Moines @ Cheyenne Denver WASHINGTON Colorado Springs Fresno # TULE Las Vegas HIPROC MUSKOGE Nashville . TEMECULA OZARK LOS ANGELES Albuquerque Oklahoma City Amarillo Phoenix : PHOENIX **■** Tucson El Paso CHINAT Hawaiʻian Islands Legend http://fakeisthenewreal.org/reform, Neil Freeman fakeisthenewreal.org

Clustering example: image segmentation

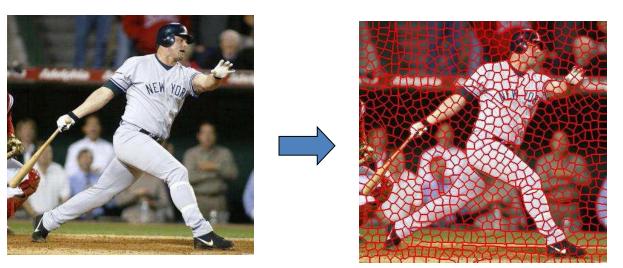
Goal: Break up the image into meaningful or perceptually similar regions



Segmentation for feature support or efficiency



[Felzenszwalb and Huttenlocher 2004]



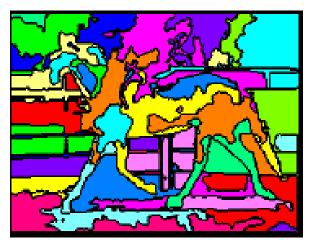
[Shi and Malik 2001] Slide: Derek Hoiem

Segmentation as a result

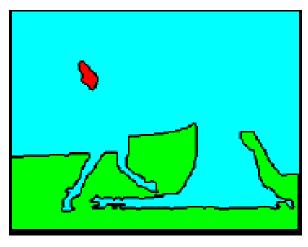


Types of segmentations

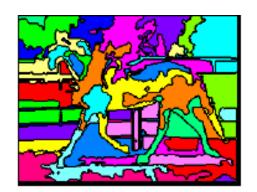


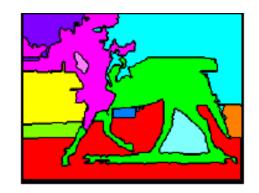


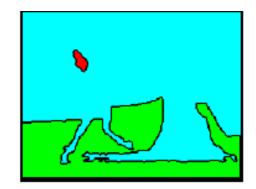
Oversegmentation



Undersegmentation







Multiple Segmentations

Clustering: group together similar points and represent them with a single token

Key Challenges:

- 1) What makes two points/images/patches similar?
- 2) How do we compute an overall grouping from pairwise similarities?

Slide: Derek Hoiem

How do we cluster?

- K-means
 - Iteratively re-assign points to the nearest cluster center
- Agglomerative clustering
 - Start with each point as its own cluster and iteratively merge the closest clusters
- Mean-shift clustering
 - Estimate modes of pdf
- Spectral clustering
 - Split the nodes in a graph based on assigned links with similarity weights

Clustering for Summarization

Goal: cluster to minimize variance in data given clusters

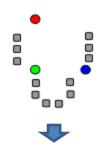
Preserve information

$$\mathbf{c}^*, \boldsymbol{\delta}^* = \underset{\mathbf{c}, \boldsymbol{\delta}}{\operatorname{argmin}} \ \frac{1}{N} \sum_{j}^{N} \sum_{i}^{K} \mathcal{S}_{ij} \left(\mathbf{c}_{i} - \mathbf{x}_{j} \right)^2$$
Whether \mathbf{x}_{j} is assigned to \mathbf{c}_{i}

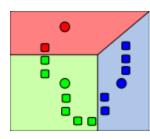
Slide: Derek Hoiem

K-means algorithm

1. Randomly select K centers



2. Assign each point to nearest center



3. Compute new center (mean) for each cluster

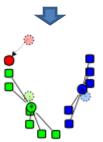
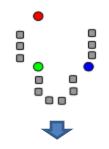


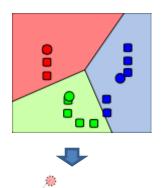
Illustration: http://en.wikipedia.org/wiki/K-means_clustering

K-means algorithm

1. Randomly select K centers



2. Assign each point to nearest center



Back to 2

3. Compute new center (mean) for each cluster

Illustration: http://en.wikipedia.org/wiki/K-means_clustering

K-means

- 1. Initialize cluster centers: \mathbf{c}^0 ; t=0
- 2. Assign each point to the closest center

$$\boldsymbol{\delta}^{t} = \underset{\boldsymbol{\delta}}{\operatorname{argmin}} \, \frac{1}{N} \sum_{i}^{N} \sum_{i}^{K} \delta_{ij} \left(\mathbf{c}_{i}^{t-1} - \mathbf{x}_{j} \right)^{2}$$

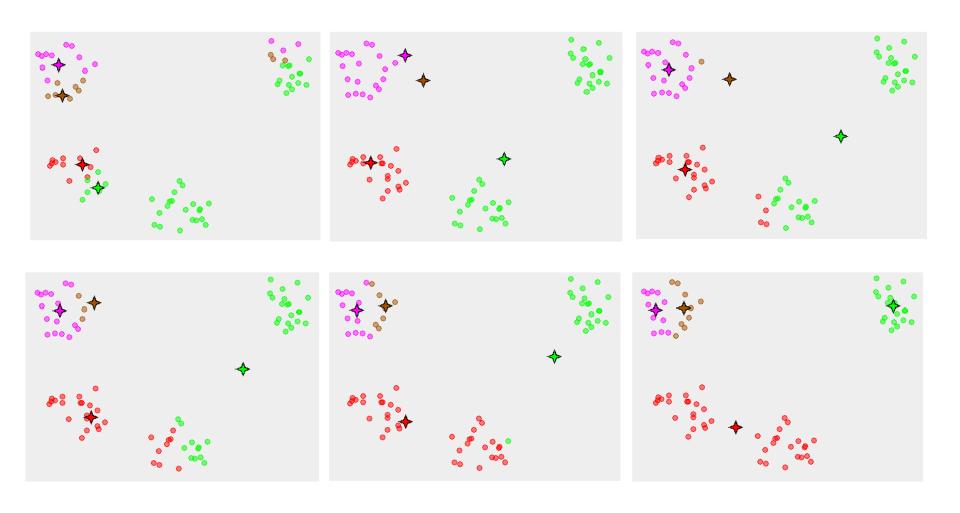
3. Update cluster centers as the mean of the points

$$\mathbf{c}^{t} = \underset{\mathbf{c}}{\operatorname{argmin}} \, \frac{1}{N} \sum_{i}^{N} \sum_{j}^{K} \delta_{ij}^{t} \left(\mathbf{c}_{i} - \mathbf{x}_{j} \right)^{2}$$

4. Repeat 2-3 until no points are re-assigned (t=t+1)

Slide: Derek Hoiem

K-means converges to a local minimum



K-means: design choices

- Initialization
 - Randomly select K points as initial cluster center
 - Or greedily choose K points to minimize residual
- Distance measures
 - Traditionally Euclidean, could be others
- Optimization
 - Will converge to a local minimum
 - May want to perform multiple restarts

K-means clustering using intensity or color

Image

Clusters on intensity

Clusters on color







How to evaluate clusters?

Generative

– How well are points reconstructed from the clusters?

Discriminative

- How well do the clusters correspond to labels?
 - Purity
- Note: unsupervised clustering does not aim to be discriminative

Slide: Derek Hoiem

How to choose the number of clusters?

- Validation set
 - Try different numbers of clusters and look at performance
 - When building dictionaries (discussed later), more clusters typically work better

Slide: Derek Hoiem

K-Means pros and cons

Pros

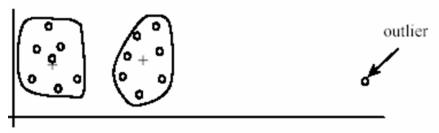
- Finds cluster centers that minimize conditional variance (good representation of data)
- Simple and fast*
- Easy to implement

Cons

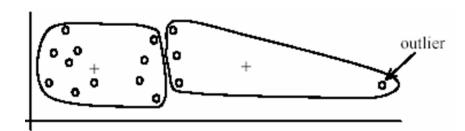
- Need to choose K
- Sensitive to outliers
- Prone to local minima
- All clusters have the same parameters (e.g., distance measure is nonadaptive)
- *Can be slow: each iteration is O(KNd) for N d-dimensional points

Usage

Rarely used for pixel segmentation



(B): Ideal clusters

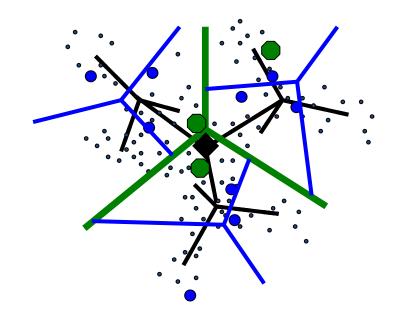


Building Visual Dictionaries

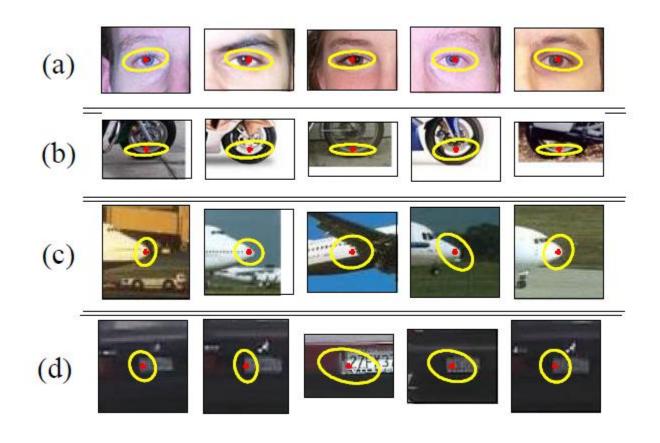
- Sample patches from a database
 - E.g., 128 dimensional
 SIFT vectors



- 2. Cluster the patches
 - Cluster centers are the dictionary
- Assign a codeword (number) to each new patch, according to the nearest cluster



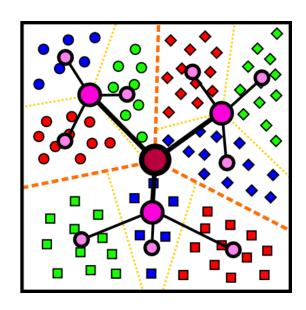
Examples of learned codewords



Most likely codewords for 4 learned "topics" EM with multinomial (problem 3) to get topics

Which algorithm to use?

- Quantization/Summarization: K-means
 - Aims to preserve variance of original data
 - Can easily assign new point to a cluster



Quantization for computing histograms

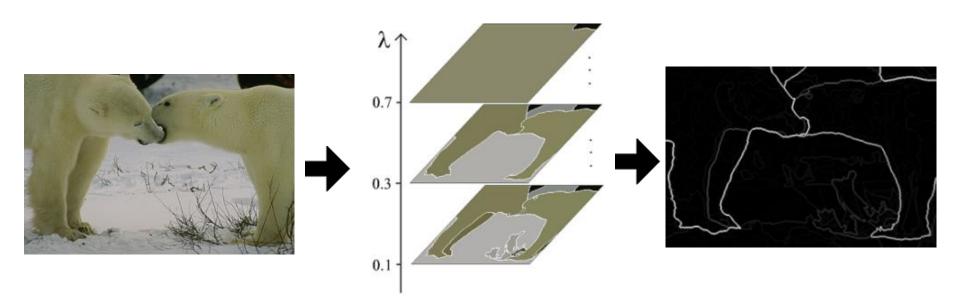


Summary of 20,000 photos of Rome using "greedy k-means"

http://grail.cs.washington.edu/projects/canonview/

Which algorithm to use?

- Image segmentation: agglomerative clustering
 - More flexible with distance measures (e.g., can be based on boundary prediction)
 - Adapts better to specific data
 - Hierarchy can be useful



http://www.cs.berkeley.edu/~arbelaez/UCM.html

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dimensionality reduction

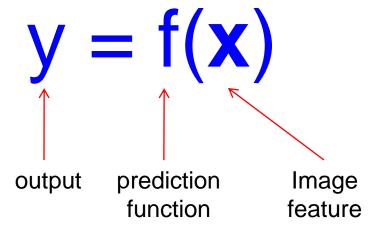
Discrete

Continuous

The machine learning framework

 Apply a prediction function to a feature representation of the image to get the desired output:

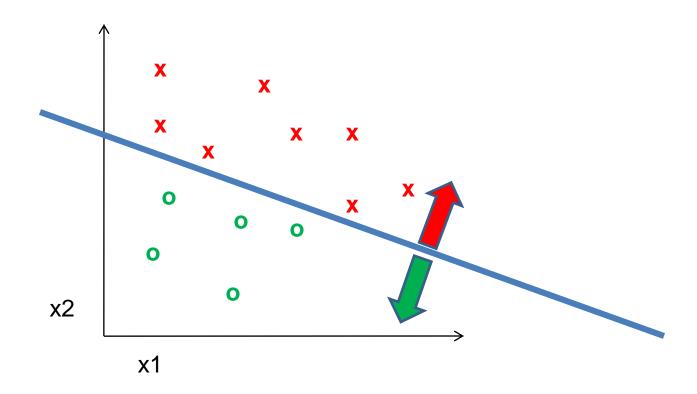
The machine learning framework



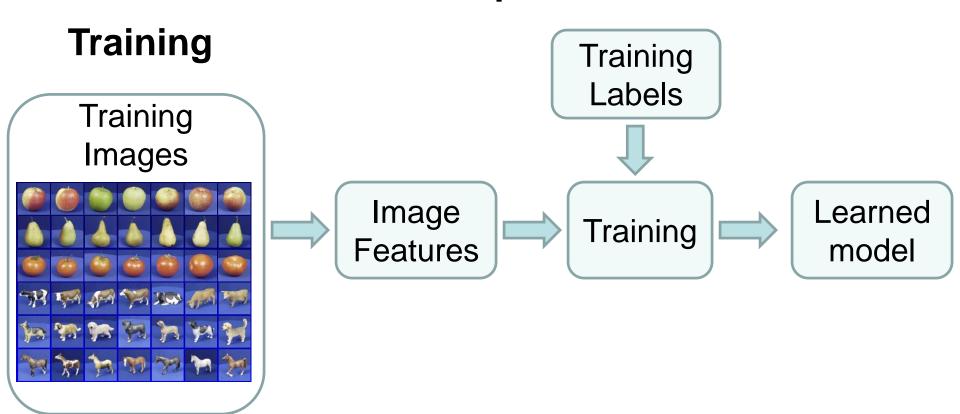
- Training: given a training set of labeled examples {(x₁,y₁), ..., (x_N,y_N)}, estimate the prediction function f by minimizing the prediction error on the training set
- Testing: apply f to a never before seen test example x and output the predicted value y = f(x)

Learning a classifier

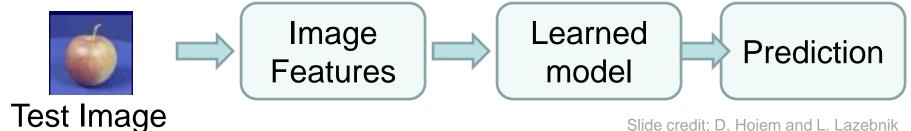
Given some set of features with corresponding labels, learn a function to predict the labels from the features



Steps



Testing



Slide credit: D. Hoiem and L. Lazebnik

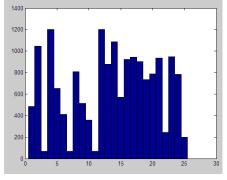
Features

Raw pixels

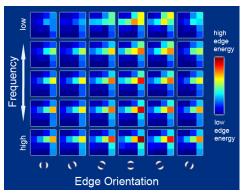
Histograms

GIST descriptors









• . . .

One way to think about it...

 Training labels dictate that two examples are the same or different, in some sense

 Features and distance measures define visual similarity

 Classifiers try to learn weights or parameters for features and distance measures so that visual similarity predicts label similarity

Many classifiers to choose from

- SVM
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- Boosted Decision Trees
- K-nearest neighbor
- RBMs
- Deep Convolutional Network
- Etc.

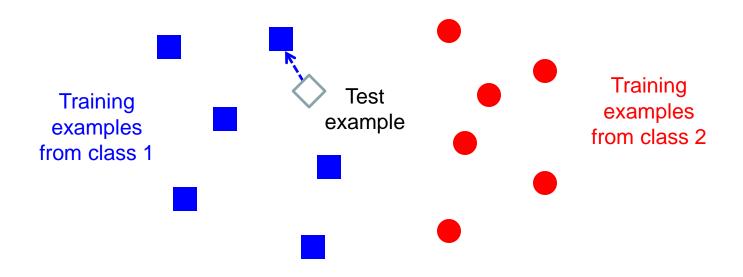
Which is the best one?

Claim:

The decision to *use* machine learning is more important than the choice of a *particular* learning method.

^{*}Deep learning seems to be an exception to this, at the moment, probably because it is learning the feature representation.

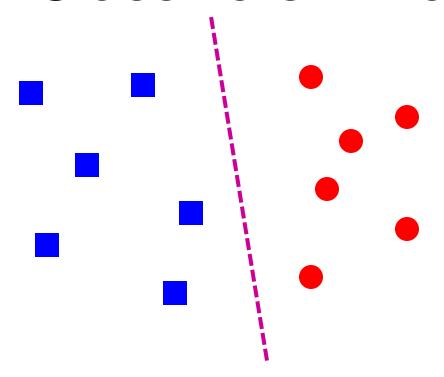
Classifiers: Nearest neighbor



$f(\mathbf{x})$ = label of the training example nearest to \mathbf{x}

- All we need is a distance function for our inputs
- No training required!

Classifiers: Linear

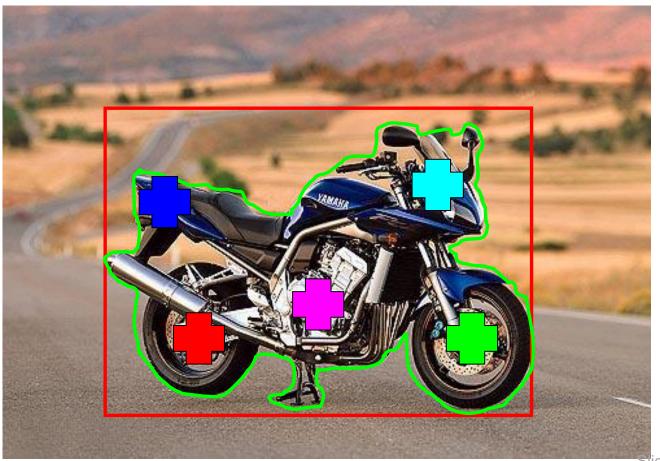


$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + \mathbf{b})$$

Recognition task and supervision

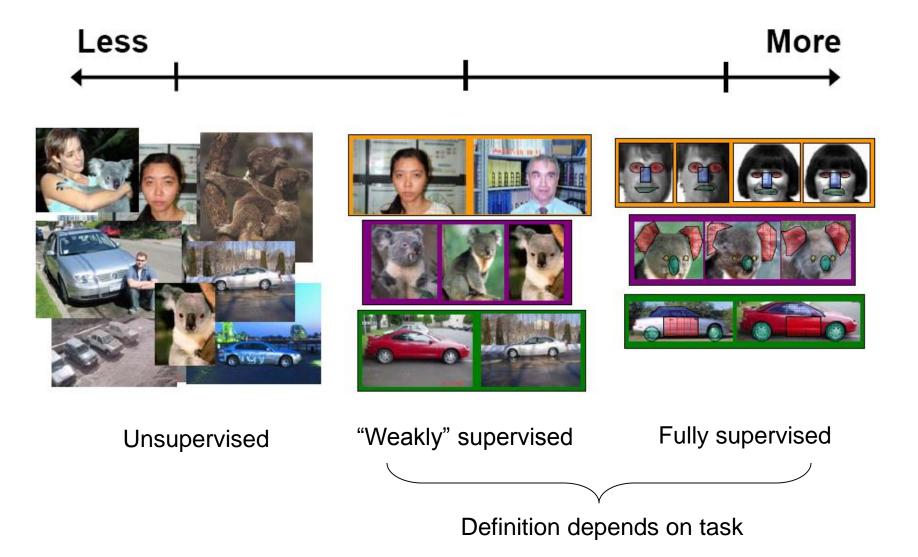
 Images in the training set must be annotated with the "correct answer" that the model is expected to produce

Contains a motorbike

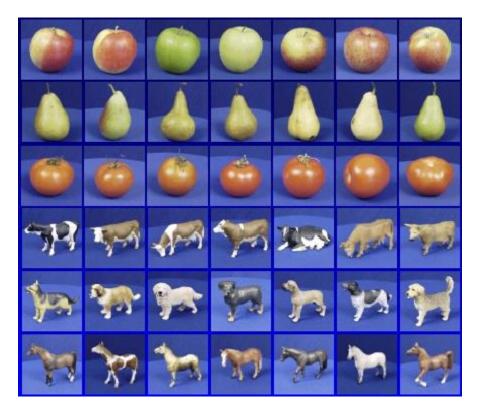


Slide credit: L. Lazebnik

Spectrum of supervision



Generalization



Training set (labels known)



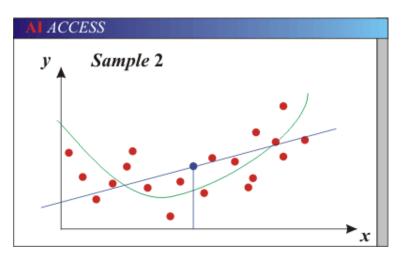
Test set (labels unknown)

 How well does a learned model generalize from the data it was trained on to a new test set?

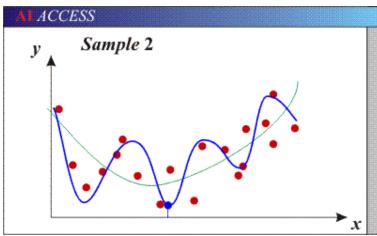
Generalization

- Components of generalization error
 - Bias: how much the average model over all training sets differ from the true model?
 - Error due to inaccurate assumptions/simplifications made by the model.
 - Variance: how much models estimated from different training sets differ from each other.
- Underfitting: model is too "simple" to represent all the relevant class characteristics
 - High bias (few degrees of freedom) and low variance
 - High training error and high test error
- Overfitting: model is too "complex" and fits irrelevant characteristics (noise) in the data
 - Low bias (many degrees of freedom) and high variance
 - Low training error and high test error

Bias-Variance Trade-off



 Models with too few parameters are inaccurate because of a large bias (not enough flexibility).



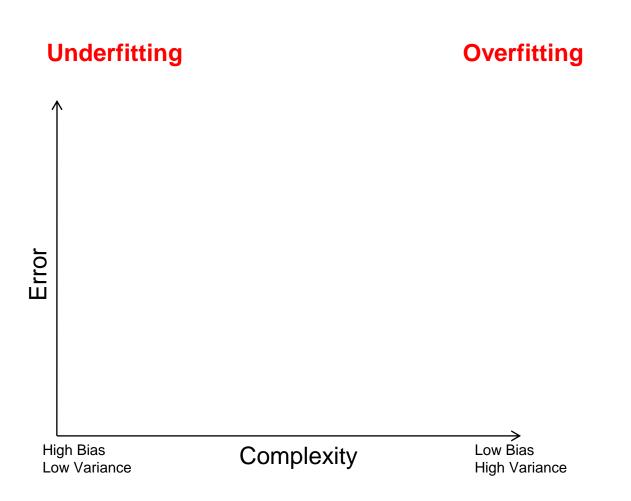
 Models with too many parameters are inaccurate because of a large variance (too much sensitivity to the sample).

Bias-Variance Trade-off

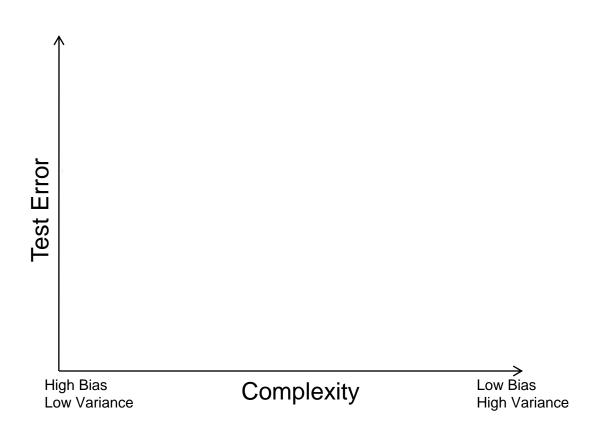
See the following for explanations of bias-variance (also Bishop's "Neural Networks" book):

http://www.inf.ed.ac.uk/teaching/courses/mlsc/Notes/Lecture4/BiasVariance.pdf

Bias-variance tradeoff



Bias-variance tradeoff



Effect of Training Size

Fixed prediction model

Number of Training Examples



Remember...

 No classifier is inherently better than any other: you need to make assumptions to generalize



- Three kinds of error
 - Inherent: unavoidable
 - Bias: due to over-simplifications
 - Variance: due to inability to perfectly estimate parameters from limited data

How to reduce variance?

Choose a simpler classifier

Regularize the parameters

Get more training data

Very brief tour of some classifiers

- K-nearest neighbor
- SVM
- Boosted Decision Trees
- Neural networks
- Naïve Bayes
- Bayesian network
- Logistic regression
- Randomized Forests
- RBMs
- Etc.

Generative vs. Discriminative Classifiers

Generative Models

- Represent both the data and the labels
- Often, makes use of conditional independence and priors
- Examples
 - Naïve Bayes classifier
 - Bayesian network
- Models of data may apply to future prediction problems

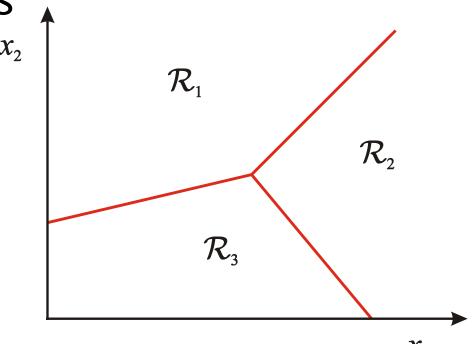
Discriminative Models

- Learn to directly predict the labels from the data
- Often, assume a simple boundary (e.g., linear)
- Examples
 - Logistic regression
 - SVM
 - Boosted decision trees
- Often easier to predict a label from the data than to model the data

Classification

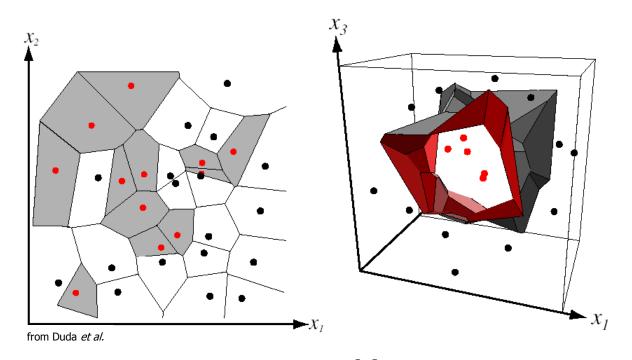
Assign input vector to one of two or more classes

 Any decision rule divides input space into decision regions separated by decision boundaries



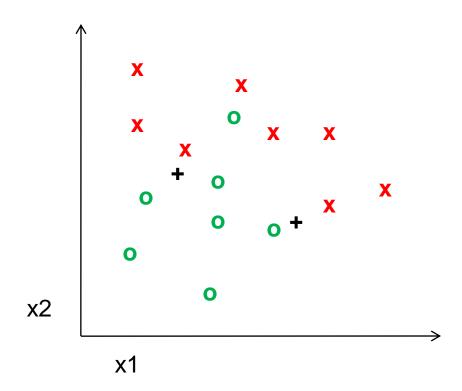
Nearest Neighbor Classifier

 Assign label of nearest training data point to each test data point

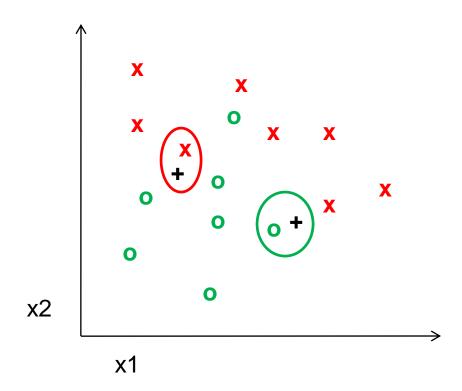


Voronoi partitioning of feature space for two-category 2D and 3D data

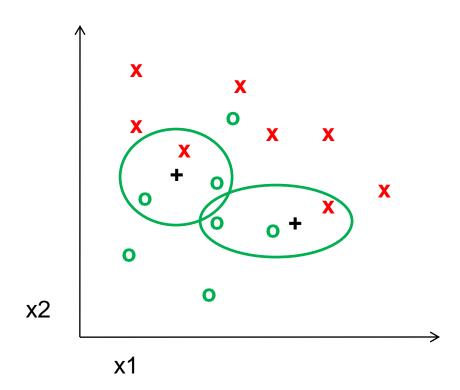
K-nearest neighbor



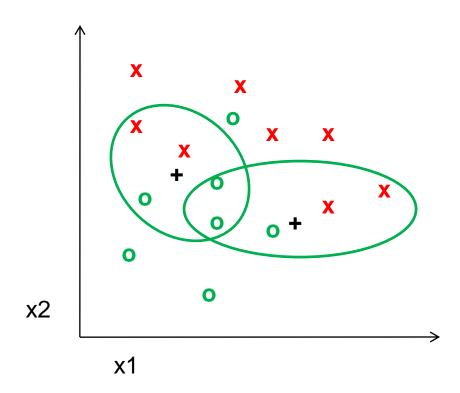
1-nearest neighbor



3-nearest neighbor



5-nearest neighbor

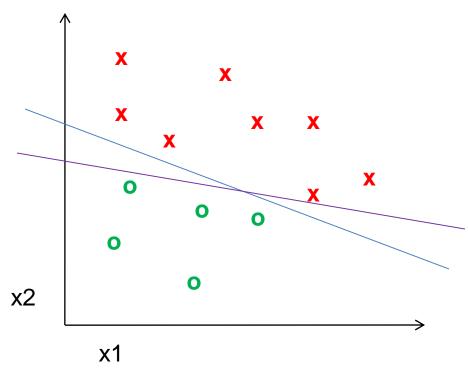


Using K-NN

• Simple, a good one to try first

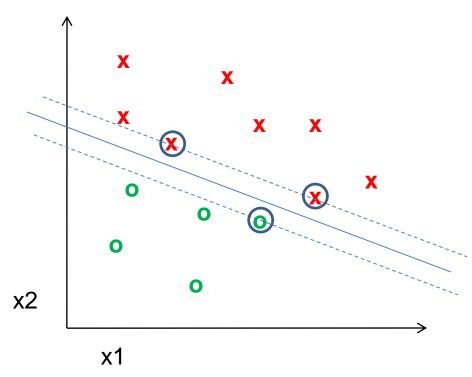
 With infinite examples, 1-NN provably has error that is at most twice Bayes optimal error

Classifiers: Linear SVM



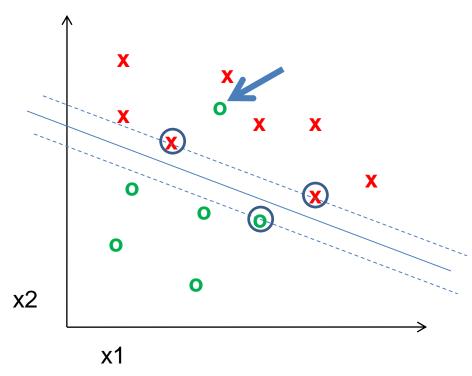
$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + \mathbf{b})$$

Classifiers: Linear SVM



$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + \mathbf{b})$$

Classifiers: Linear SVM



$$f(\mathbf{x}) = \operatorname{sgn}(\mathbf{w} \cdot \mathbf{x} + \mathbf{b})$$

What about multi-class SVMs?

- Unfortunately, there is no "definitive" multiclass SVM formulation
- In practice, we have to obtain a multi-class SVM by combining multiple two-class SVMs
- One vs. others
 - Traning: learn an SVM for each class vs. the others
 - Testing: apply each SVM to test example and assign to it the class of the SVM that returns the highest decision value
- One vs. one
 - Training: learn an SVM for each pair of classes
 - Testing: each learned SVM "votes" for a class to assign to the test example

SVMs: Pros and cons

Pros

- Many publicly available SVM packages: http://www.kernel-machines.org/software
- Kernel-based framework is very powerful, flexible
- SVMs work very well in practice, even with very small training sample sizes

Cons

- No "direct" multi-class SVM, must combine two-class SVMs
- Computation, memory
 - During training time, must compute matrix of kernel values for every pair of examples
 - Learning can take a very long time for large-scale problems

What to remember about classifiers

- No free lunch: machine learning algorithms are tools, not dogmas
- Try simple classifiers first
- Better to have smart features and simple classifiers than simple features and smart classifiers
- Use increasingly powerful classifiers with more training data (bias-variance tradeoff)

Making decisions about data

- 3 important design decisions:
 - 1) What data do I use?
 - 2) How do I represent my data (what feature)?
 - 3) What classifier / regressor / machine learning tool do I use?
- These are in decreasing order of importance
- Deep learning addresses 2 and 3 simultaneously (and blurs the boundary between them).
- You can take the representation from deep learning and use it with any classifier.