Machine Learning Crash Course



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Photo: CMU Machine Learning Department protests G20

Machine Learning Problems



The machine learning framework

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



Slide credit: L. Lazebnik

Learning a classifier

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



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?

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



x2

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



• Find a *linear function* to separate the classes:

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

Classifiers: Linear SVM



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Nonlinear SVMs

• Datasets that are linearly separable work out great:



• But what if the dataset is just too hard?



• We can map it to a higher-dimensional space:



Nonlinear SVMs

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



Nonlinear SVMs

• The kernel trick: instead of explicitly computing the lifting transformation $\varphi(\mathbf{x})$, define a kernel function K such that

$$K(\mathbf{x}_i,\mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i) \cdot \boldsymbol{\varphi}(\mathbf{x}_j)$$

(to be valid, the kernel function must satisfy *Mercer's condition*)

• This gives a nonlinear decision boundary in the original feature space:

$$\sum_{i} \alpha_{i} y_{i} \varphi(\boldsymbol{x}_{i}) \cdot \varphi(\boldsymbol{x}) + b = \sum_{i} \alpha_{i} y_{i} K(\boldsymbol{x}_{i}, \boldsymbol{x}) + b$$

C. Burges, <u>A Tutorial on Support Vector Machines for Pattern Recognition</u>, Data Mining and Knowledge Discovery, 1998

Nonlinear kernel: Example

• Consider the mapping $\varphi(x) = (x, x^2)$



$$\varphi(x) \cdot \varphi(y) = (x, x^2) \cdot (y, y^2) = xy + x^2 y^2$$
$$K(x, y) = xy + x^2 y^2$$

Kernels for bags of features

• Histogram intersection kernel:

$$I(h_1, h_2) = \sum_{i=1}^{N} \min(h_1(i), h_2(i))$$

• Generalized Gaussian kernel:

$$K(h_1, h_2) = \exp\left(-\frac{1}{A}D(h_1, h_2)^2\right)$$

• *D* can be (inverse) L1 distance, Euclidean distance, χ^2 distance, etc.

J. Zhang, M. Marszalek, S. Lazebnik, and C. Schmid, <u>Local Features and Kernels for</u> <u>Classification of Texture and Object Categories: A Comprehensive Study</u>, IJCV 2007

Summary: SVMs for image classification

- 1. Pick an image representation (e.g. histogram of quantized sift features)
- 2. Pick a kernel function for that representation
- 3. Compute the matrix of kernel values between every pair of training examples
- 4. Feed the kernel matrix into your favorite SVM solver to obtain support vectors and weights
- 5. At test time: compute kernel values for your test example and each support vector, and combine them with the learned weights to get the value of the decision function

What about multi-class SVMs?

- Unfortunately, there is no "definitive" multi-class 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: <u>http://www.kernel-machines.org/software</u>
 - 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

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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. "Bias" sounds negative. "Regularization" sounds nicer.
 - 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 tradeoff



Bias-variance tradeoff



Effect of Training Size

Fixed prediction model



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
- How to reduce bias?
 - Choose a more complex, more expressive classifier
 - Remove regularization
 - (These might not be safe to do unless you get more training data)

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 (biasvariance tradeoff)

Machine Learning Considerations

- 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.

Machine Learning Problems



- Andrew Ng's ranking of machine learning impact
 - 1. Supervised Learning
 - 2. Transfer Learning
 - 3. Unsupervised Learning* (Often "self-supervised" learning)
 - 4. Reinforcement Learning



James thinks 2 and 3 might have switched ranks.