CS 188: Artificial Intelligence

Learning Theory, Decision Trees, and Optimization

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[Slides drawn from Nicholas Tomlin, Dan Klein, and Pieter Abbeel for CS188 at UC Berkeley. All CS188 materials are available at http://ai.berkeley.edu.]

Summary of Key Ideas

- Optimize probability of label given input
- max *w* $ll(w) = \max$ *w* \sum

$$
\sum_i \log P(y^{(i)} | x^{(i)}; w)
$$

- Continuous optimization
	- Gradient ascent:
		- Compute steepest uphill direction = gradient $(=$ just vector of partial derivatives)
		- Take step in the gradient direction
		- Repeat (until held-out data accuracy starts to drop $=$ "early stopping")
- Deep neural nets
	- Last layer $=$ still logistic regression
	- Now also many more layers before this last layer
		- = computing the features
		- \rightarrow the features are learned rather than hand-designed
	- Universal function approximation theorem
		- If neural net is large enough
		- **•** Then neural net can represent any continuous mapping from input to output with arbitrary accuracy
		- But remember: need to avoid overfitting / memorizing the training data \rightarrow early stopping!
	- Automatic differentiation gives the derivatives efficiently

Inductive Learning

Inductive Learning (Science)

- Simplest form: learn a function from examples
	- A target function: *g*
	- Examples: input-output pairs $(x, g(x))$
	- E.g. *x* is an email and $g(x)$ is spam / ham
	- E.g. *x* is a house and $g(x)$ is its selling price

▪ Problem:

- Given a hypothesis space *H*
- Given a training set of examples x_i
- Find a hypothesis $h(x)$ such that $h \sim g$
- Includes:
	- Classification (outputs = class labels)
	- Regression (outputs $=$ real numbers)
- **•** How do perceptron and naïve Bayes fit in? $(H, h, g, \text{etc.})$

Inductive Learning

▪ Curve fitting (regression, function approximation):

- Consistency vs. simplicity
- Ockham's razor

Consistency vs. Simplicity

- Fundamental tradeoff: bias vs. variance
- Usually algorithms prefer consistency by default (why?)
- Several ways to operationalize "simplicity"
	- Reduce the hypothesis space
		- Assume more: e.g. independence assumptions, as in naïve Bayes
		- Have fewer, better features / attributes: feature selection
		- Other structural limitations (decision lists vs trees)
	- Regularization
		- Smoothing: cautious use of small counts
		- Many other generalization parameters (pruning cutoffs today)
		- Hypothesis space stays big, but harder to get to the outskirts

Reminder: Features

- Features, aka attributes
	- Sometimes: TYPE=French
	- **•** Sometimes: $f_{\text{Type=French}}(x) = 1$

Decision Trees

- Compact representation of a function:
	- Truth table
	- Conditional probability table
	- Regression values
- True function
	- **•** Realizable: in H

Expressiveness of DTs

• Can express any function of the features

 $P(C|A,B)$

▪ However, we hope for compact trees

Comparison: Perceptrons

▪ What is the expressiveness of a perceptron over these features?

- For a perceptron, a feature's contribution is either positive or negative
	- If you want one feature's effect to depend on another, you have to add a new conjunction feature
	- **E.g. adding "PATRONS=full** \land **WAIT = 60" allows a perceptron to model the interaction between the two** atomic features
- DTs automatically conjoin features / attributes
	- Features can have different effects in different branches of the tree!
- Difference between modeling relative evidence weighting (NB) and complex evidence interaction (DTs)
	- Though if the interactions are too complex, may not find the DT greedily

Hypothesis Spaces

How many distinct decision trees with n Boolean attributes?

- = number of Boolean functions over n attributes
- $=$ number of distinct truth tables with $2ⁿ$ rows
- $= 2^{(2^n)}$
- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees
- How many trees of depth 1 (decision stumps)?
	- = number of Boolean functions over 1 attribute = number of truth tables with 2 rows, times n
	- $= 4n$
	- E.g. with 6 Boolean attributes, there are 24 decision stumps
- More expressive hypothesis space:
	- Increases chance that target function can be expressed (good)
	- Increases number of hypotheses consistent with training set (bad, why?)
	- Means we can get better predictions (lower bias)
	- But we may get worse predictions (higher variance)

Decision Tree Learning

- Aim: find a small tree consistent with the training examples
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree

```
function DTL(examples, attributes, default) returns a decision tree
if examples is empty then return default
else if all examples have the same classification then return the classification
else if attributes is empty then return MODE(examples)
else
     best \leftarrow CHOOSE-ATTRIBUTE(attributes, examples)
     tree \leftarrow a new decision tree with root test bestfor each value v_i of best do
          examples_i \leftarrow \{elements of examples with best = v_i\}subtree \leftarrow DTL(examples_i, attributes - best, \text{MoDE}(examples))add a branch to tree with label v_i and subtree subtree
     return tree
```
Choosing an Attribute

▪ Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"

▪ So: we need a measure of how "good" a split is, even if the results aren't perfectly separated out

Entropy and Information

▪ Information answers questions

- The more uncertain about the answer initially, the more information in the answer
- Scale: bits
	- Answer to Boolean question with prior <1/2, 1/2>?
	- **-** Answer to 4-way question with prior $\langle 1/4, 1/4, 1/4, 1/4 \rangle$?
	- Answer to 4-way question with prior <0, 0, 0, 1>?
	- **•** Answer to 3-way question with prior $\langle 1/2, 1/4, 1/4 \rangle$?
- A probability p is typical of:
	- A uniform distribution of size $1/p$
	- A code of length $log 1/p$

Entropy

- **General answer: if prior is** $\langle p_1, ..., p_n \rangle$ **:**
	- Information is the expected code length

$$
H(\langle p_1, \dots, p_n \rangle) = E_p \log_2 1/p_i
$$

=
$$
\sum_{i=1}^n -p_i \log_2 p_i
$$

- Also called the entropy of the distribution
	- Range [0, 1]
	- More uniform = higher entropy
	- More values = higher entropy
	- More peaked = lower entropy
	- Rare values almost "don't count"

Information Gain

- Back to decision trees!
- For each split, compare entropy before and after
	- **•** Difference is the information gain
	- Problem: there's more than one distribution after split!

Next Step: Recurse

- Now we need to keep growing the tree!
- Two branches are done (why?)
- What to do under "full"?
	- See what examples are there…

Example: Learned Tree

▪ Decision tree learned from these 12 examples:

- Substantially simpler than "true" tree
	- A more complex hypothesis isn't justified by data
- Also: it's reasonable, but wrong

Example: Miles Per Gallon

40 Examples 40 Examples

Find the First Split

• Look at information gain for each attribute

- Note that each attribute is correlated with the target!
- What do we split on?

Result: Decision Stump

Second Level

Reminder: Overfitting

- Overfitting:
	- When you stop modeling the patterns in the training data (which generalize)
	- And start modeling the noise (which doesn't)
- We had this before:
	- Naïve Bayes: needed to smooth
	- Perceptron: early stopping

Significance of a Split

- Starting with:
	- Three cars with 4 cylinders, from Asia, with medium HP
	- 2 bad MPG
	- 1 good MPG
- What do we expect from a three-way split?
	- Maybe each example in its own subset?
	- Maybe just what we saw in the last slide?
- Probably shouldn't split if the counts are so small they could be due to chance
- A chi-squared test can tell us how likely it is that deviations from a perfect split are due to chance*
- **Each split will have a significance value,** p_{CHANCE}

Keeping it General

▪ Pruning:

- Build the full decision tree
- Begin at the bottom of the tree
- Delete splits in which

$p_{\text{CHANCE}} > \text{MaxP}_{\text{CHANCE}}$

- Continue working upward until there are no more prunable nodes
- Note: some chance nodes may not get pruned because they were "redeemed" later

Bonus: Pruning example

• With Max $P_{CHANCE} = 0.1$:

Regularization

- MaxP_{CHANCF} is a regularization parameter
- Generally, set it using held-out data (as usual)

Two Ways of Controlling Overfitting

- Limit the hypothesis space
	- E.g. limit the max depth of trees
	- Easier to analyze
- **Regularize the hypothesis selection**
	- E.g. chance cutoff
	- Disprefer most of the hypotheses unless data is clear
	- Usually done in practice

Other Optimizers

Recall: Batch Gradient Ascent

$$
\max_{w} \quad ll(w) = \max_{w} \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$
\n
$$
g(w)
$$

\n- init
$$
w
$$
\n- for $iter = 1, 2, \ldots$
\n- $w \leftarrow w + \alpha * \sum_{i} \nabla \log P(y^{(i)} | x^{(i)}; w)$
\n

Recall: Stochastic Gradient Ascent

$$
\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

Observation: once gradient on one training example has been computed, might as well incorporate before computing next one

> ▪ init $\texttt{for iter} = 1, 2, ...$ ▪ pick random j *w* $w \leftarrow w + \alpha * \nabla \log P(y^{(j)} | x^{(j)}; w)$

Recall: Mini-batch Gradient Ascent

$$
\max_{w} \quad ll(w) = \max_{w} \quad \sum_{i} \log P(y^{(i)} | x^{(i)}; w)
$$

Observation: gradient over small set of training examples (=mini-batch) can be computed in parallel, might as well do that instead of a single one

\n- init
$$
w
$$
\n- for $\text{iter} = 1, 2, \ldots$
\n- pick random subset of training examples J
\n- $w \leftarrow w + \alpha * \sum_{j \in J} \nabla \log P(y^{(j)} | x^{(j)}; w)$
\n

Concept #1: Computing Second-Order Derivatives

Newton's Method (in 1D):

- Want to optimize: $\max_{\theta} f(\theta)$
- Apply Taylor expansion:

 $f(\theta + h) \approx f(\theta) + f'(\theta)h + \frac{1}{2}f''(\theta)h^2$

Find value of h that maximizes this:

$$
0 = \frac{\partial}{\partial h} \Big[f(\theta) + f'(\theta)h + \frac{1}{2} f''(\theta)h^2 \Big]
$$

= f'(\theta) + f''(\theta)h

Rearrange terms to get update:

$$
h = -\frac{f'(\theta)}{f''(\theta)} \qquad \theta_{t+1} = \theta_t + h = \theta_t - \frac{f'(\theta)}{f''(\theta)}
$$

Caveat: can be computationally expensive or difficult to compute in higher dimensions

Concept #2: Momentum

- Potential issues with vanilla SGD:
	- Can take a long time to converge if the learning rate is too low
	- Can bounce around in "ravines" without making much progress toward a local optimum

Concept #2: Momentum

Stochastic Gradient Descent with Momentum

- **•** Keep a running sum of old updates: $v_t = \gamma v_{t-1} + \eta \nabla_{\theta} f(\theta_t)$
- **•** Perform a standard gradient descent step: $\theta_{t+1} = \theta_t v_t$
	- **•** (or gradient ascent step: $\theta_{t+1} = \theta_t + v_t$)

Nesterov Accelerated Gradient (NAG)

▪ Key idea: "anticipate" where momentum will take you and compute the gradient at that point instead. Can think of this as momentum with planning

$$
v_t = \gamma v_{t-1} + \eta \nabla_{\theta} f(\theta_t - \gamma v_{t-1})
$$

$$
\theta_{t+1} = \theta_t - v_t
$$

green vector = accumulated gradient brown vector $=$ jump, red vector = correction,

blue vectors = standard momentum

• Recall: learning rates

- Determines how much we update weights in the direction of the gradient
- Often: want to set this in terms of how much it updates the weights
- Often: want to lower learning rate over time (*learning rate scheduling*)

$$
\theta_{t+1} = \theta_t - \eta \nabla_{\theta} f(\theta_t)
$$

. Key idea: different learning rates for each parameter

- We can make larger or smaller updates depending on how important a feature is
- Small updates for frequent features; big updates for rare features
- This idea underlies: Adagrad, RMSProp, Adam, etc.

Adagrad

• Compute the gradient at i **-th parameter:**

 $g_{t,i} = \nabla_{\theta}(\theta_{t,i})$

▪ Make an update based on adaptive learning rate:

$$
\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{G_{t,ii} - \epsilon}} \cdot g_{t,i}
$$

- **•** Where each G_t is a diagonal matrix where entry i, i is the sum of squares of the gradients up to timestep t
	- Biggest issue with this method: sum of squares of gradients continues to grow over time

RMSProp

▪ Based on decaying running average of gradients:

$$
E[g^2]_t = 0.9 \cdot E[g^2]_{t-1} + 0.1 \cdot g_t^2
$$

▪ Adaptive learning rate based on running average instead of accumulated sum:

$$
\theta_{t+1,i} = \theta_{t,i} - \frac{\eta}{\sqrt{E[g^2]_{t,i} - \epsilon}} \cdot g_{t,i}
$$

Adaptive Moment Estimation (Adam)

▪ Combining momentum with adaptive learning rates

$$
m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t
$$

$$
v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2
$$

▪ Bias correction to prevent running averages from tending toward zero:

$$
\widehat{m_t} = \frac{m_t}{1 - \beta_1} \qquad \widehat{\nu_t} = \frac{\nu_t}{1 - \beta_2}
$$

▪ Then update parameters:

$$
\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\widehat{v_t}} + \epsilon} \widehat{m_t}
$$

Visualizations

Summary: Key Ideas in Optimization

▪ Gradient descent

- **Batch: update based on the whole dataset**
- SGD: update based on a single randomly chosen training example
- Minibatch: update based on *k* randomly chosen training examples
- Beyond gradient descent:
	- Second order optimization (e.g., Newton's method)
	- Momentum (Nesterov's accelerated gradient, Adam)
	- Adaptive learning rates (Adagrad, RMSProp, Adam, etc.)

Learn more: https://www.ruder.io/optimizing-gradient-descent/

Question Time!

Object Detection

ImageNet Error Rate 2010-2014

MS COCO Image Captioning Challenge

"man in black shirt is playing guitar."

"construction worker in orange safety vest is working on road."

"two young girls are playing with lego toy."

"boy is doing backflip on wakeboard."

"girl in pink dress is jumping in air."

"black and white dog jumps over bar."

"young girl in pink shirt is swinging on swing."

"man in blue wetsuit is surfing on wave."

Karpathy & Fei-Fei, 2015; Donahue et al., 2015; Xu et al, 2015; many more

Speech Recognition

Machine Translation

Google Neural Machine Translation (in production)

