Large-Scale Machine Learning (1)

CS246: Mining Massive Datasets
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New Topic: ML!

- **High dim. data**
  - Locality sensitive hashing
  - Clustering
  - Dimensionality reduction

- **Graph data**
  - PageRank, SimRank
  - Community Detection
  - Spam Detection

- **Infinite data**
  - Filtering data streams
  - Web advertising
  - Queries on streams

- **Machine learning**
  - Decision Trees
  - Neural Networks
  - Parallel SGD

- **Apps**
  - Recommender systems
  - Association Rules
  - Duplicate document detection
Supervised Learning

**Given some data:**

- “Learn” a function to map from the **input** to the **output**

**Given:**

Training examples \((x_i, y_i = f(x_i))\) for some unknown function \(f\)

**Find:**

A good approximation to \(f\)
Many Other ML Paradigms

- **Supervised:**
  - Given “labeled data” \( \{x, y\} \), learn \( f(x) = y \)

- **Unsupervised:**
  - Given only “unlabeled data” \( \{x\} \), learn \( f(x) \)

- **Semi-supervised:**
  - Given some labeled \( \{x, y\} \) and some unlabeled data \( \{x\} \), learn \( f(x) = y \)

- **Active learning:**
  - When we predict \( f(x) = y \), we then receive true \( y^* \)

- **Transfer learning:**
  - Learn \( f(x) \) so that it works well on new domain \( f(z) \)
Would like to do prediction: estimate a function $f(x)$ so that $y = f(x)$

Where $y$ can be:
- **Real number**: Regression
- **Categorical**: Classification
- **Complex object**:
  - Ranking of items, Parse tree, etc.

Data is labeled:
- Have many pairs $\{(x, y)\}$
  - $x$ ... vector of binary, categorical, real valued features
  - $y$ ... class, or a real number
**Supervised Learning**

- **Task:** Given data \((X, Y)\) build a model \(f()\) to predict \(Y’\) based on \(X’\)
- **Strategy:** Estimate \(y = f(x)\) on \((X, Y)\)
  
  Hope that the same \(f(x)\) also works to predict unknown \(Y’\)
  
  - The “hope” is called generalization
    - **Overfitting:** If \(f(x)\) predicts well \(Y\) but is unable to predict \(Y’\)
  
  - We want to build a model that generalizes well to unseen data
Brawn or Brains?

In 2001, Microsoft researchers ran a test to evaluate 4 of different approaches to ML-based language translation.

Findings:

- Size of the dataset used to train the model **mattered more** than the model itself.
- As the dataset grew large, performance difference between the models became small.

The Unreasonable Effectiveness of Data

- In 2017, Google revisited the same type of experiment with the latest Deep Learning models in computer vision.

Findings:

- Performance increases logarithmically based on volume of training data.
- Complexity of modern ML models (i.e., deep neural nets) allows for even further performance gains.

Large datasets + large ML models => amazing results!!

Decision Trees
Decision Tree Learning

- Given one attribute (e.g., lifespan), try to predict the value of new people’s lifespans by means of some of the other available attribute

- **Input attributes:**
  - $d$ features/attributes: $x^{(1)}, x^{(2)}, \ldots x^{(d)}$
  - Each $x^{(j)}$ has domain $O_j$
    - Categorical: $O_j = \{red, blue\}$
    - Numerical: $H_j = (0, 10)$
  - $Y$ is output variable with domain $O_Y$:
    - Categorical: Classification, Numerical: Regression

- **Data D:**
  - $n$ examples $(x_i, y_i)$ where $x_i$ is a $d$-dim feature vector, $y_i \in O_Y$ is output variable

- **Task:**
  - Given an input data vector $x$ predict output label $y$
A Decision Tree is a tree-structured plan of a set of attributes to test in order to predict the output.
Decision Trees

- **Decision trees:**
  - Split the data at each internal node
  - Each leaf node makes a prediction

- **Lecture today:**
  - Binary splits: $X^{(i)} < v$
  - Numerical attributes
  - Regression
How to make predictions?

- **Input**: Example $x_i$
- **Output**: Predicted $\hat{y}_i$

- “Drop” $x_i$ down the tree until it hits a leaf node
- Predict the value stored in the leaf that $x_i$ hits
Decision Trees: feature space

- Alternative view:
**How to construct a tree?**

- **Training dataset** $D^*$, $|D^*| = 100$ examples

![Tree Diagram]

- Number of examples traversing the edge

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9/26/19
Imagine we are currently at some node $G$
- Let $D_G$ be the data that reaches $G$

There is a decision we have to make: Do we continue building the tree?
- **If yes**, which variable and which value do we use for a **split**?
  - Continue building the tree recursively
- **If not**, how do we make a prediction?
  - We need to build a "**predictor node**"
3 steps in constructing a tree

Algorithm 1

Require: Node $n$, Data $D \subseteq D^*$

1: $(n \rightarrow \text{split}, D_L, D_R) = \text{FindBestSplit}(D)$  \hspace{1cm} (1)
2: if StoppingCriteria($D_L$) then
3:   $n \rightarrow \text{left\_prediction} = \text{FindPrediction}(D_L)$ \hspace{1cm} (2)
4: else
5: BuildSubtree $(n \rightarrow \text{left}, D_L)$
6: if StoppingCriteria($D_R$) then
7:   $n \rightarrow \text{right\_prediction} = \text{FindPrediction}(D_R)$ \hspace{1cm} (3)
8: else
9: BuildSubtree $(n \rightarrow \text{right}, D_R)$

- Requires at least a single pass over the data!
How to construct a tree?

(1) How to split? Pick attribute & value that optimizes some criterion

- **Regression: Purity**
  - Find split \((X^{(i)}, v)\) that creates \(D, D_L, D_R\): parent, left, right child datasets and maximizes:

\[
|D| \cdot \text{Var}(D) - (|D_L| \cdot \text{Var}(D_L) + |D_R| \cdot \text{Var}(D_R))
\]

- \(\text{Var}(D) = \frac{1}{n} \sum_{i \in D} (y_i - \bar{y})^2\) ... variance of \(y_i\) in \(D\)
(1) How to split? Pick attribute & value that optimizes some criterion

- **Classification:**
  - Information Gain
    - Measures how much a given attribute $X$ tells us about the class $Y$
    - $IG(Y \mid X)$: We must transmit $Y$ over a binary link. How many bits on average would it save us if both ends of the line knew $X$?
Entropy: What’s the smallest possible number of bits, on average, per symbol, needed to transmit a stream of symbols drawn from $X$’s distribution?

The entropy of $X$: $H(X) = -\sum_{j=1}^{m} p(X_j) \log p(X_j)$

- “High Entropy”: $X$ is from a uniform (boring) distribution
  - A histogram of the frequency distribution of values of $X$ is flat
- “Low Entropy”: $X$ is from a varied (peaks/valleys) distribution.
  - A histogram of the frequency distribution of values of $X$ would have many lows and one or two highs
Suppose I want to predict $Y$ and I have input $X$

- $X =$ College Major
- $Y =$ Likes “Casablanca”

From this data we estimate

- $P(Y = Yes) = 0.5$
- $P(X = Math \& Y = No) = 0.25$
- $P(X = Math) = 0.5$
- $P(Y = Yes \mid X = History) = 0$

Note:

- $H(Y) = -\frac{1}{2}\log_2(\frac{1}{2}) - \frac{1}{2}\log_2(\frac{1}{2}) = 1$
- $H(X) = 1.5$
Suppose I want to predict $Y$ and I have input $X$

- $X =$ College Major
- $Y =$ Likes “Casablanca”

**Def: Specific Conditional Entropy**

- $H(Y \mid X = v) =$ The entropy of $Y$ among only those records in which $X$ has value $v$

**Example:**

- $H(Y \mid X = Math) = 1$
- $H(Y \mid X = History) = 0$
- $H(Y \mid X = CS) = 0$
Suppose I want to predict $Y$ and I have input $X$

- $X$ = College Major
- $Y$ = Likes “Casablanca”

**Def: Conditional Entropy**

- $H(Y \mid X) = \text{The average specific conditional entropy of } Y$
- $= \text{if you choose a record at random what will be the conditional entropy of } Y$, conditioned on that row’s value of $X$
- $= \text{Expected number of bits to transmit } Y$ if both sides will know the value of $X$
- $= \sum_j P(X = v_j)H(Y \mid X = v_j)
Suppose I want to predict $Y$ and I have input $X$

- $H(Y \mid X) =$ The average specific conditional entropy of $Y$

$$= \sum_j P(X = v_j) H(Y \mid X = v_j)$$

Example:

<table>
<thead>
<tr>
<th>$v_j$</th>
<th>$P(X=v_j)$</th>
<th>$H(Y\mid X=v_j)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Math</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>History</td>
<td>0.25</td>
<td>0</td>
</tr>
<tr>
<td>CS</td>
<td>0.25</td>
<td>0</td>
</tr>
</tbody>
</table>

So: $H(Y\mid X)=0.5*1+0.25*0+0.25*0 = 0.5$
Why Information Gain?

- Suppose I want to predict $Y$ and I have input $X$

  - Def: Information Gain
    - $IG(Y|X) = I$ must transmit $Y$. How many bits on average would it save me if both ends of the line knew $X$?
    
    $$IG(Y|X) = H(Y) - H(Y | X)$$

- Example:
  - $H(Y) = 1$
  - $H(Y | X) = 0.5$
  - Thus $IG(Y|X) = 1 - 0.5 = 0.5$
Suppose you are trying to predict whether someone is going to live past 80 years. From historical data you might find:

- $IG(\text{LongLife} | \text{HairColor}) = 0.01$
- $IG(\text{LongLife} | \text{Smoker}) = 0.4$
- $IG(\text{LongLife} | \text{Gender}) = 0.25$
- $IG(\text{LongLife} | \text{LastDigitOfSSN}) = 0.00001$

$IG$ tells us how much information about $Y$ is contained in $X$. So attribute $X$ that has high $IG(Y|X)$ is a good split!
3 steps in constructing a tree

Algorithm 1: BuildSubtree

Require: Node \( n \), Data \( D \subseteq D^* \)

1. \((n \rightarrow \text{split}, D_L, D_R) = \text{FindBestSplit}(D)\) \hspace{1cm} (1)
2. if \( \text{StoppingCriteria}(D_L) \) then
3. \( n \rightarrow \text{left\_prediction} = \text{FindPrediction}(D_L)\) \hspace{1cm} (3)
4. else
5. \( (n \rightarrow \text{left}, D_L) \)
6. if \( \text{StoppingCriteria}(D_R) \) then
7. \( n \rightarrow \text{right\_prediction} = \text{FindPrediction}(D_R)\)
8. else
9. \( (n \rightarrow \text{right}, D_R) \)

BuildSubtree

BuildSubtree
(2) When to stop?

- Many different heuristic options
- Two ideas:
  - (1) When the leaf is “pure”
    - The target variable does not vary too much: $\text{Var}(y) < \varepsilon$
  - (2) When # of examples in the leaf is too small
    - For example, $|D| \leq 100$
(3) How to predict?

- Many options
  - Regression:
    - Predict average $y_i$ of the examples in the leaf
    - Build a linear regression model on the examples in the leaf
  - Classification:
    - Predict most common $y_i$ of the examples in the leaf
Building Decision Trees Using MapReduce
Problem: Building a tree

- Given a large dataset with hundreds of attributes
- **Build a decision tree!**

**General considerations:**
- **Tree is small** (can keep it memory):
  - Shallow (~10 levels)
- **Dataset too large to keep in memory**
- **Dataset too big to scan over on a single machine**
- **MapReduce to the rescue!**

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**Algorithm 1** `BuildSubTree`

Require: Node $n$, Data $D \subseteq D^*$

1. $(n \rightarrow \text{split}, D_L, D_R) = \text{FindBestSplit}(D)$
2. if StoppingCriteria($D_L$) then
3.     $n \rightarrow \text{left\_prediction} = \text{FindPrediction}(D_L)$
4. else
5.     **BuildSubTree**($n \rightarrow \text{left}, D_L$)
6. if StoppingCriteria($D_R$) then
7.     $n \rightarrow \text{right\_prediction} = \text{FindPrediction}(D_R)$
8. else
9.     **BuildSubTree**($n \rightarrow \text{right}, D_R$)
Parallel Learner for Assembling Numerous Ensemble Trees [Panda et al., VLDB ‘09]

- A sequence of MapReduce jobs that builds a decision tree
- Spark MLlib Decision Trees are based on PLANET

**Setting:**

- Hundreds of numerical (discrete & continuous, but not categorical) attributes
- Target variable is numerical: Regression
- Splits are binary: $X^{(i)} < v$
- Decision tree is small enough for each Mapper to keep it in memory
- Data too large to keep in memory
MapReduce: Given a set of split candidates compute their quality

Keeps track of the model and decides how to grow the tree
The tree will be built in levels
- One level at a time:

Steps:
- 1) Master decides candidate splits \((n, X^{(j)}, v)\)
- 2) MapReduce computes quality of those splits
- 3) Master then grows the tree for a level
- 4) Goto (1)
Hard part: Computing “quality” of a split
1) Master tells the Mappers which splits \((n, X^{(i)}, v)\) to consider
2) Each Mapper gets a subset of data and computes partial statistics for a given split
3) Reducers collect partial statistics and output the final quality for a given split \((n, X^{(i)}, v)\)
4) Master makes final decision where to split
We build the tree level by level

- One MapReduce step builds one level of the tree

Mapper

- Considers a number of candidate splits \((\text{node}, \text{attribute}, \text{value})\) on its subset of the data
- For each split it stores partial statistics
- Partial split-statistics is sent to Reducers

Reducer

- Collects all partial statistics and determines best split

Master grows the tree for one level
- **Mapper** loads the DT model and info about which attribute splits (split is a tuple <NodeID, Attribute, Value>) to consider
  - Each mapper sees a subset of the data D*
  - Mapper “drops”/classifies each datapoint d using the tree to find the leaf node L where d lands
  - For each leaf node L mapper keeps statistics about
    - (1) the data reaching L
    - (2) the data in left/right subtree under some split S
- **Reducer** aggregates the statistics (1), (2) and determines the best split for each tree node
PLANE: Components

- **Master**
  - Monitors everything (runs multiple MapReduce jobs)

- **Three types of MapReduce jobs:**
  - (1) **MapReduce Initialization** (run once first)
    - For each attribute identify values to be considered for splits
  - (2) **MapReduce FindBestSplit** (run multiple times)
    - MapReduce job to find best split (when there is too much data to fit in memory)
  - (3) **MapReduce InMemoryBuild** (run once last)
    - Similar to **BuildSubTree** (but for small data)
    - Grows an entire sub-tree once the data fits in memory

- **Model file**
  - A file describing the state of the model
PLANET: Components

(1) Master Node
(2) MapReduce Initialization (run once first)
(3) MapReduce FindBestSplit (run multiple times)
(4) MapReduce InMemoryBuild (run once last)
Master controls the entire process

Determines the state of the tree and grows it:

1. Decides if nodes should be split
2. If there is little data entering a tree node, Master runs an InMemoryBuild MapReduce job to grow the entire subtree below that node
3. For larger nodes, Master launches MapReduce FindBestSplit to evaluate candidates for best split
   - Master also collects results from FindBestSplit and chooses the best split for a node
4. Updates the model
PLANET: Components

1. Master Node
2. MapReduce **Initialization** (run once first)
3. MapReduce **FindBestSplit** (run multiple times)
4. MapReduce **InMemoryBuild** (run once last)
Initialization: Attribute metadata

- **Initialization job:** Identifies all the attribute values which need to be considered for splits
  - Initialization process generates “attribute metadata” to be loaded in memory by other tasks

- **Main question:** Which splits to even consider?

- **A split is defined by a triple:**
  - (node $n$, attribute $X^{(j)}$, value $v$)
Initialization: Attribute metadata

- **Which splits to even consider?**
  - For small data we can sort the values along a particular feature and consider every possible split
  - But data values may not be uniformly populated so many splits may not really make a difference

\[ X(j): 1.2 \, 1.3 \, 1.4 \, 1.6 \, 2.1 \, 7.2 \, 8.1 \, 9.8 \, 10.1 \, 10.2 \, 10.3 \, 10.4 \, 11.5 \, 11.7 \, 12.8 \, 12.9 \]

- **Idea:** Consider a limited number of splits such that splits “move” about the same amount of data
Splits for numerical attributes:

- For attribute $X^{(j)}$ we would like to consider every possible value $v \in O_j$
- Compute an approx. equi-depth histogram on $D^*$
  - Idea: Select buckets such that counts per bucket are equal

Use boundary points of histogram as splits
Goal: Equal number of elements per bucket (\(B\) buckets total)

- Construct by first **sorting** and then taking \(B-1\) equally-spaced splits

Faster construction:
- Sample & take equally-spaced splits in the sample
  - Nearly equal buckets
PLANET: Components

1. Master Node
2. MapReduce Initialization (run once first)
3. MapReduce FindBestSplit (run multiple times)
4. MapReduce InMemoryBuild (run once last)
Goal: For a particular split node \( n \) find attribute \( X^{(i)} \) and value \( v \) that maximize Purity:

\[
|D| \cdot \text{Var}(D) - (|D_L| \cdot \text{Var}(D_L) + |D_R| \cdot \text{Var}(D_R))
\]

- \( D \) ... training data \((x_i, y_i)\) reaching the node \( n \)
- \( D_L \) ... training data \( x_i \), where \( x_i^{(i)} < v \)
- \( D_R \) ... training data \( x_i \), where \( x_i^{(i)} \geq v \)

\[
\text{Var}(D) = \frac{1}{n} \sum_{i \in D} y_i^2 - \left( \frac{1}{n} \sum_{i \in D} y_i \right)^2
\]
To compute Purity we need

\[ \text{Var}(D) = \frac{1}{n} \sum_{i \in D} y_i^2 - \left( \frac{1}{n} \sum_{i \in D} y_i \right)^2 \]

Important observation: Variance can be computed from sufficient statistics: \( N, S=\Sigma y_i, Q=\Sigma y_i^2 \)

- Each Mapper \( m \) processes subset of data \( D_m \), and computes \( N_m, S_m, Q_m \) for its own \( D_m \)

Reducer combines the statistics and computes global variance and then Purity:

\[ \text{Var}(D) = \frac{1}{\sum_m N_m} \sum_m Q_m - \left( \frac{1}{\sum_m N_m} \sum_m S_m \right)^2 \]
FindBestSplit: Map

**Mapper:**

- Initialized by loading results of *Initialization task*
  - **Current model** (to find which node each datapoint $x_i$ ends up)
  - **Attribute metadata** (all split points for each attribute)
  - Load the set of *candidate splits*: \{(node, attribute, value)\}

- For each data record run the Map algorithm:
  - For each tree node store statistics of the data entering the node and at the end emit (to all reducers):
    - $<\text{NodeID}, \{ S=\Sigma y, Q=\Sigma y^2, N=\Sigma 1 \} >$
  - For each split store statistics and at the end emit:
    - $<\text{SplitID}, \{ S, Q, N \} >$
      - SplitID = (node id, attribute $X^{(j)}$, split value $v$)
Reducer:

1. Load all the `<NodeID, List {S_m, Q_m, N_m}>` pairs and aggregate the per node statistics.
2. For all the `<SplitID, List {S_m, Q_m, N_m}>` aggregate the statistics.

\[ Var(D) = \frac{1}{\sum_m N_m \sum_m Q_m} \sum_m Q_m - \left( \frac{1}{\sum_m N_m \sum_m S_m} \sum_m S_m \right)^2 \]

For each NodeID, output the best split found.
**Overall system architecture**

- **Master gives the mappers:**
  1. Tree
  2. Set of nodes
  3. Set of candidate splits

  ![Diagram](image)

  **Nodes:** F, G, H, I
  **Split candidates:** (G, $X^{(1)}, v^{(1)})$, (G, $X^{(2)}, v^{(2)})$, (H, $X^{(3)}, v^{(3)})$, (H, $X^{(4)}, v^{(4)})$

  Mappers output 2 types of key-value pairs:
  - (NodeID: S,Q,N)
  - (Split: S,Q,N)

  For every (NodeID, Split) Reducer(s) compute the Purity and output the best split.
Example: Need to split nodes F, G, H, I

Map and Reduce:

FindBestSplit::Map (each mapper)
- Load the current model M
- Drop every example \( x_i \) down the tree
- If it hits \( G \) or \( H \), update in-memory hash tables:
  - For each node: \( T_n: (\text{Node}) \rightarrow \{S, Q, N\} \)
  - For each \((\text{Split, Node})\): \( T_{n,j,s}: (\text{Node, Attribute, SplitValue}) \rightarrow \{S, Q, N\}\)
- Map::Finalize: output the key-value pairs from above hashtables

FindBestSplit::Reduce (each reducer)
- Collect:
  - \( T_1: <\text{Node, List}\{S, Q, N\}> \rightarrow <\text{Node, } \{\Sigma S, \Sigma Q, \Sigma N\}> \)
  - \( T_2: <(\text{Node, Attr., Val}), \text{List}\{S, Q, N\}> \rightarrow <(\text{Node, Attr., Val}), \{\Sigma S, \Sigma Q, \Sigma N\} > \)
- Compute Purity for each node using \( T_1, T_2 \)
- Return best split to Master (which then decides on globally best split)
Back to the Master

- Collects outputs from FindBestSplit reducers
  \(<\text{Split.NodeID, Attribute, Value, Purity}>\)

- For each node decides the best split
  - If data in \(D_L/D_R\) is small enough, later run a MapReduce job \textit{InMemoryBuild} on the node
  - Else run MapReduce \textit{FindBestSplit} job for both nodes
Decision Trees: Conclusion
Decision Trees

- **Characteristics**
  - Classification & Regression
    - Multiple (~10) classes
  - Real valued and categorical features
  - Few (hundreds) of features
  - Usually dense features
  - Complicated decision boundaries
    - Early stopping to avoid overfitting!

- **Example applications**
  - User profile classification
  - Landing page bounce prediction
Decision Trees

- Decision trees are the single most popular data mining tool:
  - Easy to understand
  - Easy to implement
  - Easy to use
  - Computationally cheap
  - It’s possible to mitigate overfitting (i.e., with ensemble methods)
  - They do classification as well as regression!
Learning Ensembles

- Learn multiple trees and combine their predictions
  - Gives better performance in practice
- **Bagging:**
  - Learns multiple trees over independent samples of the training data
    - For a dataset $D$ on $n$ data points: Create dataset $D'$ of $n$ points but sample from $D$ with replacement:
      - 33% points in $D'$ will be duplicates, 66% will be unique
  - Predictions from each tree are averaged to compute the final model prediction
Bagging Decision Trees
How to create random samples of D?

- Compute a hash of a training record’s id and tree id
- Use records that hash into a particular range to learn a tree
- This way the same sample is used for all nodes in a tree

**Note:** This is sampling D without replacement (but samples of D should be created with replacement)
Train a **Bagged Decision Tree**

But use a modified tree learning algorithm that selects (at each candidate split) a **random subset of the features**

- If we have \( d \) features, consider \( \sqrt{d} \) random features

**This is called: Feature bagging**

- **Benefit:** Breaks correlation between trees
  - If one feature is very strong predictor, then every tree will select it, causing trees to be correlated.

**Random Forests achieve state-of-the-art results in many classification problems!**