CS6220: DATA MINING TECHNIQUES

Sequence Data

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November 22, 2015

Announcement

TRACE faculty survey
myNEU->self service tab

- Homeworks
 - HW5 will be the last homework

• Midterm Exam

Methods to Learn

	Matrix Data	Text Data	Set Data	Sequence Data	Time Series	Graph & Network	Images
Classification	Decision Tree; Naïve Bayes; Logistic Regression SVM; kNN			нмм		Label Propagation*	Neural Network
Clustering	K-means; hierarchical clustering; DBSCAN; Mixture Models; kernel k-means*	PLSA				SCAN*; Spectral Clustering*	
Frequent Pattern Mining			Apriori; FP-growth	GSP; PrefixSpan			
Prediction	Linear Regression				Autoregression		
Similarity Search					DTW	P-PageRank	
Ranking						PageRank	



What is sequence data?

Sequential pattern mining

Hidden Markov Model

Summary

Sequence Database

 A sequence database consists of sequences of ordered elements or events, recorded with or without a concrete notion of time.

SID	sequence
10	<a(<u>abc)(a<u>c</u>)d(cf)></a(<u>
20	<(ad)c(bc)(ae)>
30	<(ef)(<u>ab</u>)(df) <u>c</u> b>
40	<eg(af)cbc></eg(af)cbc>

Sequence Data

• What is sequence data?



Hidden Markov Model

Summary

Sequence Databases & Sequential

Patterns

- Transaction databases vs. sequence databases
- Frequent patterns vs. (frequent) sequential patterns
- Applications of sequential pattern mining
 - Customer shopping sequences:
 - First buy computer, then CD-ROM, and then digital camera, within 3 months.
 - Medical treatments, natural disasters (e.g., earthquakes), science & eng. processes, stocks and markets, etc.
 - Telephone calling patterns, Weblog click streams
 - Program execution sequence data sets
 - DNA sequences and gene structures

What Is Sequential Pattern Mining?

 Given a set of sequences, find the complete set of *frequent* subsequences

A <u>sequence</u>: < (ef) (ab) (df) c b >

A <u>sequence database</u>

SID	sequence					
10	<a(<u>abc)(a<u>c</u>)d(cf)></a(<u>					
20	<(ad)c(bc)(ae)>					
30	<(ef)(<u>ab</u>)(df) <u>c</u> b>					
40	<eg(af)cbc></eg(af)cbc>					

An element may contain a set of items. Items within an element are unordered and we list them alphabetically.

<a(bc)dc> is a <u>subsequence</u> of <<u>a(abc)(ac)d(c</u>f)>

Given <u>support threshold</u> min_sup =2, <(ab)c> is a <u>sequential</u> <u>pattern</u>

Sequence

- Event / element
 - An non-empty set of items, e.g., e=(ab)
- Sequence
 - An ordered list of events, e.g., $s = \langle e_1 e_2 \dots e_l \rangle$
- Length of a sequence
 - The number of instances of items in a sequence
 - The length of \leq (ef) (ab) (df) c b > is 8 (Not 5!)

Subsequence

Subsequence

- For two sequences $\alpha = \langle a_1 a_2 \dots a_n \rangle$ and $\beta = \langle b_1 b_2 \dots b_m \rangle$, α is called a subsequence of β if there exists integers $1 \leq j_1 < j_2 < \dots < j_n \leq m$, such that $a_1 \subseteq b_{j_1}, \dots, a_n \subseteq b_{j_n}$
- Supersequence
 - If α is a subsequence of β , β is a supersequence of α

<a(bc)dc> is a <u>subsequence</u> of <<u>a(abc)(ac)d(c</u>f)>

Sequential Pattern

• Support of a sequence α

- Number of sequences in the database that are supersequence of α
- $Support_{S}(\alpha)$
- α is frequent if $Support_S(\alpha) \ge \min_support$
- A frequent sequence is called sequential pattern
 - l-pattern if the length of the sequence is l



A <u>sequence database</u>

SID	sequence
10	<a(<u>abc)(a<u>c</u>)d(cf)></a(<u>
20	<(ad)c(bc)(ae)>
30	<(ef)(<u>ab</u>)(df) <u>c</u> b>
40	<eg(af)cbc></eg(af)cbc>

Given <u>support threshold</u> min_sup =2, <(ab)c> is a <u>sequential</u> <u>pattern</u>

Challenges on Sequential Pattern Mining

- A huge number of possible sequential patterns are hidden in databases
- A mining algorithm should
 - find the complete set of patterns, when possible, satisfying the minimum support (frequency) threshold
 - be highly efficient, scalable, involving only a small number of database scans
 - be able to incorporate various kinds of userspecific constraints

Sequential Pattern Mining Algorithms

- Concept introduction and an initial Apriori-like algorithm
 - Agrawal & Srikant. Mining sequential patterns, ICDE'95
- Apriori-based method: GSP (Generalized Sequential Patterns: Srikant & Agrawal @ EDBT'96)
- Pattern-growth methods: FreeSpan & PrefixSpan (Han et al.@KDD'00; Pei, et al.@ICDE'01)
- Vertical format-based mining: SPADE (Zaki@Machine Leanining'00)
- Constraint-based sequential pattern mining (SPIRIT: Garofalakis, Rastogi, Shim@VLDB'99; Pei, Han, Wang @ CIKM'02)
- Mining closed sequential patterns: CloSpan (Yan, Han & Afshar @SDM'03)

The Apriori Property of Sequential Patterns

- A basic property: Apriori (Agrawal & Sirkant'94)
 - If a sequence S is not frequent
 - Then none of the super-sequences of S is frequent
 - E.g, <hb> is infrequent \rightarrow so do <hab> and <(ah)b>

Seq. ID	Sequence
10	<(bd)cb(ac)>
20	<(bf)(ce)b(fg)>
30	<(ah)(bf)abf>
40	<(be)(ce)d>
50	<a(bd)bcb(ade)></a(bd)bcb(ade)>

Given <u>support threshold</u> min_sup =2

GSP—Generalized Sequential Pattern Mining

- GSP (Generalized Sequential Pattern) mining algorithm
 - proposed by Agrawal and Srikant, EDBT'96
- Outline of the method
 - Initially, every item in DB is a candidate of length-1
 - for each level (i.e., sequences of length-k) do
 - scan database to collect support count for each candidate sequence
 - generate candidate length-(k+1) sequences from length-k frequent sequences using Apriori
 - repeat until no frequent sequence or no candidate can be found
- Major strength: Candidate pruning by Apriori

Finding Length-1 Sequential Patterns

- Examine GSP using an example
- Initial candidates: all singleton sequences

 Scan database once, count support for candidates

$IIIII_Sup - Z$						
Seq. ID	Sequence					
10	<(bd)cb(ac)>					
20	<(bf)(ce)b(fg)>					
30	<(ah)(bf)abf>					
40	<(be)(ce)d>					
50	<a(bd)bcb(ade)></a(bd)bcb(ade)>					



GSP: Generating Length-2 Candidates

51 length-2 Candidates

	<a>		<c></c>	<d></d>	<e></e>	<f></f>
<a>	<aa></aa>	<ab></ab>	<ac></ac>	<ad></ad>	<ae></ae>	<af></af>
	<ba></ba>	<bb></bb>	<bc></bc>	<bd></bd>	<be></be>	<bf></bf>
<c></c>	<ca></ca>	<cb></cb>	<cc></cc>	<cd></cd>	<ce></ce>	<cf></cf>
<d></d>	<da></da>	<db></db>	<dc></dc>	<dd></dd>	<de></de>	<df></df>
<e></e>	<ea></ea>	<eb></eb>	<ec></ec>	<ed></ed>	<ee></ee>	<ef></ef>
<f></f>	<fa></fa>	<fb></fb>	<fc></fc>	<fd></fd>	<fe></fe>	<ff></ff>

	<a>		<c></c>	<d></d>	<e></e>	<f></f>
<a>		<(ab)>	<(ac)>	<(ad)>	<(ae)>	<(af)>
			<(bc)>	<(bd)>	<(be)>	<(bf)>
<c></c>				<(cd)>	<(ce)>	<(cf)>
<d></d>					<(de)>	<(df)>
<e></e>						<(ef)>
<f></f>						

Without Apriori property, 8*8+8*7/2=92 candidates

Apriori prunes 44.57% candidates

How to Generate Candidates in General?

- From L_{k-1} to C_k
- Step 1: join
 - s_1 and s_2 can join, if dropping first item in s_1 is the same as dropping the last item in s_2
 - Examples:
 - <(12)3> join <(2)34> = <(12)34>
 - <(12)3> join <(2)(34)> = <(12)(34)>

Step 2: pruning

• Check whether all length k-1 subsequences of a candidate is contained in L_{k-1}

The GSP Mining Process



	Seq. ID	Sequence	
	10	<(bd)cb(ac)>	
	20	<(bf)(ce)b(fg)>	
$min_sup = 2$	30	<(ah)(bf)abf>	
	40	<(be)(ce)d>	
	50	<a(bd)bcb(ade)></a(bd)bcb(ade)>	

Candidate Generate-and-test: Drawbacks

- A huge set of candidate sequences generated.
 - Especially 2-item candidate sequence.
- Multiple Scans of database needed.
 - The length of each candidate grows by one at each database scan.
- Inefficient for mining long sequential patterns.
 - A long pattern grow up from short patterns
 - The number of short patterns is exponential to the length of mined patterns.

*The SPADE Algorithm

- SPADE (<u>Sequential PAttern Discovery using Equivalent Class</u>) developed by Zaki 2001
- A vertical format sequential pattern mining method
- A sequence database is mapped to a large set of
 - Item: <SID, EID>
- Sequential pattern mining is performed by
 - growing the subsequences (patterns) one item at a time by Apriori candidate generation

The SPADE Algorithm

SID	EID	Items
1	1	a
1	2	abc
1	3	ac
1	4	d
1	5	cf
2	1	ad
2	2	с
2	3	\mathbf{bc}
2	4	ae
3	1	ef
3	2	ab
3	3	df
3	4	с
3	5	b
4	1	е
4	2	g
4	3	af
4	4	С
4	5	b
4	6	с

2	a	k	b		
SID	EID	SID	EID	•••	
1	1	1	2		
1	2	2	3		
1	3	3	2		
2	1	3	5		
2	4	4	5		
3	2				
4	3				

Join two tables

	$\mathbf{a}\mathbf{b}$			ba		
SID	EID (a)	EID(b)	SID	EID (b)	EID(a)	
1	1	2	1	2	3	
2	1	3	2	3	4	
3	2	5				
4	3	5				
	i	aba		• • •		

aba				5 IF 150
SID	EID (a)	EID(b)	EID(a)	•••
1	1	2	3	
2	1	3	4	

Data Mining: Concepts and Techniques

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Bottlenecks of GSP and SPADE

- A huge set of candidates could be generated
 - 1,000 frequent length-1 sequences generate s huge number of length-2 candidates! $1000 \times 1000 + \frac{1000 \times 999}{2} = 1,499,500$
- Multiple scans of database in mining
- Breadth-first search
- Mining long sequential patterns
 - Needs an exponential number of short candidates
 - A length-100 sequential pattern needs 10³⁰

candidate sequences!

$$\sum_{i=1}^{100} \binom{100}{i} = 2^{100} - 1 \approx 10^{30}$$

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Prefix and Suffix (Projection)

Assume a pre-specified order on items, e.g., alphabetical order

- <a>, <aa>, <a(ab)> and <a(abc)> are <u>prefixes</u> of sequence <a(abc)(ac)d(cf)>
 - Note <a(ac)> is not a prefix of <a(abc)(ac)d(cf)>
- Given sequence <a(abc)(ac)d(cf)>

Prefix	Suffix (Prefix-Based Projection)
<a>	<(abc)(ac)d(cf)>
<aa></aa>	<(_bc)(ac)d(cf)>
<a(ab)></a(ab)>	<(_c)(ac)d(cf)>

Mining Sequential Patterns by Prefix Projections

- Step 1: find length-1 sequential patterns
 - <a>, , <c>, <d>, <e>, <f>
- Step 2: divide search space. The complete set of seq. pat. can be partitioned into 6 subsets:
 - The ones having prefix <a>;
 - The ones having prefix ;

• The ones having prefix <f>

SID	sequence
10	<a(abc)(ac)d(cf)></a(abc)(ac)d(cf)>
20	<(ad)c(bc)(ae)>
30	<(ef)(ab)(df)cb>
40	<eg(af)cbc></eg(af)cbc>

Finding Seq. Patterns with Prefix <a>

- Only need to consider projections w.r.t. <a>
 - <a>-projected database:
 - (abc)(ac)d(cf)>
 - <(_d)c(bc)(ae)>
 - <(_b)(df)cb>
 - <(_f)cbc>

SID	sequence
10	<a(abc)(ac)d(cf)></a(abc)(ac)d(cf)>
20	<(ad)c(bc)(ae)>
30	<(ef)(ab)(df)cb>
40	<eg(af)cbc></eg(af)cbc>

- Find all the length-2 seq. pat. Having prefix <a>: <aa>, <ab>,
 (ab)>, <ac>, <ad>, <af>
 - Further partition into 6 subsets
 - Having prefix <aa>;

 Having prefix <af> November 22, 2015

Why are those 6 subsets?

- By scanning the <a>-projected database once, its locally frequent items are identified as
 - *a* : 2, *b* : 4, _*b* : 2, *c* : 4, *d* : 2, and *f* : 2.
- Thus all the length-2 sequential patterns prefixed with <*a*> are found, and they are:
 - <aa>: 2, <ab>: 4, <(ab)>: 2, <ac>: 4, <ad>: 2,
 and <a f>: 2.

Completeness of PrefixSpan



Efficiency of PrefixSpan

- No candidate sequence needs to be generated
- Projected databases keep shrinking
- Major cost of PrefixSpan: Constructing projected databases

• Can be improved by pseudo-projections

Speed-up by Pseudo-projection

- Major cost of PrefixSpan: projection
 - Postfixes of sequences often appear repeatedly in recursive projected databases
- When (projected) database can be held in main memory, use pointers to form projections s=<a(abc)(ac)d(cf)>
 <a>

2)

- Pointer to the sequence s|<a>: (,
- Offset of the postfix

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Data Mining: Concepts and Techniques

sl<ab>:

<(abc)(ac)d(cf)>

Pseudo-Projection vs. Physical Projection

- Pseudo-projection avoids physically copying postfixes
 - Efficient in running time and space when database can be held in main memory
- However, it is not efficient when database cannot fit in main memory
 - Disk-based random accessing is very costly
- Suggested Approach:
 - Integration of physical and pseudo-projection
 - Swapping to pseudo-projection when the data set fits in memory

Performance on Data Set C10T8S8I8



Performance on Data Set Gazelle



runtime (in seconds)

No

Effect of Pseudo-Projection



Sequence Data

• What is sequence data?

- Sequential pattern mining
- Hidden Markov Model 🦊

Summary

A Markov Chain Model



- Markov property: Given the present state,
 future states are independent of the past
 states
- At each step the system may change its state from the current state to another state, or remain in the same state, according to a certain probability distribution
- The changes of state are called *transitions*, and the probabilities associated with various statechanges are called *transition probabilities*
- Transition probabilities
 - Pr(x_i=a | x_{i-1}=g)=0.16
 - Pr(x_i=c|x_{i-1}=g)=0.34
 - $Pr(x_i=g | x_{i-1}=g)=0.38$
 - Pr(x_i=t | x_{i-1}=g)=0.12

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Data Mining: Principles and Algorithms

38

Definition of Markov Chain Model

- A Markov chain model is defined by
 A Markov chain model is defined by
 - A set of states
 - Some states emit symbols
 - Other states (e.g., the begin state) are silent
 - A set of transitions with associated probabilities
 - The transitions emanating from a given state define

a distribution over the possible next states

Markov Chain Models: Properties

- Given some sequence x of length L, we can ask how probable the sequence is given our model
- For any probabilistic model of sequences, we can write this probability as

$$Pr(x) = Pr(x_L, x_{L-1}, ..., x_1)$$

= Pr(x_L | x_{L-1}, ..., x₁) Pr(x_{L-1} | x_{L-2}, ..., x₁)... Pr(x₁)

 key property of a (1st order) Markov chain: the probability of each x_i depends only on the value of x_{i-1}

$$Pr(x) = Pr(x_{L} | x_{L-1}) Pr(x_{L-1} | x_{L-2}) ... Pr(x_{2} | x_{1}) Pr(x_{1})$$
$$= Pr(x_{1}) \prod_{i=2}^{L} Pr(x_{i} | x_{i-1})$$

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The Probability of a Sequence for a Markov Chain Model



Pr(cggt)=Pr(c)Pr(g|c)Pr(g|g)Pr(t|g)

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*Example Application

CpG islands

- CG dinucleotides are rarer in eukaryotic genomes than expected given the marginal probabilities of C and G
- but the regions upstream of genes are richer in CG dinucleotides than elsewhere – CpG islands
- useful evidence for finding genes
- Application: Predict CpG islands with Markov chains
 - one to represent CpG islands
 - one to represent the rest of the genome

*Markov Chains for Discrimination

- Suppose we want to distinguish CpG islands from other sequence regions
- Given sequences from CpG islands, and sequences from other regions, we can construct
 - a model to represent CpG islands
 - a null model to represent the other regions
- can then score a test sequence by:

$$score(x) = \log \frac{\Pr(x \mid CpGModel)}{\Pr(x \mid nullModel)}$$

*Markov Chains for Discrimination

• Why use

$$score(x) = \log \frac{\Pr(x \mid CpGModel)}{\Pr(x \mid nullModel)}$$

According to Bayes' rule

$$Pr(CpG \mid x) = \frac{Pr(x \mid CpG) Pr(CpG)}{Pr(x)}$$
$$Pr(null \mid x) = \frac{Pr(x \mid null) Pr(null)}{Pr(x)}$$

 If we are not taking into account of prior probabilities of two classes, we just need to compare Pr(x|CpG) and Pr(x|null)

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*Higher Order Markov Chains

- The Markov property specifies that the probability of a state depends only on the probability of the previous state
- But we can build more "memory" into our states by using a higher order Markov model
- In an n-th order Markov model

$$\Pr(x_i \mid x_{i-1}, x_{i-2}, \dots, x_1) = \Pr(x_i \mid x_{i-1}, \dots, x_{i-n})$$

*Higher Order Markov Chains

- An n-th order Markov chain over some alphabet A is equivalent to a first order Markov chain over the alphabet of n-tuples: Aⁿ
- Example: A 2nd order Markov model for DNA can be treated as a 1st order Markov model over alphabet
 - AA, AC, AG, AT
 - CA, CC, CG, CT
 - GA, GC, GG, GT
 - TA, TC, TG, TT

*A Fifth Order Markov Chain



Pr(gctaca)=Pr(gctac)Pr(a|gctac)

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Hidden Markov Model

- A hidden Markov model (HMM): A statistical model in which the system being modeled is assumed to be a Markov process with unknown parameters
 - The state is not directly visible, but variables influenced by the state are visible
 - Each state has a probability distribution over the possible output tokens. Therefore the sequence of tokens generated by an HMM gives some information about the sequence of states.
- The challenge is to determine the hidden parameters from the observable data. The extracted model parameters can then be used to perform further analysis
- An HMM can be considered as the simplest dynamic Bayesian network

Learning and Prediction Tasks

Learning

- Given a model, a set of training sequences
- Find model parameters that explain the training sequences with relatively high probability (goal is to find a model that *generalizes* well to sequences we haven't seen before)

Classification

- Given a set of models representing different sequence classes, a test sequence
- Determine which model/class best explains the sequence

Segmentation

- Given a model representing different sequence classes, a test sequence
- Segment the sequence into subsequences, predicting the class of each subsequence

The Parameters of an HMM

Transition Probabilities

$$a_{kl} = \Pr(\pi_i = l \mid \pi_{i-1} = k)$$

Probability of transition from state k to state l

Emission Probabilities

$$e_k(b) = \Pr(x_i = b \mid \pi_i = k)$$

• Probability of emitting character b in state k

An HMM Example



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Three Important Questions

- How likely is a given sequence?
 - The Forward algorithm
- What is the most probable "path" for generating a given sequence?
 - The Viterbi algorithm
- How can we learn the HMM parameters given a set of sequences?

• The Forward-Backward (Baum-Welch) algorithm 11/22/2015 Data Mining: Principles and

Algorithms

How Likely is a Given Sequence?

 The probability that the path is taken and the sequence is generated:



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How Likely is a Given Sequence?

The probability over all paths is

$$\Pr(x_1...x_L) = \sum_{\pi} \Pr(x_1...x_L, \underbrace{\pi_0...\pi_N}_{\pi})$$

- But the number of paths can be exponential in the length of the sequence...
- The Forward algorithm enables us to compute this efficiently
 - Define *f_k(i)* to be the probability of being in state *k* having observed the first *i* characters of sequence x
 - To compute *Pr(x)*, the probability of being in the end state having observed all of sequence x
 - Can define this recursively
 - use dynamic programming

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The Forward Algorithm

- Initialization
 - f₀(0) = 1 for start state;
 - f_i(0) = 0 for other state
- Recursion
 - For emitting state (i = 1, ... L)

$$f_l(i) = e_l(x_i) \sum_k f_k(i-1)a_{kl}$$

Termination

$$Pr(x) = Pr(x_1...x_L) = \sum_k f_k(L)a_{kN}$$

N: ending state; denoted as 0 in textbook

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Forward Algorithm Example



Given the sequence x=TAGA

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Forward Algorithm Example

- Initialization
 - $f_0(0)=1$, $f_1(0)=0...f_5(0)=0$
- Computing other values
 - $f_1(1)=e_1(T) * (f_0(0)a_{01}+f_1(0)a_{11})$ =0.3* (1*0.5+0*0.2)=0.15



• $f_2(1)=e_2(T) * (f_0(0)a_{02}+f_2(0)a_{22})=0.4 * (1 * 0.5+0 * 0.8)$ • $f_1(2)=e_1(A) * (f_0(1)a_{01}+f_1(1)a_{11})$ = 0.4 * (0 * 0.5+0.15 * 0.2)

• $Pr(TAGA) = f_5(4) = f_3(4)a_{35} + f_4(4)a_{45}$

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Three Important Questions

- How likely is a given sequence?
- What is the most probable "path" for generating a given sequence?
- How can we learn the HMM parameters given a set of sequences?

Find the most probable "path" for generating a given sequence

- Decoding
 - $\pi^* = \operatorname{argmax}_{\pi} P(\pi | x)$
- Given a length L sequence, how many possible underlying paths?
 - | Q |^L
 - Where |Q| is the number of possible state

Finding the Most Probable Path: The Viterbi Algorithm

- Define v_k(i) to be the probability of the most probable path accounting for the first i characters of x and ending in state k
- We want to compute v_N(L), the probability of the most probable path accounting for all of the sequence and ending in the end state
- Can define recursively
- Can use DP to find v_N(L) efficiently

Initialization (i = 0): $v_0(0) = 1, v_k(0) = 0$ for k > 0(1)Recursion $(i = 1 \dots L)$: $v_l(i) = e_l(x_i) \max_k(v_k(i-1)a_{kl})$ (2) $ptr_i(l) = argmax_k(v_k(i-1)a_{kl})$ $P(x, \pi^*) = max_k(v_k(L) | a_{kN})$ Termination: (3)





Total number of paths: 4^6=4096; Number of candidate paths in Viterbi=4

Three Important Questions

- How likely is a given sequence?
- What is the most probable "path" for generating a given sequence?
- How can we learn the HMM parameters given a set of sequences?

Learning Without Hidden State

 Learning is simple if we know the correct path for each sequence in our training set



 estimate parameters by counting the number of times each parameter is used across the training set

Learning With Hidden State

 If we don't know the correct path for each sequence in our training set, consider all possible paths for the sequence



 Estimate parameters through a procedure that counts the expected number of times each parameter is used across the training set

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*Learning Parameters: The Baum-Welch Algorithm

- Also known as the Forward-Backward algorithm
- An Expectation Maximization (EM) algorithm
 - EM is a family of algorithms for learning probabilistic models in problems that involve hidden state
- In this context, the hidden state is the path that best explains each training sequence

*Learning Parameters: The Baum-Welch Algorithm

- Algorithm sketch:
 - initialize parameters of model
 - iterate until convergence
 - calculate the *expected* number of times each transition or emission is used
 - adjust the parameters to maximize the likelihood of these expected values

Computational Complexity of HMM Algorithms

- Given an HMM with S states and a sequence of length L, the complexity of the Forward, Backward and Viterbi algorithms is $O(S^2L)$
 - This assumes that the states are densely interconnected
- Given M sequences of length L, the complexity of Baum Welch on each iteration is $O(MS^2L)$



• What is sequence data?

Sequential pattern mining

Hidden Markov Model



Summary

- Sequential Pattern Mining
 GSP, SPADE, PrefixSpan
 - Hiddon Markov Modal
- Hidden Markov Model
 - Markov chain, HMM