CIS 519/419 Applied Machine Learning www.seas.upenn.edu/~cis519

Dan Roth <u>danroth@seas.upenn.edu</u> <u>http://www.cis.upenn.edu/~danroth/</u> 461C, 3401 Walnut

Slides were created by Dan Roth (for CIS519/419 at Penn or CS446 at UIUC), Eric Eaton for CIS519/419 at Penn, or from other authors who have made their ML slides available.

Course Overview

- Introduction: Basic problems and questions
- A detailed example: Linear classifiers; key algorithmic idea
- Two Basic Paradigms:
 - Discriminative Learning & Generative/Probablistic Learning
- Learning Protocols:
 - Supervised; Unsupervised; Semi-supervised
- Algorithms
 - Gradient Descent
 - Decision Trees
 - Linear Representations: (Perceptron; SVMs; Kernels)
 - Neural Networks/Deep Learning
 - Probabilistic Representations (naïve Bayes)
 - Unsupervised /Semi supervised: EM
 - Clustering; Dimensionality Reduction
- Modeling; Evaluation; Real world challenges
- Ethics

CIS519 Admin

Registration to Class

- Check our class website:
 - Schedule, slides, videos, policies
 - http://www.seas.upenn.edu/~cis519/fall2018/
 - Sign up, participate in our Piazza forum:
 - Announcements and discussions
 - http://piazza.com/upenn/fall2018/cis419519
 - Check out our team
 - Office hours
 - Canvas:
 - Notes, homework and videos will be open.
 - [Optional] Discussion Sessions:
 - Starting this week: Wednesday 4pm, Thursday 5pm: Python Tutorial
 - Check the website for the location

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HW0 is mandatory!

We start today

What is Learning

- The Badges Game.....
 - This is an example of the key learning protocol: supervised learning
- First question: Are you sure you got it?
 - Why?

Training data

- + Naoki Abe
- Myriam Abramson
- + David W. Aha
- + Kamal M. Ali
- Eric Allender
- + Dana Angluin
- Chidanand Apte
- + Minoru Asada
- + Lars Asker
- + Javed Aslam
- + Jose L. Balcazar
- Cristina Baroglio

- + Peter Bartlett
- Eric Baum
- + Welton Becket
- Shai Ben-David
- + George Berg
- + Neil Berkman
- + Malini Bhandaru
- + Bir Bhanu
- + Reinhard Blasig
- Avrim Blum
- Anselm Blumer
- + Justin Boyan

- + Carla E. Brodley
- + Nader Bshouty
- Wray Buntine
- Andrey Burago
- + Tom Bylander + Bill Byrne
- Claire Cardie
- + John Case
- + Jason Catlett
- Philip Chan
- Zhixiang Chen
- Chris Darken

The Badges game

+ Naoki Abe

- Eric Baum

 Conference attendees to the 1994 Machine Learning conference were given name badges labeled with + or -.

What function was used to assign these labels?

Raw test data

Shivani Agarwal Gerald F. DeJong Chris Drummond Yolanda Gil Attilio Giordana Jiarong Hong J. R. Quinlan Priscilla Rasmussen Dan Roth Yoram Singer Lyle H. Ungar

Labeled test data

- ? Shivani Agarwal
- + Gerald F. DeJong
- Chris Drummond
- + Yolanda Gil
- Attilio Giordana
- + Jiarong Hong

- J. R. Quinlan
- Priscilla Rasmussen
- + Dan Roth
- + Yoram Singer
- Lyle H. Ungar

What is Learning

- The Badges Game.....
 - This is an example of the key learning protocol: supervised learning
- First question: Are you sure you got it?
 - Why?
- Issues:
 - Which problem was easier?
 - Prediction or Modeling?
 - Representation
 - Problem setting
 - Background Knowledge
 - When did learning take place?
 - Algorithm: can you write a program that takes this data as input and predicts the label for your name?





 We consider systems that apply a function f() to input items x and return an output y = f(x).



 In (supervised) machine learning, we deal with systems whose f(x) is learned from examples.

Why use learning?

- We typically use machine learning when the function f(x) we want the system to apply is unknown to us, and we cannot "think" about it. The function could actually be simple.
- (ENGLAND, June, 1989) Christopher Robin is alive and well. He lives in England. He is the same person that you read about in the book, Winnie the Pooh. As a boy, Chris lived in a pretty home called Cotchfield Farm. When Chris was three years old, his father wrote a poem about him. The poem was printed in a magazine for others to read. Mr. Robin then wrote a book. He made up a fairy tale land where Chris lived. His friends were animals. There was a bear called Winnie the Pooh. There was also an owl and a young pig, called a piglet. All the animals were stuffed toys that Chris owned. Mr. Robin made them come to life with his words. The places in the story were all near Cotchfield Farm. Winnie the Pooh was written in 1925. Children still love to read about Christopher Robin and his animal friends. Most people don't know he is a real person who is grown now. He has written two books of his own. They tell what it is like to be famous.





Supervised learning: Training Can you suggest other learning protocols?



- Give the learner examples in $\mathcal{D}^{ ext{train}}$
- The learner returns a model g(x)

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g(x) is the model we'll use in our application

Supervised learning: Testing

Labeled Test Data **T** test (**x'**₁, y'₁) (x'_{2}, y'_{2}) (**x'**_M, y'_M)

Reserve some labeled data for testing



Supervised learning: Testing

Apply the model to the raw test data

Can you use the test data otherwise?

Evaluate by comparing predicted labels against the test labels



Supervised Learning : Examples

- Disease diagnosis
 - x: Properties of patient (symptoms, lab tests)
 - f : Disease (or maybe: recommended therapy)
- Part-of-Speech tagging
 - x: An English sentence (e.g., The can will rust)
 - f : The part of speech of a word in the sentence
- Face recognition
 - x: Bitmap picture of person's face
 - f : Name the person (or maybe: a property of)
- Automatic Steering
 - x: Bitmap picture of road surface in front of car
 - f : Degrees to turn the steering wheel

Many problems that do not seem like classification problems can be decomposed to classification problems.

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Key Issues in Machine Learning

- Modeling
 - How to formulate application problems as machine learning problems ? How to represent the data?
 - Learning Protocols (where is the data & labels coming from?)
- Representation
 - What **functions** should we learn (hypothesis spaces) ?
 - How to map raw **input** to an instance space?
 - Any rigorous way to find these? Any general approach?
- Algorithms
 - What are good algorithms?
 - How do we define success?
 - Generalization vs. over fitting
 - The computational problem

Using supervised learning

- What is our instance space?
 - Gloss: What kind of features are we using?
- What is our label space?
 - Gloss: What kind of learning task are we dealing with?
- What is our hypothesis space?
 - Gloss: What kind of functions (models) are we learning?
- What learning algorithm do we use?
 - Gloss: How do we learn the model from the labeled data?
- What is our loss function/evaluation metric?
 - Gloss: How do we measure success? What drives learning?





Designing an appropriate instance space X is crucial for how well we can predict y.

1. The instance space $oldsymbol{\mathcal{X}}$

- When we apply machine learning to a task, we first need to define the instance space X.
- Instances $x \in X$ are defined by features:
 - Boolean features:
 - Is there a folder named after the sender?
 - Does this email contains the word 'class'?
 - Does this email contains the word 'waiting'?
 - Does this email contains the word 'class' and the word 'waiting'?
 - Numerical features:
 - How often does 'learning' occur in this email?
 - What long is email?
 - How many emails have I seen from this sender over the last day/week/month?
 - Bag of tokens
 - Just list all the **tokens** in the input

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Does it add anything?

What's X for the Badges game?

- Possible features:
 - Gender/age/country of the person?
 - Length of their first or last name?
 - Does the name contain letter 'x'?
 - How many vowels does their name contain?
 - Is the n-th letter a vowel?
 - Height;
 - Shoe size

${oldsymbol{\mathcal{X}}}$ as a vector space

- X is an N-dimensional vector space (e.g. < N)
 - Each dimension = one feature.
- Each x is a feature vector (hence the boldface x).
- Think of $\mathbf{x} = [\mathbf{x}_1 \dots \mathbf{x}_N]$ as a point in $\boldsymbol{\mathcal{X}}$:



Good features are essential

- The choice of features is crucial for how well a task can be learned.
 - In many application areas (language, vision, etc.), a lot of work goes into designing suitable features.
 - This requires domain expertise.
- Think about the badges game what if you were focusing on visual features?
- We can't teach you what specific features to use for your task.
 - But we will touch on some general principles



 The label space *Y* determines what kind of supervised learning task we are dealing with

Supervised learning tasks I

- Output labels y∈Y are categorical:
 - Binary classification: Two possible labels
 - Multiclass classification: k possible labels
 - Output labels y∈Y are structured objects (sequences of labels, parse trees, etc.)
 - Structure learning



Before I <u>met</u> with him before <u>leaving</u> for Paris on <u>Thursday</u>. → Be_Included

Supervised learning tasks II

- Output labels y∈Y are numerical:
 - Regression (linear/polynomial):
 - Labels are continuous-valued
 - Learn a linear/polynomial function f(x)
 - Ranking:
 - Labels are ordinal
 - Learn an ordering $f(x_1) > f(x_2)$ over input



 We need to choose what kind of model we want to learn

A Learning Problem



Hypothesis Space

Complete Ignorance: There are $2^{16} = 65536$ possible fun	ctions 1 0 0 0 7		
over four input features.	 There are Y ^X possible functions f(x) from the instance 		
We can't figure out which one is	space X to the label space Y .		
correct until we've seen every	 Learners typically consider only a <i>subset</i> of the functions from X to Y, called the hypothesis space H . H ⊆ Y ^X 		
possible input-output pair.			
After observing seven examples we	still <u>1 0 1 1 ?</u>		
have 2 ⁹ possibilities for f	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		
Is Learning Possible?	16 1 1 1 1 ?		

Hypothesis Space (2)

Simple Rules: The form y	here are only 16 simple cor =x _i ^ x _j ^ x _k	njunctive rules	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Rule	Counterexample	Rule	<u>Counterexample</u>
У =с		X2 A X3	0011 1
X 1	1100 0	X 2 Λ X 4	0011 1
X 2	0100 0	X3 A X4	1001 1
X 3	0110 0	X 1 A X 2 A X 3	0011 1
X 4	0101 1	X 1 A X 2 A X 4	0011 1
X 1 A X 2	1100 0	X 1 A X3 A X4	0011 1
X 1 A X 3	0011 1	Χ 2 Λ Χ 3 Λ Χ 4	0011 1
X 1 A X 4	0011 1	Χ 1 Λ Χ 2 Λ Χ 3 Λ 2	X 4 0011 1

No simple rule explains the data. The same is true for **simple clauses (disjunctions)**. CIS419/519 Fall '18



of the following n variables are 1"

variables 1-of 2-of 3-of 4-of



1-of 2-of 3-of 4-of



Views of Learning

Learning is the removal of our <u>remaining</u> uncertainty:

- Suppose we knew that the unknown function was an m-of-n Boolean function, then we could use the training data to infer which function it is.
- Learning requires guessing a good hypothesis class:
 - We can start with a very small class and enlarge it until it contains an hypothesis that fits the data.
- We could be wrong !
 - Our prior knowledge might be wrong:
 - y=x4 Λ one-of (x1, x3) is also consistent
 - Our guess of the hypothesis space could be wrong
- If this is the unknown function, then we will make errors when we are given new examples, and are asked to predict the value of the function

General strategies for Machine Learning

- Develop flexible hypothesis spaces:
 - Decision trees, neural networks, nested collections.
 - Constraining the hypothesis space is done algorithmically
- Develop representation languages for restricted classes of functions:
 - Serve to limit the expressivity of the target models
 - E.g., Functional representation (n-of-m); Grammars; linear functions; stochastic models;
 - Get flexibility by augmenting the feature space
- In either case:
 - Develop algorithms for finding a hypothesis in our hypothesis space, that fits the data
 - And hope that they will generalize well

Administration

- The class is still full.
 - There will be some changes until midnight tonight.
 - But there will be chances to petition and get in as people drop.
- You all need to complete HWO!
- 1st quiz was due last night.
- HW 1 will be released next week.
- Questions?
 - Please ask/comment during class.
- No Class on Wednesday
- Office hours, as usual;
 - I will have one today, but not on Wednesday.

Key Issues in Machine Learning

- Modeling
 - How to formulate application problems as machine learning problems ? How to represent the data?
 - Learning Protocols (where is the data & labels coming from?)
- Representation
 - What functions should we learn (hypothesis spaces) ?
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An Example: Context Sensitive Spelling

I don't know {whether, weather} to laugh or cry

This is the Modeling Step

How can we make this a learning problem?

What is the hypothesis space?

We will look for a function
 f: Sentences → {whether, weather}

Input/Instance space?

- We need to define the domain of this function better.
- <u>An option</u>: For each word w in English define a Boolean feature x_w:
 [x_w =1] iff w is in the sentence
- This maps a sentence to a point in {0,1}^{50,000}
- In this space: some points are <u>whether</u> points

some are <u>weather</u> points

Learning Protocol?

Supervised? Unsupervised?

Representation Step: What's Good?

sgn(z) =0 if z<0;
1 otherwise</pre>

$$w^T \cdot x = \sum_{i=1}^n w_i x$$

- Learning problem:
 Find a function that
 best separates the data
- What function?
- What's best?
- (How to find it?)

Linear = linear in t e feature space **x**= data representation; **v** = the classifier (**w**, **x**, column vectors of cimensionality n) **y** = sgn {w^Tx}



• A possibility: Define the learning problem to be:

 A (linear) function that best separates the data CIS419/519 Fall '18

Expressivity

$$f(\mathbf{x}) = \operatorname{sgn} \{ w^T \cdot x - \theta \} = \operatorname{sgn} \{ \sum_{i=1}^n w_i x_i - \theta \}$$

- Many functions are Linear
 - Conjunctions:
 - $y = x_1 \wedge x_2 \wedge x_5$
 - $y = sgn\{1 \cdot x_1 + 1 \cdot x_2 + 1 \cdot x_5 3\};$ $w = (1, 0, 1, 0, 1) \theta = 3$

Probabilistic Classifiers as well

- At least m of n:
 - y = at least 2 of {x₁, x₃, x₅}
 - $y = sgn\{1 \cdot x_1 + 1 \cdot x_2 + 1 \cdot x_5 2\}\};$ $w = (1, 0, 1, 0, 1) \theta = 2$
- Many functions are not
 - Xor: $y = (x_1 \land x_2) \lor (\neg x_1 \land \neg x_2)$
 - Non trivial DNF: $y = (x_1 \land x_2) \lor (x_3 \land x_4)$
- But can be made linear
- Note: all the variables above are Boolean variables

Functions Can be Made Linear

- Data points are not linearly separable in one dimension
- Not separable if you insist on using a specific class of functions (e.g., linear)



Blown Up Feature Space

Data are separable in <x, x²> space



Exclusive-OR (XOR)

•
$$(x_1 \wedge x_2) \vee (\neg \{x_1\} \wedge \neg \{x_2\})$$

In general: a parity function.

•
$$x_i \in \{0, 1\}$$

•
$$f(x_1, x_2, ..., x_n) = 1$$

iff $\sum x_i$ is even

This function is not linearly separable.



Functions Can be Made Linear

<u>A real Weather/Whether</u> <u>example</u> **Discrete Case**

$x_1 x_2 x_4 \vee x_2 x_4 x_5 \vee x_1 x_3 x_7$ $x_1 x_2 x_4 \vee x_2 x_4 x_5 \vee x_1 x_3 x_7$ New discriminator is



Representation (1)

Feature Types:

(what does the algorithm know about the input):

- 1,2. relative position (+/-1) has this pos/w
- 3. Conjunctions of size two
- 4. word w occurs in (-2,+2) window around target **Note:** 4 feature **types**; many features

The feature resulting from instantiating the type in the given data

Some statistics (not part of the learning process; just for the understanding of the problem)

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1p=Det 0.972222 0 34 1w=the 0.961538 0 24 -1p=Punc 1p=Pro 0.96 0 23 -1p=V 1p=Adv 0.96 0 23 or 0.959184 3 93 1p=Adj 0.957447 1 44 not 0.956522 1 43 -1p=V 1p=Pro 0.956522 0 21 1p=Det 2p=Ns 0.954545 0 20 -1p=V 1p=Det 0.954545 0 20 1w=he 0.952381 0 19 -1p=Prep 1p=Pro 0.952381 0 19 -2w=to -1p=V 0.952381 0 19 1p=Pro 2p=Vpp 0.947368 0 17 question 0.947368 0 17 1p=Pro 0.946237 4 87 -1w=, 1p=Pro 0.944444 0 16 -1p=Punc 0.941176 2 47 should 0.941176 0 15 1w=thev 0.941176 0 15 -1p=V 1w=the 0.941176 0 15 -1p=Ns 1p=Adj 0.9375 0 14 1p=Pro 2p=Was 0.9375 0 14 1p=Pro 2p=Vpt 0.9375 0 14 -1p=Punc 1p=Adj 0.9375 0 14 -2p=Ns -1p=Punc 0.933333 1 27 Adj 2p=Prep 0.933333 0 13 1p=Ns 2p=Vpp 0.933333 0 13 -1p=Conj 1p=Pro 0.933333 0 13 you 0.933333 0 13 1p=Ns 2p=Was 0.933333 0 13 1w=it 0.933333 0 13 1p=Punc 1p=Prep 0.933333 0 13 -1w-, 1- 0.928571 0 12 -1p=Punc 1p=Ns 0.928571 1 25 -1p=V 1p=Adj 0.928571 0 12 1p=Ns 2w=was 0.928571 0 12

Representation (2)

Extracting features from the data:

(what does the algorithm know about the input):

1,2. relative position (+/-1); pos/w

3. Conjunctions of size two

4. Occurrence of a word in a window around the target

Note: 2 feature types; many features

For each feature type, the data gives rise to multiple

features; you don't know which, before you see the data.

But << whether >> the murder of El Benefactor in Ciudad Trujillo means freedom for the people of the Caribbean fiefdom is a question that cannot now be answered .

If Russian pupils have to take these languages , how come American students have a choice << whether >> or not to take a language , but have to face so many exceptions ? ?

The rescue squad is to be praised immensely for the fine work they do in all kinds of << weather >> .

Besides the lack of an adequate ethical dimension to the Governor's case , one can ask seriously << whether >> our lead over the Russians in quality and quantity of nuclear weapons is so slight as to make the tests absolutely necessary .

It is another question << whether >> `` they '' -- or a single general , off in a corner of China , secure for a few (galvanizing ? ?

And little Zeme North , a Dora with real spirit and verve , was fascinating << whether >> she was singing of her love for Floyd , the cop who becomes sewer commissioner and then is promoted into garbage , or just dancing to display her exuberant feelings .

A few drops of rain just before midnight , when Sarah Vaughan was in the midst of her first number , scattered the more timid members of the audience briefly , but at this hour and with Sarah on the stand , most of the listeners didn't care << whether >> they got wet .

Expressed differently : if the price for becoming a faithful follower of Jesus Christ is some form of self-destruction , << whether >> of the body or of the mind -- sacrificium corporis , sacrificium intellectus -- then there is no alternative but that the price remain unpaid .

Thus , if what is at issue is << whether >> `` All S is P '' , it is indifferent whether `` Some S is not P '' or `` No S is P '' , since in either case the judgment in question is false .

Thus , if what is at issue is whether `` All S is P '' , it is indifferent << whether >> `` Some S is not P '' or `` No S is P '' , since in either case the judgment in question is false .

Such efforts almost always find themselves compelled to ask << whether >> Adam was created capable of growing old and then older and then still older , in short , whether Adam's life was intended to be part of the process of time .

Such efforts almost always find themselves compelled to ask whether Adam was created capable of growing old and then older and then still older , in short , << whether >> Adam's life was intended to be part of the process of time .

It is idle to ask why we are no longer disturbed if somebody , professing the deepest piety , decides anew that it is of no importance << whether >> or not Christ transformed the water into wine at eleven A.M. on the third of August , A.D. 32 .

Representation (3)

Each example corresponds to one target occurrence; all the features for this target are collected into a vector, and the label is added.

Here:

- Sparse Representation of the feature vector. Why?

- Variable size: Why?

Here the first index (0/1) is the label)

- 1,2,3,11,48,51,82,87,92,105,176,198,199,279,327,413,439,482,498,747,963,964,965,975,1029,1072,1166,1176:
- 1,6,9,42,43,44,45,47,73,155,157,216,226,238,240,322,441,497,498,757,829,971,978,987,995,1000,1047,1060,1073,1077,1078,1086,1116,1118,1119,1132,1138,11 39,1141,1172:
- 0,57,94,109,112,119,153,305,387,482,759,855,963,964,965,1002,1050,1068,1142,1207,1226:
- 1,7,52,60,65,141,197,240,469,497,772,963,964,965,989,1045,1067,1072:
- 1,6,16,57,69,116,137,153,156,201,213,280,302,304,322,325,432,468,497,830,986,987,1058,1143:
- 1,17,26,32,36,46,119,148,157,239,292,299,322,329,433,474,497,919,963,964,978,1001,1045,1061,1071,1116,1131,1209:
- 1,8,15,17,20,25,57,103,116,224,370,414,458,497,719,956,963,964,987,1068:
- 1,6,21,27,29,41,58,67,69,155,238,271,304,460,497,963,964,1027,1111:
- 1,54,69,78,91,100,110,115,153,156,195,250,283,302,305,325,497,656,753,756,833,957,977,986,1065,1066:
- 1,6,9,37,69,153,156,302,305,325,443,497,597,729,986,1013,1040,1065,1111,1116:
- 1,7,12,32,36,39,89,116,152,154,157,222,240,329,827,938,943,963,1045,1188:
- 1,21,27,41,67,68,98,121,133,162,232,240,329,489,497,886,963,964,965,1045:
- 1,6,9,42,43,44,45,47,69,155,156,157,216,238,441,497,757,833,954,963,964,966,968,971,987,995,1040,1078,1086,1101,1118,1143,1172:
- 1,6,7,21,24,27,29,35,38,41,56,58,61,67,87,125,156,157,223,232,238,455,489,497,774,1203:
- 1,6,8,17,62,99,116,147,156,220,237,240,275,276,284,298,322,326,486,497,499,559,561,961,963,964,970,1039:
- 1,6,13,17,28,62,90,93,101,103,119,147,158,161,169,194,237,240,275,276,305,322,323,326,482,487,491,497,961,963,970,987,1029,1045:
- 1,2,3,6,11,21,27,41,48,61,67,87,98,121,125,133,162,204,217,229,256,305,322,329,439,497,517,630,964,965:
- 1,6,8,14,17,75,89,103,116,119,154,156,157,182,229,296,497,499,536,679,684,700,784,888,927,966,971,976,987,1040,1058,1086,1106,1143,1190:
- 1,99,116,117,205,212,237,305,322,455,499,601,943,989,999,1068,1071,1091,1127:
- 0,119,217,440,487,491,497,743,791,847,938,987,1016,1046,1061,1071,1116,1129,1145,1168,1196:
- 0,305,322,329,482,812,963,964,965,1002,1045,1050,1068,1142,1196,1207:
- 0,37,49,127,153,172,201,324,354,490,497,498,531,689,908,963,964,965,966,972,987,994,1000,1007,1028,1045,1047,1049,1052,1056,1057,1065,1066,1072,1081,1 086,1094,1116,1117,1120,1122,1135,1138,1140,1143,1204:
- 0,87,198,321,446,497,908,954,963,964,966,974,987,997,1001,1015,1045,1052,1072,1116,1120,1140:
- 1,7,9,57,73,80,157,197,226,237,240,295,356,437,442,484,493,497,893,917,1067,1072,1101,1120:
- 1,9,57,356,428,453,485,493,497,893,963,964,965,1032,1045,1072,1120:
- 1 6 7 21 24 29 20 61 69 80 87 167 208 211 228 296 204 264 419 427 442 606

Administration

- "Easy" Registration Period is over.
 - But there will be chances to petition and get in as people drop.
 - If you want to switch 419/519, talk with Nicholas Mancuso <u>nmancuso@seas.upenn.edu</u>
- You all need to complete HWO!
- 2nd quiz was due last night.
- HW 1 will be released on Wednesday this week.
- Questions?
 - Please ask/comment during class.
- Change in my office hours:
 - Today: 3-4 pm; Wednesday 1:30-2:30

Third Step: How to Learn?

- A possibility: Local search
 - Start with a linear threshold function.
 - See how well you are doing.
 - Correct
 - Repeat until you converge.
- There are other ways that do not search directly in the hypotheses space
 - Directly compute the hypothesis



A General Framework for Learning

- Goal: predict an unobserved output value y 2 Y based on an observed input vector x 2 X
- Estimate a functional relationship y~f(x) from a set {(x,y)_i}_{i=1,n}
- Most relevant Classification: $y \in \{0,1\}$ (or $y \in \{1,2,...k\}$)
 - (But, within the same framework can also talk about Regression, y 2 <)

Simple loss function: # of mistakes [...] is a indicator function

- What do we want f(x) to satisfy?
 - We want to minimize the Risk: $L(f()) = E_{x,y}([f(x)\neq y])$
 - Where: E _{x,y} denotes the expectation with respect to the true distribution.

Learning (II)

We want to minimize the Loss: $L(f()) = E_{X,Y}([f(X) \neq Y])$

- Where: E _{x,y} denotes the expectation with respect to the true distribution.
- We cannot minimize this loss

Side note: If the distribution over $X \pounds Y$ is known,predict: $y = \operatorname{argmax}_{y} P(y|x)$ This is the best possible (the optimal Bayes' error).

- Instead, we try to minimize the empirical classification error.
- For a set of training examples {(x_i, y_i)}_{i=1,m}
- Try to minimize: $L'(f()) = 1/m \sum_{i} [f(x_i) \neq y_i]$ (m=# of examples)
 - (Issue I: why/when is this good enough? Not now)
- This minimization problem is typically NP hard.
- To alleviate this computational problem, minimize a new function a convex upper bound of the (real) classification error function:

I(f(x),y) =[f(x) \neq y] = {1 when f(x) \neq y; 0 otherwise}

Algorithmic View of Learning: an Optimization Problem

- A Loss Function L(f(x),y) measures the penalty incurred by a classifier f on example (x,y).
- There are many different loss functions one could define:
 - Misclassification Error:

L(f(x),y) = 0 if f(x) = y;

• Squared Loss:

 $L(f(x),y) = (f(x) - y)^2$

Input dependent loss:

L(f(x),y) = 0 if f(x) = y; c(x) otherwise

1 otherwise A continuous con

A continuous convex loss function allows a simpler optimization algorithm.

f(x) -y

Loss





Putting it all together:

A Learning Algorithm

Third Step: How to Learn?

- A possibility: Local search
 - Start with a linear threshold function.
 - See how well you are doing.
 - Correct
 - Repeat until you converge.
- There are other ways that do not search directly in the hypotheses space
 - Directly compute the hypothesis



Learning Linear Separators

(LTU=Linear Threshold Unit)

$$f(\mathbf{x}) = \operatorname{sgn} \{ w^T \cdot x - \theta \} = \operatorname{sgn} \{ \sum_{i=1}^n w_i x_i - \theta \}$$

- x^T= (x₁,x₂,...,x_n) ∈ {0,1}ⁿ is the feature based encoding of the data point
- $w^T = (w_1, w_2, \dots, w_n) \in \mathbb{R}^n$ is the target function.
- θ determines the shift
 with respect to the origin



Canonical Representation

$$f(\mathbf{x}) = \operatorname{sgn} \{ w^T \cdot x \cdot \theta \} = \operatorname{sgn} \{ \sum_{i=1}^n w_i x_i - \theta \}$$

- Note: sgn { $w^T \cdot x \theta$ } = sgn { $w'^T \cdot x'$ }
- Where:
 - x' = (x, -1) and w' = (w, θ)
- Moved from an n dimensional representation to an (n+1) dimensional representation, but now can look for hyperplanes that go through the origin.
- Basically, that means that we learn both w and θ

General Learning Principle

- **Our goal** is to find a w that *minimizes* the expected risk $E(w) = E_{x,y} Q(x, y, w)$
- We cannot do it.

The Risk (Err) E:

a function of w

- **Instead,** we approximate E(w) using a finite training set of independent samples (x_i, y_i)
- **E(w)** ~=~ $1/m \sum_{1,m} Q(x_i, y_i, w)$
- To find the *minimum*, we use a batch gradient descent algorithm
- That is, we successively compute estimates w^t of the optimal parameter vector w:

wt+1 = wt -
$$\mathbf{r}$$
 $\mathbf{E}(\mathbf{w}) = wt - 1/m \sum_{1,m} \mathbf{r}$ $\mathbf{Q}(\mathbf{x}_{i}, \mathbf{y}_{i}, \mathbf{w})$
CIS419/519 Fall '18 there is "time" or "iteration" #

The loss Q: a function of x, w and y

W

W

To find a local minimum of a function using gradient descent, we take steps proportional to the negative of the gradient of the function at the current point.

Η

Gradient Descent

- We use gradient descent to determine the weight vector that minimizes E(w) (= Err (w));
- Fixing the set D of examples, E=Err is a function of w

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 At each step, the weight vector is modified in the direction that produces the steepest descent along the error surface.



To find a local minimum of a function using gradient descent, we take steps proportional to the negative of the gradient of the function at the current point.

LMS: An Optimization Algorithm

- Our Hypothesis Space is the collection of Linear Threshold Units
- Loss function:
 - Squared loss: LMS (Least Mean Square, L₂)
 - $Q(x, y, w) = \frac{1}{2} (w^T x y)^2$



LMS: An Optimization Algorithm

(i (subscript) – vector component; j (superscript) - time; d – example #)

Assumption: $x \in \mathbb{R}^n$; $u \in \mathbb{R}^n$ is the target weight vector; the target (label) is $t_d = u^T \cdot x$ Noise has been added; so, possibly, no weight vector is consistent with the data.

- Let w⁽ⁱ⁾ be the current weight vector we have
- Our prediction on the d-th example **x** is:

$$O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$$

- Let t_d be the target value for this example
- The error the current hypothesis makes on the data set is:

$$E(w) = \operatorname{Err}(w^{j}) = \frac{1}{2} \sum_{d \in D} (t_{d} - O_{d})^{2}$$



Gradient Descent

To find the best direction in the <u>weight space</u> w we compute the gradient of E with respect to each of the components of

$$\nabla E(w) = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \dots, \frac{\partial E}{\partial w_n}\right]$$

- This vector specifies the direction that produces the steepest increase in E;
- We want to modify w in the direction of $-\nabla E(w)$
- Where (with a fixed step size R):

$$w^{t} = w^{t-1} + \Delta w$$
$$\Delta w = -R \nabla E(w)$$

Gradient Descent: LMS

• We have: $E(w) = \text{Err}(w^j) = \frac{1}{2} \sum_{d \in D} (t_d - O_d)^2$

$$\frac{\partial \mathsf{E}}{\partial \mathsf{W}_{i}} = \frac{\partial}{\partial \mathsf{W}_{i}} \frac{1}{2} \sum_{\mathsf{d} \in \mathsf{D}} (\mathsf{t}_{\mathsf{d}} - \mathsf{O}_{\mathsf{d}})^{2} =$$

Therefore:

$$= \frac{1}{2} \sum_{d \in D} \frac{\partial}{\partial W_i} (t_d - O_d)^2 =$$

$$= \frac{1}{2} \sum_{d \in D} 2(t_d - O_d) \frac{\partial}{\partial W_i} (t_d - W_d \bullet X_d) =$$

$$= \sum_{d \in D} (t_d - O_d) (-X_{id})$$

Alg1: Gradient Descent: LMS

Weight update rule:

$$\Delta w_i = R \sum_{d \in D} (t_d - O_d) x_{id}$$

- Gradient descent algorithm for training linear units:
 - Start with an initial random weight vector
 - For every example d with target value t_d do:
 - Evaluate the linear unit $O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$
 - Update w by adding Δw_i to each component
 - Continue until E below some threshold

This algorithm always converges to a local minimum of E(w), for small enough steps. Here (LMS for linear regression), the surface contains only a single global minimum, so the algorithm converges to a weight vector with minimum error, regardless of whether the examples are linearly separable.

The surface may have local minimum if the loss function is different.

Alg 2: Incremental (Stochastic) Gradient Descent:

(LMS)

Weight update rule:

$$\Delta w_i = R(t_d - O_d) x_{id}$$

Dropped the averaging operation. Instead of averaging the gradient of the loss over the complete training set, choose at random a sample (x,y) (or a subset of examples) and update w^t

- Gradient descent algorithm for training linear units:
 - Start with an initial random weight vector
 - For every example d with target value t_d do:
 - Evaluate the linear unit $O_d = w^{(j)T} \cdot x = \sum_{i=1}^n w_i^{(j)} x_i$
 - update w by <u>incrementally</u> by adding Δw_i to each component (update without summing over all data)
 - Continue until E below some threshold
- In general does not converge to global minimum
- But, on-line algorithms are sometimes advantageous...
- Decreasing R with time guarantees convergence CIS419/519 Fall '18

Learning Rates and Convergence

- In the general (non-separable) case the learning rate R must decrease to zero to guarantee convergence.
- The learning rate is called the step size. There are more sophisticated algorithms that choose the step size automatically and converge faster.
- Choosing a better starting point also has impact.
- The gradient descent and its stochastic version are very simple algorithms, but almost all the algorithms we will learn in the class can be traced back to gradient decent algorithms for different loss functions and different hypotheses spaces.

Computational Issues

- Assume the data is linearly separable.
- Sample complexity:
 - Suppose we want to ensure that our LTU has an error rate (on new examples) of less than ε with high probability (at least (1-δ))
 - How large does m (the number of examples) must be in order to achieve this ? It can be shown that for n dimensional problems

m = O(1/ ε [ln(1/ δ) + (n+1) ln(1/ ε)].

- Computational complexity: What can be said?
 - It can be shown that there exists a polynomial time algorithm for finding consistent LTU (by reduction from linear programming).
 - [Contrast with the NP hardness for 0-1 loss optimization]
 - (On-line algorithms have inverse quadratic dependence on the margin)

Other Methods for LTUs

- Fisher Linear Discriminant:
 - A direct computation method
- Probabilistic methods (naïve Bayes):
 - Produces a stochastic classifier that can be viewed as a linear threshold unit.
- Winnow/Perceptron
 - A multiplicative/additive update algorithm with some sparsity properties in the function space (a large number of irrelevant attributes) or features space (sparse examples)
- Logistic Regression, SVM...many other algorithms