CPSC 340: Machine Learning and Data Mining

Course Review/Preview Fall 2016

Some images from this lecture are taken from Google Image Search.

Admin

- Assignment 6:
 - 1 late day to hand in next Monday, 2 for Wednesday, 3 for Friday.
- Final:
 - December 12 (8:30am HEBB 100)
 - Covers Assignments 1-6.
 - List of topics posted.
 - Final from last year will be posted after class.
 - Closed-book, cheat sheet: 4-pages each double-sided.

Last Time: Semi-Supervised Learning

- In semi-supervised learning we have:
 - Usual labeled examples {X,y}.
 - An additional set of unlabeled examples \tilde{X} .
- Exam analogy for types of supervised/semi-supervised learning:
 - Regular supervised learning:
 - You are given the practice final with answers.
 - You want to get the answers right on the real final.
 - Inductive SSL:
 - You are given the practice final with answers.
 - You also have the finals from previous years (but no answers).
 - You want to get the answers right on the real final.
 - Transdutive SSL:
 - You are given the practice final with answers.
 - You want to get the answers right on a take-home final.
 - You can study while knowing what questions you need to answer.

Last Time: Graph-Based Semi-Supervised Learning

• Graph-based (transductive) SSL uses weighted graph on examples:



• Find labels minimizing cost penalizing disagreements on edges.

KNN bode

- Similar to KNN, but labels get 'propagated' through unlabeled \tilde{x}_i . – Can label cluster or manifold.
- Directly works on labeling: only need the graph, not the features. — Interpretation as random walk in graph or in terms of a Markov chain.

Today: Course Review

- The age of "big data" is upon us.
- Data mining and machine learning are key tools to analyze big data.
- Very similar to statistics, but more emphasis on:
 - 1. Computation
 - 2. Test error.
 - 3. Non-asymptotic performance.
 - 4. Models that work across domains.
- Enormous and growing number of applications.
- The field is growing very fast:
 - ~2500 attendees at NIPS 2 years ago, ~5800 next week (Influence of \$\$\$, too).
- Today: review of topics we covered, overview of topics we didn't.

Data Representation and Exploration

- We first talked about feature representation of data:
 - Each row in a table corresponds to one 'object'.
 - Each column in that row contains a 'feature' of the object.



- Discussed numerical/discrete features, feature transformations.
- Discussed summary statistics like mean, quantiles, variance.
- Discussed data visualizations like boxplots and scatterplots.

Supervised Learning and Decision Trees

- Supervised learning builds model to map from features to labels.
 - Most successful machine learning method.

Egg	Milk	Fish	Wheat	Shellfish	Peanuts	•••	Sick?
0	0.7	0	0.3	0	0		1
0.3	0.7	0	0.6	0	0.01		1
0	0	0	0.8	0	0		0

- Decision trees consist of a sequence of single-variables 'rules':
 - Simple/interpretable but not very accurate.



• Greedily learn from by fitting decision stumps and splitting data.

Training, Validation, and Testing

- In machine learning we are interesting in the test error.
 - Performance on new data.
- IID: training and new data drawn independently from same distribution.
- Overfitting: worse performance on new data than training data.
- Fundamental trade-off:
 - How low can make the training error? (Complex models are better here.)
 - How does training error approximate test error? (Simple models are better here.)
- Golden rule: we cannot use test data during training.
- But validation set or cross-validation allow us to approximate test error.
- No free lunch theorem: there is no 'best' machine learning model.

Probabilistic Classifiers and Naïve Bayes

• Probabilistic classifiers consider probability of correct label.

- $p(y_i = "spam" | x_i) vs. p(y_i = "not spam" | x_i).$

• Generative classifiers model probability of the features:

$$p(y_i = "spam" | x_i) \propto p(x_i | y_i = "spam") p(y_i = "spam")$$

- For tractability, often make strong independence assumptions.
 - Naïve Bayes assumes independence of features given labels:

$$p(x_i|y_i) = \frac{d}{1/p}(x_{ij}|y_i)$$

• Decision theory: predictions when errors have different costs. (ost of false negative \neq cost false positive

Parametric and Non-Parametric Models

- Parametric model size does not depend on number of objects 'n'.
- Non-parametric model size depends on 'n'.
- K-Nearest Neighbours:
 - Non-parametric model that uses label of closest x_i in training data.
 - Accurate but slow at test time.

- Curse of dimensionality:
 - Problem with distances in high dimensions.
- Universally consistent methods:
 - achieve lowest possible test error as 'n' goes to infinity.

Ensemble Methods and Random Forests

- Ensemble methods are classifiers that have classifiers as input:
 - Boosting: improve training error of simple classifiers.
 - Averaging: reduce overfitting of complex classifiers.
- Random forests:
 - Ensemble method that averages random trees fit on bootstrap samples.
 - Fast and accurate, one of the best "out of the box" classifiers.





Clustering and K-Means

- Unsupervised learning considers features X without labels.
- Clustering is task of grouping similar objects.



- K-means is a classic clustering method:
 - Represent each cluster by its mean value.
 - Learning alternates between updating means and assigning to clusters.
 - Sensitive to initialization, but some guarantees with k-means++.

Density-Based Clustering

- **Density-based clustering** is a non-parametric clustering method:
 - Based on finding dense connected regions.
 - Allows finding non-convex clusters.





Ensemble and Hierarhical Clustering

- Ensemble clustering combines clusterings.
 - But need to account for label switching problem.
- Hierarchical clustering groups objects at multiple levels.



Outlier Detection

- Outlier detection is task of finding "significantly different" objects.
 - Global outliers are different from all other objects.
 - Local outliers fall in normal range, but are different from neighbours.



- Approaches:
 - Model-based: fit model, check probability under model (z-score).
 - Graphical approaches: plot data, use human judgement (scatterplot).
 - Cluster-based: cluster data, find points that don't belong.
 - Distance-based: outlierness test of "abnormally far form neighbours".

Association Rules

- Association rules find items that are frequently bought together.
 - (S => T): if you buy 'S' then you are likely to buy 'T'.
 - Rules have support, P(S=1), and confidence, P(T=1 | S=1).
- A priori algorithm finds all rules with high support/confidence.

Found to be Infrequent

- Probabilistic inequalities reduce search space.
- Amazon's item-to-item recommendation:
 - Compute similarity of 'user vectors' for items.

$$COS(x_{i}, x_{j}) = \frac{x_{i}^{T}x_{j}}{\|x_{i}\| \|x_{j}\|}$$

Linear Regression and Least Squares

Xi

• We then returned to supervised learning and linear regression:

- Write label as weighted combination of features: $y_i = w^T x_i$.

• Least squares is the most common formulation:

$$f(w) = \sum_{i=1}^{n} (w x_i - y_i)^2$$

- Solution is a linear system: $(X^TX)w = X^Ty$
- Non-zero y-intercept (bias) by adding a feature $x_{ii} = 1$.
- Model non-linear effects by change of basis:

Regularization, Robust Regression, Gradient Descent

• L2-regularization adds a penalty on the L2-norm of 'w':

$$f(w) = \frac{1}{2} ||Xw - y||^2 + \frac{1}{2} ||w||^2$$

- Several magical properties and usually lower test error.
- Robust regression replaces squared error with absolute error:
 - Less sensitive to outliers.
 - Absolute error has smooth approximations.
- Gradient descent lets us find local minimum of smooth objectives.

– Find global minimum for convex functions.

Binary Classification and Logistic Regression

• Binary classification using regression by taking the sign:

$$y_i = sign(w^T x_i)$$



- But squared error penalizes for being too right ("bad errors").
 - Ideal 0-1 loss is discontinuous/non-convex.
 - Logistic loss is smooth and convex approximation:

$$f(w) = \sum_{i=1}^{n} \log(|+exp(-y_i w^T x_i))$$

Support Vector Machines

• SVMs for separable data maximize margin for separable data:



• For non-separable data, hinge loss minimizes penalizes violations:



Kernel Trick

• Non-separable data can be separable in high-dimensional space:



• Kernel trick: linear regression using similarities instead of features.

$$\hat{\gamma} = \hat{K}(K+\lambda I)' \gamma \quad \text{with} \quad K = ZZ' \quad \text{and} \quad \hat{k} = \hat{Z}Z'$$

- If you can compute inner product, you don't to store basis z_i .
- Can have exponential/infinite basis.

Stochastic Gradient

- Stochastic gradient methods are appropriate when 'n' is huge.
 Take step in negative gradient of random training example.
- Less progress per iteration, but iterations don't depend on 'n'.
 - Fast convergence at start.
 - Slow convergence as accuracy improves.
- With infinite data:
 - Optimizes test error directly (cannot overfit).
 - But often difficult to get working.



Feature Selection and L1-Regularization

- Feature selection is task of finding "relevant" variables.
 - Can be hard to precisely define "relevant".
- Hypothesis testing methods:
 - Do tests trying to make variable 'j' conditionally independent of y.
 - Ignores effect size.
- Search and score methods:
 - Define score (LO-norm) and search for variables that optimize it.
 - Finding optimal combination is hard, but heuristics exist (forward select).
- L1-regularization:
 - Formulate as a convex problem.
 - Very fast but prone to false positives.



Maximum Likelihood Estimation

• We discussed maximum likelihood estimation:

• And how this is equivalent to minimizing negative log-likelihood:

$$f(w) = -\sum_{i=1}^{n} \log(p(y_i | x_{i,w}))$$

- Makes connection between probabilities and loss functions:
 - Gaussian likelihood => squared loss.
 - Laplace likelihood => absolute loss.
 - Sigmoid likelihood => logistic regression.

MAP Estimation

• We discussed MAP estimation:

$$p(w|X,y) \propto p(y|X,w)p(w)$$

"posterior" "likelihood" prior"

- Prior can take into account that complex models can overfit.

• Makes connection between probabilities and regularization:

If
$$p(y_i | x_{i,yw}) = \frac{1}{1 + exp(-y_i w^T x_i)}$$
 and $p(w_j) \propto \exp(-\frac{3}{2} w_j^2)$
then MAP estimate is minimum of $f(w) = \sum_{j=1}^{n} \log(1 + exp(-y_i w^T x_j)) + \frac{3}{2} ||w||^2$

Softmax Loss for Multi-Class Classification

- Sometimes it's easier to define a likelihood than a loss function.
 - Softmax probability:

$$p(y_i = c \mid x_i, W) \propto exp(w_c^T x_i)$$

- We have a vector wc for each class 'c', and classify by choosing largest w_c^Tx_i.
- Leads to softmax loss for multi-class classification:

$$f(w) = -\sum_{i=1}^{n} \log(p(y_i | x_i, W))$$

=
$$\sum_{i=1}^{n} -w_{y_i}^{T} x_i + \log(\sum_{c=1}^{k} \exp(w_c^{T} x_i))$$

Can define other losses based on other probabilities or probability ratios.

Latent-Factor Models

• Latent-Factor models approximate x_i with low-dimensional z_i:



Principal Component Analysis

• Principal component analysis (PCA): LFM based on squared error.

$$f(W_{j}Z) = \sum_{i=1}^{n} \sum_{j=1}^{d} (w_{j}^{T}z_{i} - x_{ij})^{2} = ||ZW - X||_{F}^{2}$$

- With 1 factor, minimizes 'orthogonal' distance: Principal component analysis
- To give unique solution:
 - Constrain factors to have norm of 1.
 - Constrain factors to have inner product of 0.
 - Fit factors sequentially.
- Found by SVD or alternating minimization.



Beyond PCA

- Non-negative matrix factorization:
 - Latent-factor model with non-negative constraints.
 - Sparsity due to non-negativity means we learn 'parts'.
- Could use different loss functions or regularizers:
 - Robust PCA.
 - Sparse PCA.
- Collaborative filtering:
 - Use LFMs to "fill in" missing values in matrix.
 - SVDfeature combines this with linear models.







Multi-Dimensional Scaling

loge distance

- Multi-dimensional scaling:
 - Non-parametric visualization.
 - Find low-dimensional 'z_i' that preserve distances.
- Classic MDS and Sammon mapping are similar to PCA.
- ISOMAP uses graph to approximate geodesic distance on manifold.



• T-SNE encourages 'repulsion' of close points.



Neural Networks and Deep Learning

- Neural networks combine latent-factor and linear models.
 - Linear-linear model is degenerate, so introduce non-linearity:
 - Sigmoid or ReLU function.
 - Backpropagation uses chain rule to compute gradient.
- Deep learning considers many layers of latent factors. Neural network with 3 hidden layers $V_i = w^T h(W^{(3)}h(W^{(2)}h(W^{(1)}x_i)))$
- A lot of tricks are needed to make deep learning work:
 - Parameter initialization
 - Setting stochastic gradient step sizes.
 - L2-regularization, early stopping, dropout.



Convolutional Neural Networks

- Convolutional neural networks:
 - Incorporate convolutional and max-pooling layers.



- Unprecedented performance on vision tasks.
- Lots of neat new applications:





Berry Field, June 1909 Hamilton,





Semi-Supervised Learning

- Semi-supervised learning considers labeled and unlabeled data.
 - Sometimes helps but in some settings it cannot.



- Inductive SSL: use unlabeled to help supervised learning.
- Transductive SSL: only interested in these particular unlabeled examples.
- Self-training methods alternate between labeling and fitting model.

Random Walks and Markov Chains

- We often have data organized according to a graph:
 - Could construct graph based on features and KNNs.
 - Or if you have a graph, you don't need features.
- Models based on random walks on graphs:
 - PageRank: how often does infinitely-long random walk visit page?
 - Graph-based SSL: which label does random walk reach most often?
- Markov chains are probabilistic models of sequences:
 - 1. Sampling using random walk.
 - 2. Inference using matrix multiplication.
 - 3. Stationary distribution using principal eigenvector.
- Most common model of sequential data.

CPSC 340: Overview

1. Intro to supervised learning (using counting and distances).

- Training vs. testing, parametric vs. non-parametric, ensemble methods.
- Fundamental trade-off, no free lunch, universal consistency.
- 2. Intro to unsupervised learning (using counting and distances).
 - Clustering, outlier detection, association rules.
- 3. Linear models and gradient descent (for supervised learning)
 - Loss functions, change of basis, regularization, feature selection.
 - Gradient descent and stochastic gradient.
- 4. Latent-factor models (for unsupervised learning)
 - Typically using linear models and gradient descent.
- 5. Neural networks (for supervised and multi-layer latent-factor models).
- 6. Markov chains
 - Random walk models for sequences and data living on graphs.

CPSC 340 vs. CPSC 540

- Goals of CPSC 340 this term: practical machine learning.
 - Make accessible by avoiding some technical details/topics/models.
 - Present most of the fundamental ideas, sometimes in simplified ways.
 - Choose models that are widely-used in practice.
- Goals of CPSC 540 next term: research-level machine learning.
 - Covers complicated details/topics/models that we avoided.
 - Targeted at people with algorithms/math/stats/sciComp background.
 - Goal is to be able to understand ICML/NIPS papers at the end of course.
- Rest of this lecture:
 - What did we not cover? ⇔ What I'm planning to cover in CPSC 540.

1. Large-Scale Machine Learning

- We'll also fill in details of topics we've ignored:
 - How do we convexity of general multivariate functions? $\chi^{\tau} \rho \times \xi \rho$
 - How many iterations of gradient descent do we need? $f(w^{t}) - f(w^{*}) \leq (1 - \frac{M}{L})^{t} [f(w^{0}) - f(w^{*})]$
 - How do we solve non-smooth optimization problems?

 $f(w) = c^{T}w$ with Awsb - How can get sparsity in terms of 'groups' or 'patterns' of variables?

$$f(w) = \frac{1}{2} ||X_w - y||^2 + \sum_{i \in G} ||w_g||_2$$

- How can we apply kernels to general linear models?

$$f^{*}(z) = \sup_{w \in D} \{w^{T}z - f(w)\}$$

2. Density Estimation

- Methods for estimating multivariate distributions p(x).
 - Abstract problem, includes most of ML as a special case.
 - But going beyond simple Gaussian and independent models.
- Classic models:
 - Mixture models.
 - Non-parametric models.
 - Markov chains.



• More latent-factor models: factor analysis, ICA, topic models.

Trait	Description				
Openness	Being curious, original, intellectual, creative, and open to new ideas.				
Conscientiousness	Being organized, systematic, punctual, achievement- oriented, and dependable.				
Extraversion	Being outgoing, talkative, sociable, and enjoying social situations.				
Agreeableness	Being affable, tolerant, sensitive, trusting, kind, and warm.				
Neuroticism	Being anxious, irritable, temperamental, and moody.				





3. Structured Prediction and Graphical Models

• Structured prediction:

- Instead of class label 'y_i', our output is a general object.



- Conditional random fields and structured support vector machines.
- Relationship of graph to dynamic programming (treewidth).
- Variational and Markov chain Monte Carlo for inference/decoding.
- Unsupervised deep learning: Boltzmann machines and GANs.

4. Bayesian Statistics

- Key idea: treat the model as a random variable.
 - Now use the rules of probability to make inferences.
 - Learning with integration rather than differentiation.
- Can do things with Bayesian statistics that can't otherwise be done.
 - Bayesian model averaging.
 - Hierarchical models.
 - Optimize regularization parameters and things like 'k'.
 - Allow infinite number of latent factors.
 - Non-IID data.





5. Recurrent Neural Networks

- How can we add memory to deep learning?
 - Recurrent neural nets, long short-term memory, neural Turing machine.



6. Online and Active Learning (Time Permitting)

- Online learning:
 - Training examples are streaming in over time.
 - Want to predict well in the present.
 - Not necessarily IID.
- Active learning:
 - Generalization of semi-supervised learning.
 - Model can choose which example to label next.

6. Causal Learning (Time Permitting)

- Causal learning:
 - Observational prediction (CPSC 340):
 - Do people who take Cold-FX have shorter colds?
 - Causal prediction:
 - Does taking Cold-FX cause you to have shorter colds?
 - Counter-factual prediction:
 - You didn't take Cold-FX and had long cold, would taking it have made it shorter?
- Modeling the effects of actions.
- Predicting the direction of causality.

7. Reinforcement Learning (Time Permitting)

- Reinforcement learning puts everything together:
 - Use observations to build a model of the world (learning).
 - We care about performance in the present (online).
 - We have to make decisions (active).
 - Our decisions affect the world (causal).

https://www.youtube.com/watch?v=Ih8EfvOzBOY https://www.youtube.com/watch?v=SH3bADiB7uQ https://www.youtube.com/watch?v=nUQsRPJ1dYw





Final Slide: Data Science Job Board

- Data Science Job Board: <u>http://makedatasense.ca/jobs</u>
 - Set up by students to connect employers/employees.
 - More companies looking for people than people looking for jobs.
 - Make a profile if you are looking for a job in this area.



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Data Science Job Board

Browse Data Science jobs and post your own Data Scientist profile for other companies to see.

Click here to browse jobs and post your profile