COMP 330 Notes

0.1 Short History of Data Science

- Science of extracting actionable knowledge from data sets
 - Data sets are often large and complex
 - Large too big to fit in the RAM of a server machine(128 256 GB)
 - Complex Non tabular data, often multi-modal
- Statistics foundation of Data Science
 - Emerges in the 1600s centered around economic and demographic data
 - Probability developed in the 17th century Pascal and Fermat Motivated by study of gambling
 - Cholera Example(1854 Broad Street Cholera Outbreak) Mapping cholera cases to find an outbreak source
 - Becomes more rigorous in late 1800s
 - * Ronald Risher null hypothesis, linear discriminator
 - * Pearson and Neyman "Type II" error, test power, confidence intervals
- Computer Science and Big Data
 - IBM IMS early systems, designed in 1966 for the Apollo program
 - Inventoried materials for Saturn V moon rocket and Apollo space vehicle
- Machine Learning
 - Subset of "AI" (Artificial Intelligence)
 - AI task of programming an "intelligent agent"
 - * Able to solve novel problems
 - * Emergent behavior
 - * Can do things not specifically programmed to do
 - * Goes back to Leibnez, Hobbes, Descartes'
 - * Leibniz "Calculus ratiocintor"
 - · 17th century
 - · Precursor to mathematical logic
 - · Imagines an inference engine able to reason
 - * Artificial Neural Networks
 - · First computational model proposed in 1943 inspired by brain
 - · McCulloch and Pitts ANs can perform logic
 - · Contemporary with ENIAC

- · Minsky builds SNARC(Stochastic Neural Analog Reinforcement Calculator)
- · Early ANNs: compute model not AI
- * AI: term invented by John McCarthy in 1956
- * Early quick success
 - · AI as search: goals, subgoals, backtracking
 - · Newell and Simon "General Problem Solver"
 - · Arthur Lee Samuel Samuel Checkers-playing Program
 - · Eliza: 1964 1966 MIT AI Lab mock therapist first serious attempt to pass "Turing Test" not close to passing
 - · Turing Test based on Turing's "Computing Machinery and Intelligence"
 - 1. Three "players": Interrogator, Computer, Human
 - 2. Interrogator passes written questions to both
 - 3. Tries to determine which one is human
- * Early Hype but ominous signs
 - · Automatic Language Processing Advisory Committee Critical of machine translation work
 - · Minsky and Papert "Perceptrons" seemed to kill off NN
 - · "AI: A General Survey" by Lighthill formed basis for decision by British government to end support for AI research in all but two universities
- * Decline of AI
 - · Speech Understanding Research program(DARPA)
 - 1. Harpy recognized more than 1000 words but had severe limitations
 - 2. Led to massive cutback in DARPA AI funding
 - · 1990 Death of Fifth-Generation project
 - 1. In the 80's, Japanese invested $\ 400\ \mathrm{million}(1990\ \mathrm{dollars})$ not much to show

- Rise of ML

- * AI traditionally relies on smart programmers
 - · May be able to "reason" and search for a better solution
 - · Could chain together rules but didn't really learn
- * Ends with advent of ML
 - · ML is an AI that learns from retrospective data or experience
 - · ML is often statistical in nature
- * Backpropogation Rumelhart, Hinton, Williams use BP to train a NN via gradient descent
 - · Forerunner of all modern "deep learning"
 - · Easier way to optimize weights of a NN
- * Reinforcement Learning(Q-learning) Watkins

- · Paradigm where ML learns via experience
- · Not pre-collected data
- * Association rule mining kicks off field of "data mining"
- * Random Forests Ensemble decision tree method
- * Support Vector Machines "Max margin" method, works well for large number features, little data
- * LSTM Type of NN which can remember state over sequential data
- NVIDIA and CUDA Architecture (2007)
 - * SGI graphics engineers move to NVIDIA in 1999
 - * Graphics pipeline added in NVIDIA GPUs
 - * CG programming language for GPUs, C for Graphics
 - * GPGPU
 - * cuDNN
- ImageNet classification of images, spurred vision research
- Word2Vec Word embedding, easy to use ML methods on text data
- GANS Generative Adversarial Networks can generate images, two neural networks:
 - * One to generate data
 - * One to recognize real from fake data
- Image Classification ML algorithms can out-perform human experts at important tasks finding tumors

1 Relational Databases 1

- Database collection of data, set of programs for managing that data
- In past, dominant data model was the network or navigational model data was a set of records with pointers between them
 - DB code written in COBOL
 - Code was written for specific storage model
 - Changing storage / indexing required modification
 - Led to little flexibility
- 1970 development of relational model
 - Data stored in relations
 - Relation is a table of tuples or records
 - Attributes of a tuple have no sub-structure (are atomic)
 - Querying done via "relational calculus" declarative language

- * Give a mathematical description of the tuples you want
- * System figures out how to get those for you
- * Data independence, code has no data access specs, can change physical org, no code re-writes
- Relation Schema all data stored in tables or relations relation scheme consists of:
 - Relation name
 - Set of attribute_name, attribute_type pairs each pair is referred to as an attribute or column
 - Usually denoted using NAME (attribute_name, attribute_type)
 - Defined as a set of sets
 - * If $T_1, T_2, ... T_n$ are the *n* attribute types, where each T_i is a set of possible values (for integers, $-2^{31}, 2^{31} 1$, for strings)
 - * A realization of the scheme(aka relation) is a subset of $T_1 \times T_2 \times ... \times T_n$ huge set of all possible combinations of all possible values of each of its attributes
 - A corresponding relation for LIKES (DRINKER string, BEER string) could be {("Luis", "Modelo"), ("Sinan", "PBR")} referred to as a table
 - * Entries in the relation are referred to as "rows", "tuples", or "records"
 - Entire table is an instance of the relation schema
- In the relational model, given $R(A_1, A_2, ...A_n)$, a set of attributes $K = \{K_1, ..., K_m\}$ is a key(subset of the attributes in a relation that uniquely identifies each row in the relation) if
 - For any valid realization R' of R
 - For all t_1, t_2 in R'...
 - If $t_1[K_1] = t_2[K_1]$ and $t_1[K_2] = t_2[K_2]$ and ... $t_1[K_m] = t_2[K_m]$
 - Then $t_1 = t_2$
- Relation scheme can have many keys
- Those that are minimal are candidate keys no subset of the attributes is a key
- One is designated as the primary key denoted with an underline
- Surrogate Key no real-world meaning, added to simplify primary key only job is to uniquely identify each student
- Connecting Relations need some notion between tuple references
 - DRINKER(DRINKER, FNAME, LNAME)
 - LIKES(DRINKER, BEER)
 - LIKES.DRINKER refers to DRINKER.DRINKER but not the other way around

- * One person can like multiple beers but cannot have multiple entires for the same person in the DRINKER table but can have in the LIKES table
- * Can have a drinker than does not like beer but cannot have a beer that is liked by a non-drinker someone can be in the drinker table and not in the likes table but a drinker cannot be in the likes table while not being in the drinker table
- Using Foreign Keys given relation schemas R_1, R_2 :
 - * Say a set of attributes K_1 from R_1 is a foreign key to a set of attributes K_2 from R_2 if
 - * K_2 is a candidate key for R_2 and
 - * For any valid realizations R'_1, R'_2 of $R_1, R_2...$
 - * For each $t_1 \in R_1'$ it MUST be the case that there exists $t_2 \in R_2'$ such that
 - * $t_1[K_{1,1}] = t_2[K_{2,1}]$ and $t_1[K_{1,2}] = t_2[K_{2,2}]$ and ... $t_1[K_{1,m}] = t_2[K_{2,m}]$
 - * Foreign key k_1 must be a set of attributes that uniquely identify a record in another table R_2
 - * The combination of attribute values present in every tuple of R_1 must also be present in R_2
- Cascading Deletes having elements in one foreign key of child table but not in parent table - would delete all entries of that element
- Failed Inserts database system does not allow merging if foreign key in child table has an element while the same key in parent table R does not occur

2 Relational Databases 2

- Relational Calculus is a variant on first-order logic
- "Give me all tuples t where P(t) holds
 - -P(t) is a predicate boolean function can use logical operations and quantification (first order logic)
 - Important Equivalence $\forall X(P(X))$ is equivalent to $\neg \exists (X)(\neg P(X))$

3 Relational Calculus and Algebra

Using syntax $\{t|P(t)\}$ Relational Calculus

- Start with {} and add the "such that" bar "|"
- Add what you are looking for to the left of the "|" description of the tuples you want back

- Provide predicate that evaluates to True over all variables that appear on the left if predicate is True, then tuple will be included
- Could treat as a pseudocode to find the relevant data

Relational Algebra - "abstract machine" of relational databases

- Algebra set(domain) with a number of operations this domain is closed under those operations
- In RA the domain is the set of all valid relations set of operations include $\pi, \sigma, \times, \bowtie$, $\cap, \cup, -$
- Projection removes attributes $\pi_A(R)$
 - -A is set of attributes of relation R
 - Removes all attributes not in A from R
 - Cardinality of output can differ from R can remove tuples if there are duplicates
 - Output is a relation
 - Like "select" in R
- Selection removes tuples $\sigma_B(R)$
 - B is a boolean predicate that can be applied to a single tuple from R
 - Simply removes all tuples not accepted by B
 - Output is a relation
 - Like "filter"
- Rename $\rho_{A/B}(R)$ renames attribute B to A in relation R output is a relation
 - $-\rho^{(A_1,A,2,\dots,A_n)}(R)$ renames relation R to S and renames all attributes as specified output is a relation
 - Like "Rename"
- Assignment $X \leftarrow \text{RA}$ statement
 - Assigns output of an RA statement, which is a relation, to a temporary relation
 for convenience
- Join: Cartesian Product combines tuples, join is cartesian product
 - $-R \times S$ returns $r \cdot s$ for all $r \in R, s \in S$
 - Like an inner join
 - Cardinality is $|r \times s|$
- Theta Join shorthand for $\sigma_B(R \times S)$ is $R \bowtie_B S$ interested in only some of the tuples generated by the cross product

- Natural Join want to join two relations
 - Using an equality check on all attributes having the same name
 - Then project away redundant attributes
 - Shorthand R * S
 - Like inner join

Set-Based Operations

- Types and numbers of input attributes must match
- Attribute names come from LHS
- $-R \cup S$ all tuples in R or in S
- $-R \cap S$ all tuples in R and in S
- -R-S all tuples in R and not in S

4 SQL 1

De-facto standard DB programming language - consists of

- Declarative DML
- Imperative DML
- DDL(data definition language) tells how you define schemas

In SQL:

- Duplicates are not automatically eliminated
- Not all SQL implementations(mySQL vs SQLserver etc.) are compatible
 - Support different set of operators
 - Date and time syntax
 - Comparison case sensitivity
- SQL extends RC / RA
 - Aggregate functions
 - Schema modifications

All RA have SQL equivalents:

- Projection SELECT
- Join FROM

- Selection WHERE
- Union UNION
- Intersection JOIN / EXISTS / IN
- Difference EXCEPT
- Rename AS technically optional, could just be "FREQUENTS f" instead of "FREQUENTS as f"
- Assignment INTO

Declarative Query Structure:

```
SELECT <attribute list>
FROM <tables>
WHERE <condition>(Optional)
```

- Should also include what relation the attribute comes from even if it does not matter(e.g. "f.Drinker")
- Since SQL does not clean up duplicates, need DISTINCT keyword
- Can cartesian join through the syntax "FREQ SERVES as S"

As Keyword:

- Rename from RA
- Works on tables as well as attributes
- Actual keyword "AS" is optional

Where Clause:

- \bullet < attribute >=< value >
- ullet < attribute > BETWEEN[value1]AND[value2]
- < attribute > IN([value1], [value2], ...)
- \bullet < attribute > LIKE'SST%' true if LHS is a string that starts with "SST"
- \bullet < $attribute > LIKE'SST_-'$ matches strings that start with "SST" and one character after
- < attribute > IS NULL and [attribute] IS NOT NULL
- Logical combinations with AND and OR

- Mathematical functions $\langle \rangle, ! =, \rangle, \langle, ...$
- Subqueries

Subqueries:

• Can have subquery in the WHERE clause - linked with keywords

• EXISTS

- EXISTS < subquery >
- If subquery returns at least one tuple, the clause evaluates to TRUE
- Also a NOT EXISTS subquery must return no tuples
- Like existential quantifer

IN

- < expression > IN < subquery > / < expression > NOTIN < subquery >
- Checks a value from a resultant table from a subquery is in that table

• ALL

- < expression > < boolOP > ALL < subquery >
- TRUE if every item in the subquery makes the boolOP evaluate to TRUE
- Like for all

• SOME

- < expression > < boolOP > SOME/ANY < subquery >
- TRUE if some item in the subquery can make the boolOP evaluate to TRUE
- As we iterate over tuples of outer query inner query is evaluated for each tuple
- Some can be evaluated just once if not reliant on other parts of the our query
- Some require the subquery to be evaluated for every value assignment in the outer query

Views:

- "Common" (non-materialized) views are just macros
 - Unexecuted query
 - Can be used in place of a table
 - Convenient way to simplify a query
 - Query is executed when view is used by another query
 - Its results are not stored

Style

- Declarative SQL codes tend to be very short
- Good because effort, bugs \propto code length
- Bad because sometimes difficult to understand
- Always alias tuple variables and indent carefully
- Only one major keyword per line
- Pick a capilization schema and religiously stick to it
- Make frequent use of views

5 SQL 2

Can compute simple statistics using SQL:

- SUM
- AVERAGE(AVG)
- MAX
- MIN

Can also compute aggregate at a finer level of granularity using GROUP BY

```
SELECT r.BEER, AVERAGE (r.RATING)
FROM RATES r
GROUP BY r.BEER
```

- First groups relation into subsets
- Every tuple in the subset has the same value for r.BEER
- Aggregate run over each subset independently
- Can only have the attribute being grouped by in SELECT outside of an aggregate function in an aggregate query
- For NULL:
 - COUNT(*) will count every row
 - COUNT(< attribute >) will count NON-NULL values
 - AVG, MIN, and MAX will ignore NULL
 - GROUP BY includes a row for NULL

- Subquery in FROM:
 - Can have a subquery in FROM clause
 - Treated as a temporary table
 - MUST be assigned an alias
- Can use TOP (n) to get top of a relation
 - Can optionally use PERCENT keyword
 - Can add WITH TIES
 - Can also choose ASC or DESC
 - ORDER BY can be used without TOP

6 SQL 3

- HAVING allows us to check for conditions on aggregate functions
- JOINS
 - TABLE t1 JOIN TABLE2 t2 ON pred
 - TABLE t1 INNER JOIN TABLE2 t2 ON pred
 - Exact Same, classic join
 - TABLE t1 NATURAL JOIN TABLE2 t2 no need for attributes since common attributes are found
- Can do CROSS JOINs which are cross product: TABLE t1 CROSS JOIN TABLE2 t2 is the same as TABLE1 t1, TABLE2 t2
- In FROM, can have joins of the form

TABLE t1 LEFT OUTER JOIN TABLE2 t2 ON pred TABLE t1 RIGHT OUTER JOIN TABLE2 t2 ON pred TABLE1 t1 FULL OUTER JOIN TABLE2 t2 ON pred

- Includes all tuples from the outer side
- Assigns NULLS if there is no matching tuple
- Pick one and stick with it
- Every attribute type can take the value NULL
 - NULL is a special value
 - Used to signal a missing value

- Nearly all non-comparison ops taking NULL as input return NULL ISNULL(exp)
- SQL uses 3-value logic:
 - Values are true, fale, and unknown
 - Truth tables generally make sense true and unknow give unknown, true or unknown gives true
 - Any comparison with NULL returns unknown for a where to accept the tuple, must get a true
- Data Manipulation Language(DML)
 - Data retrieval(SELECT)
 - Data insertion(INSERT)
 - Data deletion(DELETE)
 - Data modification (UPDATE)
- Data Definition Language(DDL)
 - Relation definition(CREATE TABLE)
 - Relation scheme update (ALTER TABLE)
 - Relation deletion(DROP TABLE)
 - Creating tables:

```
CREATE TABLE RATES {
DRINKER VARCHAR (30),
BEER VARCHAR (30),
SCORE INTEGER
}
```

- Can define a primary key using

```
PRIMARY KEY (DRINKER, BEER)
```

- No primary key allows for duplicates
- UNIQUE can accept NULL values can only be on primary key but multiple unique fields / combinations
- Foreign Keys:

```
ALTER TABLE RATES ADD CONSTRAINT FK
FOREIGN KEY (DRINKER, BEER)
REFERENCES LIKES (DRINKER, BEER)
```

- FK is used as a constraint to ensure that the FK values exist in the parent table
- Can manually add tuples using INTERSERT INTO relation VALUES (val1, val2, val3)

7 Imperative SQL 1

- Encapsulation make it easy for programmer
- Safety protect database from the programmer
- Performance fewer end-to-end trips
- Can respond to events, dynamic queries
- Common form of imperative code:
 - Procedure whose code is stored in the DB
 - Can be invoked from the command line, external program
 - Or from another stored procedure

```
CREATE PROCEDURE procName
/* list params */
AS BEGIN
/* code here */
END;
```

• Example: Write a stored procedure to get the peak count in a given region - return overall count if no region given

```
PEAK(NAME, ELEV, DIFF, MAP, REGION)
CREATE PROCEDURE getNumPeaks
/* list params */
@whichRegion VARCHAR (8000) = NULL
AS BEGIN
DECLARE @queryString VARCHAR(8000);
SET @queryString = 'SELECT COUNT(*) FROM PEAK' +
ISNULL(' WHERE region = ''' + @whichRegion + '''', '');
EXECUTE (@queryString);
END;
```

- All local vars need a DECLARE
- − @ used to declare variable names
- Susceptible to injection -

```
'Southern Sierra'; DROP TABLE PEAK; --
```

• Leads to the query

```
SELECT COUNT(*) FROM PEAK WHERE region = 'Southern Sierra';
DROP TABLE PEAK; --';
```

- "-" makes everything after a comment
- Then to call:

```
EXECUTE getNumPEAKS
@whichRegion = 'Corocoran to Whitney';

CREATE VIEW MyView as SELECT * FROM Employees
WHERE Department = 'Sales';
SELECT * FROM MyView;

vs.

CREATE VIEW myView AS SELECT * FROM Employees
WHERE Department = 'Sales';
GO
SELECT * FROM MyView;
```

• GO allows the SQL query to execute, without GO just compiles

```
CREATE PROCEDURE getNumPeaks
@whichRegion VARCHAR (8000),
@result INT OUTPUT

AS BEGIN

DECLARE myRes CURSOR FOR

SELECT COUNT(*) FROM peak WHERE region = @whichRegion;

OPEN myRes;

FETCH myRes INTO @result;

CLOSE myRes;

DEALLOCATE myRes;

END
```

- Now have a 'cursor'
 - Standard abstraction for dealing with record sets
 - Essentially an iterator
 - For CLOSE releases resources associated with a cursor
 - For DEALLOCATE removes output obtained from query, removes cursor's reference and frees all associated resources

• To call procedure:

```
DECLARE @myResult INT
EXECUTE getNumPeaks
@whichReqion = 'Kaweahs and West',
@result = @myResult output;
PRINT @myResult;
```

8 Imperative SQL 2

Writing a stored procedure giving the tallest height in a region

```
CREATE PROCEDURE getTallestPeak @whichRegion VARCHAR (8000), @result VARCHAR (8000) OUTPUT AS BEGIN ... END
```

Body 1: Declare control vars and cursor

```
DECLARE @peakName VARCHAR (8000);

DECLARE @bestName VARCHAR (8000);

DECLARE @peakHeight INT;

DECLARE @bestHeight INT;

SET @bestHeight = -1;

DECLARE myRes CURSOR FOR

SELECT name, elev FROM peak WHERE region = @whichRegion;
```

Body 2: Open cursor and loop to find the tallest peak

```
OPEN myRes;
FETCH NEXT FROM myRes INTO @peakName, @peakHeight;
WHILE (@@FETCH_STATUS = 0) BEGIN
IF @peakHeight > @bestHeight BEGIN
SET @bestHeight = @peakHeight;
SET @bestName = @peakName;
END
FETCH NEXT FROM myRes INTO @peakName, @peakHeight;
FND
```

FETCH

- 0 good
- -1 fail or beyond result set

- -2 fetched row missing
- -9 cursor not performing a fetch operation
- FETCH NEXT
- FETCH FIRST
- FETCH LAST
- FETCH ABSOLUTE n get nth record
- FETCH RELATIVE n go n records from here

```
Body 3: return the result
```

CLOSE myRes;

```
DEALLOCATE myRes;
SET @result = @bestName;
END;
To call:
    DECLARE @myResult VARCHAR (8000);
EXECUTE getTallestPeak
@whichRegion = 'Corocoran to Whitney',
@result = @myResult output;
PRINT @myResult;
```

- Shouldn't really write this
- TOP k would be shorter, easier, and faster
- use as much declarative code
- Only use loops, etc. when you have to
- Sometimes 3+ orders of magnitude speed difference

TSQL Functions

GO

```
CREATE FUNCTION foo (@myArg INTEGER)
RETURNS INTEGER AS BEGIN
...
RETURN (@someValue);
```

• Can be called from witin a SQL statement

Triggers - stored procedures that fire in response to some event(e.g. trigger catches updates to peak table, prints error message and does not process

```
CREATE TRIGGER checkHeight ON peak FOR UPDATE AS BEGIN \dots
```

- FOR / AFTER run only once triggering action succeeds FOR occurs before or during an update, after occurs after update
- INSTEAD OF don't run triggering action; run this instead
- Can have UPDATE, INSERT, DELETE

```
Body 1: Exit check and declarations
```

```
IF @@ROWCOUNT = O BEGIN
RETURN;
END
DECLARE myRes CURSOR FOR
SELECT d.name, d.elev, i.elev FROM inserted i, deleted d
WHERE i.name = d.name AND i.elev <> d.elev;
DECLARE @peakName VARCHAR (8000);
DECLARE @oldHeight INT;
DECLARE @newHeight INT;
```

- @@ROWCOUNT number of tuples affected
- deleted table containing old versions of records

• inserted - table containing new versions

Body 2: Loop through and reject updates

```
OPEN myRes;
FETCH NEXT FROM myRes INTO @peakName,
@oldHeight, @newHeight;
WHILE (@@FETCH_STATUS = 0) BEGIN
PRINT 'You changed the height of ' + @peakName +
' from ' + CAST (@oldHeight AS VARCHAR(100)) +
' to ' + CAST (@newHeight AS VARCHAR(100)) +
'. I am ignoring it.';
UPDATE peak SET elev = @oldHeight
WHERE name = OpeakName;
FETCH NEXT FROM myRes INTO
@peakName,
@oldHeight, @newHeight;
END
CLOSE myRes;
DEALLOCATE myRes;
No arrays, linked lists, etc. in TSQL - everything is a table
    DECLARE @myMap TABLE (
myKey INTEGER,
myValue VARCHAR (200),
PRIMARY KEY (myKey);
);
DECLARE @my2DArray TABLE (
xPos INTEGER,
yPos INTEGER,
value DOUBLE
PRIMARY KEY (xPos, yPos);
);
```

9 Connected Components & Page Rank

Connected Component:

- Subgraph where any two nodes are connected to each other by paths, not connected to other nodes in the supergraph
- Found using BFS

PageRank:

• Measure associated to graph nodes

- Shows relative importance of the nodes
- Higher PR value \implies more importance
 - A node is important when being pointed by lots of other nodes or by other important nodes
- PR models a random web surfer
- Random web surfer starts at a random page
- Randomly clicks on the out-going links to go other pages
- Can keep continue doing this(d probability) or jump to a random page(1-d)
- d is the Damping Factor
- PR value of a webpage is the probability that a random web surfer stops clicking when s/he lands on that webpage
- PR of node j = probability that random surfer lands on j
 - Can come from an in-coming link to node j
 - Can also have a random jump to node j
- PR formulation for node j for a graph n:

$$((1-d)\times 1/n)+(d\times \{PR\ value\ when\ surfer\ comes\ from\ an\ incoming\ link)$$

- Essentially a weighted average
- PR value when surfer comes from an incoming link
 - Assume each node has a PR value
 - Each link is assigned a weight by dividing PR into number of out-going links
 - PR value of a node when surfer comes from an incoming link is the sum of the weights of in-coming links
- Assuming n nodes, initialize PR of all nodes equal 1/n
- Iteratively calculate new PR values based on old values for all nodes

$$PR_{new}(node_j) = ((1-d)*1/n) + (d*\sum_{k \in \{nodes\ pointinglnode_j\}} \frac{PR_{old}(node_k)}{\#\ of\ outgoing\ links\ of\ node_k}$$

• Stop when PR values converge

$$\sum_{j} |PR_{new}(node_j) - PR_{old}(node_j)| \le \epsilon$$

- Sinks nodes with no out-going link
 - With current formulation, sum of all PR values is normalized to 1
 - If we have sinks in the graph, sum of PR values will be less than 1
 - Solution add links to all nodes from a sink including itself PR of sink will be evenly distributed to all nodes

10 Modeling

- Traditional statistical definition set of assumptions regarding the stochastic process that generated the data
- More modern a mathematical object that enables an analyst to use data to understand the past and present, and make predictions about the future
- Real data big, complex, difficult to understand
- Model is compact and simple more about simplification

Modeling Process

- Choosing the model
 - Select distribution family
 - Choosing hyperparameters external to model and not based on data

11 Gradient Descent

Optimization

- Adjusting model parameters to minimize or maximize an objective function
- Optimization at the heart of all learning frameworks
- Desired properties easily applied, scalable, fast

Gradient Descent

- Have some function $L(\theta_0, \theta_1)$, where we want $min_{\theta_0,\theta_1}L(\theta_0, \theta_1)$
- Start with some θ_0, θ_1
- Keep changing θ_0, θ_1 to reduce $L(\theta_0, \theta_1)$ until we hopefully end up at minimum

Algorithm

• Repeat until convergence:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} L(\theta_0, \theta_1), j = 0, j = 1$$

• Simultaneous update

$$temp0 := \theta_0 - \alpha \frac{\partial}{\partial \theta_0} L(\theta_0, \theta_1)$$
$$temp1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_0} L(\theta_1, \theta_1)$$
$$\theta_0 := temp0$$
$$\theta_1 := temp1$$

$$\Theta_1 \leftarrow \text{non-stupid guess for } \Theta^*$$

$$i \leftarrow 1$$

$$repeat\{$$

$$\Theta_{i+1} \leftarrow \Theta_i - \lambda \nabla L(\Theta_i);$$

$$i \leftarrow i+1;$$

$$\} while(||\Theta_i - \Theta_{i-1}||_1 > \epsilon)$$

Gradient Descent for Linear Regression

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

$$L(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_{\theta}(x^{(i)} - y^{(i)})$$

$$\frac{\partial}{\partial \theta_j} L(\theta_0, \theta_1) = 2 \cdot \frac{1}{2m} \sum_{1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot 1$$

$$\frac{\partial}{\partial \theta_0} L = \dots$$

$$\frac{\partial}{\partial \theta_1} L = 2 \cdot \frac{1}{2m} (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

$$\theta_0 := \theta_0 - \alpha \frac{1}{m} \sum_{1}^m (h_{\theta}(x^{(i)}) - y^{(i)})$$

$$\theta_1 := \theta_1 - \alpha \frac{1}{m} \sum_{1}^m (h_{\theta}(x^{(i)}) - y^{(i)}) \cdot x^{(i)}$$

11.1 Normal Equations

- \bullet Closed form solution to find regression coefficients $\theta = (X^TX)^{-1}X^Ty$
- Slower for larger n

• If X^TX is non-invertible - get redundant features or too many features

Choosing Learning Rate

- Line Search
- Bold Driver
 - Make large conservative guess for α
 - At each iteration, compute $L(\Theta i)$
 - If $L(\Theta i) < L(\Theta_{i-1})$
 - * Reaching minimum loss
 - * Incremenet α a little but
 - * Increase slowly so don't miss convergence
 - If $L(\Theta_i) \ge L(\Theta_{i-1})$
 - * Indicative of divergence
 - * Reduce α by a lot
 - * Don't update the parameters in that iteration
 - One evaluation of the loss function per iteration (less expensive than line search)
- "Batch" Gradient Descent each step of gradient descent uses all training examples
- Stochastic Gradient Descent at each step pick one random point, continue as if entire dataset was just one point
- Minibatch Gradient Descent pick small subset of data points, continue as if your entire dataset was just this subset

12 Intro to Big Data

• "Big" - too large to fit in RAM of an expensive server machine (5GB in 2002, 6 TB in 2025)

MapReduce

- Data processing paradigm
 - Leverages cluster of commodity machines
 - Distributed processing and fault tolerance
 - Requires distributed file system
 - Well-suited for calculations that can be computed independently
- To process a data set have two pieces of user-supplied code: Map function and reduce function

- Huge shared-nothing compute cluster
 - Using three data processing phases
 - A Map phase
 - A shuffle phase
 - Reduce phase
- Scalability and fault tolerance
- Functional model already existed consider map and reduce functions
 - Map, applies function onto a list
 - Reduce, recursively applies function of iterable until converges to single number

• Shared-Nothing

- Store/analyze data on large number of commodity machines
 - * Local, non-shared storage attached to each of them
 - * Only link is via a LAN
 - * Shared nothing refers to no sharing of RAM, storage NAS is common now, "pure" shared-nothing rarer

- Benefits

- * Inexpensive, built out of commodity components
- * Compute resources scales nearly linearly with money
- * Contrast to shared RAm machine with uniform memory access
- * Easier to program than shared memory systems

• The Map Phase

- Input data are stored in a huge file contains a simple list of pairs of type (key1, value1)
- Have a UDF of the form MAP(key1, value1) outputs a list of pairs of the form (key2, value2)
- In the Map phase of the MapReduce computation Map function is called for every record in the input, instances of Map run in parallel all over the cluster

• The Shuffle Phase

- Accepts all of the (key2, value2) pairs from the Map phase groups together
- After grouping all of pairs from all over the cluster having the same key2 value are merged into a single (key2, list(value2)) pair
- Called a "Shuffle" where a potential all-to-all transmission can happen, can be expensive, implemented using a hash function to map keys to nodes

- Reduce Phase
 - Apply user-supplied function of the form Reduce(key2, list(value2))
 - Outputs a list of value3 objects
 - In reduce phase of the MapReduce computation
 - * Reduce function is called for every key2 value output by the Shuffle
 - * Instances of Reduce run in parallel all over the compute cluster
 - * Output of all of those instances is collected
 - * Put in a huge output file
- Map reduce is a data processing paradigm requires with idea of distributed file system
 - Allows data to be stored / accessed across machines in a network
 - Abstracts away differences between local and remote data
 - Same API to read/write data no matter where data is located in the network
- Distributed File System MapReduce DFS sits on top of each machine's OS lives in "user space"
- On top of OS for heterogeneity and easily portable

13 Second-Order Methods

- Class of iterative optimization methods
 - Use not only first partial but second
 - Speeds convergence
 - More complex, quadratic in number of variables

13.1 Newton's Method

- Classic second order method for optimization
- Comes from Newton's method for finding zero of a function F()
- Recall that zeroes are roots / solutions
- Use approach to keep finding better approximations to the zeros of a function
 - Make an initial guess
 - Approximate $F(\theta)$ with a line tangent to F() at that guess
 - Update θ
 - $-\theta$ is the value of the model parameter

- Intuition:
 - Pick a value for theta
 - Evaluate F(theta)
 - Evaluate the derivative of the function at theta, F'(theta)
 - Revise theta based on these values
 - Repeat until convergence of theta
- Difference from Gradient Descent want to find zero of function, root finding not minimum finding
- Don't want zero in dats science max/min of loss function, so $F(\theta) \to L'(\theta)$

```
theta <- initial \\
while theta keeps changing do
theta <- theta - L'(theta) / L''(theta)</pre>
```

- Say we have multi-variate function $F: \mathbb{R}^d \to \mathbb{R}^d$, d is number of dimension
 - -ith output of F is given by the function F_i
 - So $F(\theta) = (F_1(\theta), F_2(\theta), ..., F_d(\theta))$
 - Want to find a zero of F, find $\theta = \langle \theta_1, \theta_2, ... \theta_d \rangle$ such that

$$F_1(\theta_1, \theta_2, ..., \theta_d) = 0$$

$$\vdots$$

$$F_d(\theta_1, \theta_2, ..., \theta_d) = 0$$

- To do this need to find the Jacobian of F $d \times d$ matrix of functions
- Rows cover the different parameters for a single dimension
- \bullet Columns cover the value of F for each dimension for a single parameter
- Can evaluate it at any set of parameter values, so $J_F(\theta)$ is a matrix of scalars
- For multi-variate optimization:

- Need to min/max at Θ such that

$$\begin{split} \frac{\partial L}{\partial \theta_1}(\Theta) &= 0 \\ \frac{\partial L}{\partial \theta_2}(\Theta) &= 0 \\ &\cdots \\ \frac{\partial L}{\partial \theta_d}(\Theta) &= 0 \end{split}$$

- Want Θ such that $\nabla L(\Theta) = <0,0,...,0>$
- Need to find Hessian each entry is 2nd derivative of loss function wrt to each parameter
- Each row is the Jacobian given a set of model parameters
- Pros and Cons of Newton's
 - Pros
 - * Convergence is quadratic error decreases quadratically
 - * Hundreds/ Thousands of iterations becomes tens
 - * No learning rate to set
 - * Doesn't require $F(\Theta)$ to be convex
 - Con
 - * More complicated than gradient descent
 - * Quadratic cost each iteration(linear gradient descent) Hessian is quadratic in the number of variables
 - * Cost is worse than quadratic, since matrix has to be inverted
 - * Second derivative has to exist
- Not used much in practice since in high dimensions, $d \times d$ is too big
- Usable for < 100K parameters, really hard at 1M
- Quasi-Newton methods are used instead
- Typically use just a portion or estimation of the Hessian matrix

14 Expectation Maximization

- Widely-used MLE algorithm for dealing with missing data
- Often impossible to drop(needing to be continuous and differentiable) missing data or unrealistic to replace with mean

- Formally, want to compute an MLE for $L(\theta|x_1, x_2, ..., z_1, z_2, ...)$
- x_1, x_2 are observed data, z_1, z_2 are missing
- $L(\theta|x_1, x_2, ..., z_1, z_2) = f(x_1, x_2, ...z_1, z_2, ...|\theta)$
- When z's are missing, choose θ to max

$$\int_{z_1, z_2, \dots} f(x_1, x_2, \dots, z_1, z_2, \dots | \theta) d(z_1, z_2, \dots)$$

- "Integrating out" a variable e.g. if we have height, weight pairs find probability that a pair is "tall" as $\sum_{weightw} Pr[(tall, w)]$
- Basic Idea:
 - Have an estimate Θ^{iter} for each iteration
 - Repeatedly update Θ^{iter} until convergence

$$Q(\Theta^{iter}, \Theta^{iter-1}) = E[log f(x_1, x_2, ..., z_1, z_2, ..., \Theta^{iter}) | x_1, x_2, ..., \Theta^{iter-1}]$$

- Treat $z_1, z_2...$ as random variables
- With distribution $f(z_1, z_2, ... | x_1, x_2, ... \Theta^{iter-1})$
- Q-function is expected value of LLH wrt this distribution
- Continuous version is

$$Q(\Theta^{iter}, \Theta^{iter-1}) = E[log f(x_1, x_2, ..., z_1, z_2, ... | \Theta^{iter}) | x_1, x_2, ..., \Theta^{iter-1}]$$

• If Q is discrete:

$$(\Theta^{iter}, \Theta^{iter-1}) = E \sum_{z_1, z_2, \dots} f(z_1, z_2, \dots | x_1, x_2, \dots \Theta^{iter-1}) log f(x_1, x_2, \dots, z_1, z_2, \dots | \Theta^{iter})$$

- EM Algorithm
 - Start with reasonable guess as to best Θ , call this Θ^0 , do not make parameters equivalent, will not converge
 - Choose Θ^{iter} to maximize the expected value of the log-likelihood
 - Computing $f(x_i|\Theta^{iter-1})$ requires pass over the data "E-step"
 - For Q function, let $c_{i,j} = f(z_i = j | x_i, \Theta^{iter-1})$
 - Write Q function as:

$$\sum_{z_1} \sum_{z_2} \sum_{z_3} ... (\prod_i c_{i,z_i}) log f(x_1, x_2, ..., z_1, z_2, ... | \Theta^{iter})$$

Need to maximize

15 Spark

Hadoop - "Pure" MapReduce Software

- Data reread from DFS for each MR job
- Bad for iterative data processing like gradient descent
- Can only do Map or MapReduce everything in terms of those operations
- New alternative softwares streaming and batch processing applications
- Generally oriented more towards in-memory computing more expressive APIs

Apache Spark

- Platform for efficient distributed data analytics runs on JVM
- Written in Scala bindings for Java, Scala, Python, R
- Doesn't do storage focus exclusively on compute
- RDDs Resilient Distributed Data Set(RDD) basic abstraction
 - Resilient fault tolerance
 - Distributed across machins in a cluster
 - Read-only
 - Data set buffered in RAM by Spark
 - Lazy computations done on demand
 - Ephemeral computations are discarded when not used
 - Lineage computation sequence to generate an RDD is saved

```
myRDD = sc.textFile(someFileName) #sc is Spark context
data = [1,2,3,4,5]
myRDD = sc.parallelize(data) or
myRDD = sc.parallelize(range(20000))
```

- Collect: returns the entire RDD - brings entire RDD to local environment - can lead to crashes

```
RDD.collect()
```

- Top: returns n entries based on implicit ordering

```
myRDD.top(3)
```

- Take: returns first n entries

myRDD.take(5)

- Computations series of transformations over RDDs
- Lambda nameless function that we can pass like a variable
 - Can "capture" its surroundings at creation
 - Can also accept parameters
 - Can return many items but must return something
- flatMap:

```
def countWord(fileName):
    textFile = sc.textFile(fileName)
    lines = textFile.flatMap(lambda line: line.split(" "))
```

- Process every data item in the RDD
- Apply lambda to it
- Lambda arguement to return zero or more results
- Each result added into resulting RDD
- map vs flatMap
 - Use map when want one-to-one transformation input and output have same size
 - use flatmap when you want a transformation that can generate zero or more elements from each input
- reduceByKey()

```
def countWords (fileName):
    textFile = sc.textFile (fileName)
    lines = textFile.flatMap (lambda line: line.split(" "))
    counts = lines.map (lambda word: (word, 1))
    aggCounts = counts.reduceByKey (lambda a, b: a + b)
```

- Data must be Key, Value pairs
- Shuffle so that all (K,V) pairs with same K on same machine
- Organize into $(K, (V_1, V_2, ..., V_n))$ pairs
- Use lambda to "reduce" the list to a single value
- top()

```
def countWords (fileName):
  textFile = sc.textFile (fileName)
  lines = textFile.flatMap (lambda line: line.split(" "))
  counts = lines.map (lambda word: (word, 1))
  aggCounts = counts.reduceByKey (lambda a, b: a + b)
  return aggCounts.top (200, key=lamda p: p[1])
```

- Data must be (Key, Value) pairs
- Takes two parameters, first is number to return
- Second(optional) lambda to use to obtain key for comparison
- top collects an RDD, moving from cloud to local so result is not an RDD
- Spark uses lazy evaluation if running

```
textFile = sc.textFile (fileName)
lines = textFile.flatMap (lambda line: line.split(" "))
counts = lines.map (lambda word: (word, 1))
aggCounts = counts.reduceByKey (lambda a, b: a + b)
```

- Nothing happens (other than spark remembering the ops) - does not execute until attempt made to collect an RDD
- By waiting until last second opportunities for "pipelining" exploited, only ops that require a shuffle can't be pipelined
- groupByKey()
 - Data must be (Key, Value) pairs
 - Shuffle so that all (K,V) pairs with same K on same machine
 - Organize into $(K, (V_1, V_2, ..., V_n))$ pairs
 - Store each list as a resultiterable for future processing
 - Like reduceByKey() but without reduce
- join()
 - Given two data sets rddOne, rddTwo join using

```
rddOne.join(rddTwo)
```

- Returns $(K, (V_1, V_2))$ pairs
- Constructed from all (K_1, V_1) from rddOne, (K_2, V_2) from rddTwo, where $K_1 = K_2$
- Can blow up RDD size if join is many-to-many, requires expensive shuffle

- reduce() not a transform from RDD to RDD
 - Repeatedly applies a lambda to each item in RDD to get single result
- aggregate()
 - Data must be in Key, Value pairs
 - Organized into $(K, (V_1, V_2, ..., V_n))$ pairs
 - Aggregate the list, like reduce()
 - Takes three args
 - * The "zero" to init the aggregation
 - * Lambda that takes X_1, X_2 and aggs them, where X_1 already aggregated, X_2 not
 - * Lambda that takes X_1, X_2 and aggs them, where both aggregated

16 Supervised Learning

Machine Learning Review:

- Objective: Predicting/classifying new data based on what we learn from existing data
- Requires training data to be representative of the data we want to predict/classift
- Data collection procedure is paramount
- Tasks:
 - Choosing the model family, complexity, hyperparameters
 - Learning the model "fit" the model by learning its parameters
 - Validating the model make sure model matches data
 - Applying the model use model to explain past/present and make predictions on future

Supervised Learning

- Given a bunch of (x_i, y_i) pairs
- Goal: learn how to predict value of y from x
- Called "supervised" because have examples of correct labeling
- Common Examples classification and regression
- Simplest model is a linear regression others like kNN, SVMs

Measuring Regression Performance

- View list of prediction errors $\epsilon_i = (f(t_i) x_i)$
- Can have many loss functions, corresponding to norms
- A norm is a function that maps a vector to a non-negative scalar
- Given a vector of errors ϵ_i, l_p norm defined as

$$\left(\sum_{i=1}^{n} |\epsilon_i|^p\right)^{\frac{1}{p}}$$

- l_0 sum of non-zero values
- l_1 mean absolute error
- l_2 mean squared error
- l_{∞} max absolute value

Measuring Classification Performance

- Accuracy easy to understand and compute but terrible with unbalanced classes
- Measured through a confusion matrix accuracy in terms of True Positive and True Negative, False Positive and False Negative
- False Positive Rate Number False Positive / Number False $\frac{FP}{N} = \frac{FP}{TN + FP}$
- False Negative Number False Negative / Number of True $\frac{FN}{P} = \frac{FN}{TP + FN}$
- Recall: $\frac{TP}{P} = \frac{TP}{TP + FN}$
- Precision $\frac{TP}{TP+FP}$
- Combined in F_1 score
 - $-F_1 = \frac{2 \times Precision \times Recall}{Precision + Recall}$
 - Ranges from 0-1 single number
 - Doesn't consider false positive/recall trade-off

ROC Plot

- Can modify recall by changing internal parameter in classifier
- Increase c fewer false positives, lower recall
- ROC "Receiver Operating Characteristic"
- Measures effect of increasing recall on False Positive rate plots TPR against FPR at each threshold c(ROC Plot)

 \bullet AUC-ROC curve converts plot to single number - usually between 0.5 - 1 - less than 0.5 means actively bad

Feature Engineering / Selection

- Focus in supervised learning on models
- Models are almost always less important than feature engineering
- How to vectorize features

17 GLM

Linear Regression is just a model with normal error

$$x_i, y_i \sim N(r \cdot x_i, \sigma^2)$$

 $Likelihood - \Pi_i N(y_i | r \cdot x_i, \sigma^2) = \Pi_i \sigma^{-1} (2\pi)^{-1/2} e^{-1/2(y_i - r \cdot x_i)^2 \sigma^{-2}}$

So for MLE, we try to maximize the same loss function as LR

$$-\sum_{i}(y_i-r\cdot x_i)^2$$

GLM is generalization of LR, allows error to be generated by wide variety of distribution. Any probability distribution can be writte nas

$$p(y|\theta) = b(y)exp(\theta T(y) - f(\theta))$$

Say we have prediction problem where

- Want to predict output y from an input vector x
- Natural to assume randomness or error on y is produced by some exponential family
- The ExpFam parameter θ is linearly related to x, assuming x vector-valued, θ is scalar valued

$$\theta = \sum_{j} x_j \times r_j$$

18 Overfitting

Detecting Over-Fitting

- Sniff Test
- Independent validation and test sets

• Prioritize simplest solutions

Bias-Variance Trade-Off

- Bias error from incorrect model assumptions
- Variance sensitivity of model to bad data
- Expected squared error of any prediction is

$$E[(Y - \hat{f}(x))^2]$$

- x is the data used for prediction
- \bullet Y produces the value we are trying to predict from x
- $\hat{f}(.)$ is the model we are learning

$$Var(Y) = E[Y^{2}] - E^{2}[Y]$$

$$Bias^{2}(\hat{f}(x)) = E^{2}[\hat{f}(x) - Y]$$

$$E[(Y - \hat{f}(x))^{2}] = Var(Y) + Var(\hat{f}(x)) + Bias^{2}(\hat{f}(x))$$

- Means error of supervised learner is a sum of
 - "Losseness" of relationship between x and Y, (Var(Y))
 - Sensitivity of the learner to variability of the training data $(Var(\hat{f}(x)))$
 - Inability of learner \hat{f} to learn relationship between X and Y, $Bias^2(\hat{f}(x))$

Regularization

- Give learning algorithm ability to choose complexity of model
- Simpler model lowers $Var(\hat{f}(X))$, raises inductive bias
- Complex Model raises $Var(\hat{f}(x))$, lowers inductive bias
- Balances trade-off between bias and variance to get lowest error
- Penalizes model for complexity
- Penality based on l_p norm

For logistic regression:

- p = 1 LASSO Regression
- p = 2 ridge regression

19 Outliers

Outliers - unexpected or unusual points - need some sort of reference as unusual data is not the same as an outlier

Distance-Based Outlier

- Point is an outlier if it is far from all other points
- Let $d(x_i)$ be the distance to points x_i 's kth NN in the data set
- Given data set $x_1, x_2, ...$ want to compute the set O such that
- |O| = m and $\forall (x_0 \in O, x_i \in X O), d(x_i) \leq d(x_0)$
- ullet Loop through all points, for all other points, check distance keep track of closest n neighbors
- The highest m points would then be considered outliers
- Choosing distance function use l_p norm
- Choosing m start small, gradually increase until nothing "interesting" is added
- Choose k determined using validation set, try \sqrt{N}

Model-Based Outlier

- Learn a model for what "typical" is
- Outlier is data point with low score according to the model

20 Deep Neural Networks

At highest level - nonlinear function represented usually as a graph

- Nodes neurons:
 - Little computational units
 - Computed function must be differentiable since learning is done via gradient descent
- Output of neuron is called an "activation"
- Neurons organized into layers
- Top layer is "output layer"
- Bottom layer is "input layer" activation of input neurons read directly from input features

- "Hidden Layers" between those two layers
- Each link between neurons has a "weight"

Function of Each Neuron

- Need neuron to compute some function f(v)
- Sigmoid function neuron goes from "off" to "on" smoothly so we can differentiate
- Classically two are used in NNs
 - Hypoerbolic Tangent tanh(v)
 - Logistic Function $(1 + e^{-v})^{-1}$
 - Modern Alternative is ReLU max(0, v)

21 RNNs

FNNs don't easily handle sequences

- Standard idea Use FF network with enough input units
- Pad unused tokens with special chars, set number of inputs to max sequence
- Problemated for predicting on longer sequences, last inputs are not trained very much

Elman Network

- Split hidden layer into tokens
- Tokens can be anything characters or words
- Usage of state layer after a hidden layer which feeds back into the hidden layer
- Have set of context nodes(state layer)
- Read value of hidden layer non-trainable where the value is simply remembered for one time tick

Jordan Network

- Similar to Elmann copies output values, not hidden values
- Must be producing an output at each time tick
- Can be used for sequence-to-sequence
- Easier learner but harder to remember long-term dependencies
- Not suitable for representartion learning

Training

- Classic algorithm is back-propagation
- View RNN as a compact representation of a complex graph
- Unroll the complex graph
- Use backpropagation on that weights are constrained to repeat

Vanishing Gradient

- Errors fall off exponentially as backpropped through layers
- Derivative of loss wrt activation function often much smaller than 1
- Repeatedly multiplying causes backpropped erros to end to zero
- Backprop does not affect weights in first few layers

Solutions

- Gated Neurons
- Special RNN designed to deal with vanishing gradient problem
- Use gates to control flow of information
- Move away from continuous S-shaped activation feature
- Simpler, piece-wise-linear activation functions