# CS6220: DATA MINING TECHNIQUES 

## Sequence Data

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## Reminder

## - Homework 1

- 3 students need to talk to Moon during the break
- Rakesh Viswanathan, Xin Huang, and Laxmi Rambhatla
- Midterm
- Next Tuesday (Nov. 5), 2-hour (6-8pm) in class
- Closed-book exam, and one A4 size cheating sheet is allowed
- Bring a calculator (NO cell phone)
- Cover to today's lecture


## Sequence Data

-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 | $<a(\underline{a b c})(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |
| 20 | $<(\mathrm{ad}) \mathrm{c}(\mathrm{bc})(\mathrm{ae})>$ |
| 30 | $<(\mathrm{ef})(\mathrm{ab})(\mathrm{df}) \mathrm{cb}>$ |
| 40 | $<e g(\mathrm{af}) \mathrm{cbc}>$ |

## Sequence Data

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## 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 sequence database

$$
\text { A sequence: }<(\mathrm{ef})(\mathrm{ab}) \text { (df) cb }>
$$

| SID | sequence |
| :---: | :---: |
| 10 | $<a(\operatorname{abc})(a \underline{c}) d(\mathrm{cf})>$ |
| 20 | $<(\mathrm{ad}) c(\mathrm{bc})(\mathrm{ae})>$ |
| 30 | $<(\mathrm{ef})(\mathrm{ab})(\mathrm{df}) \mathrm{cb}>$ |
| 40 | $<e \mathrm{eg}(\mathrm{af}) \mathrm{cbc}>$ | An element may contain a set of items. Items within an element are unordered and we list them alphabetically.,

<a(bc)dc> is a subsequence of <ag(abc)(ac)d(cf)>

Given support threshold min_sup $=2,<(a b) c>$ is a sequential pattern

## Sequence

- Event / element
- An non-empty set of items, e.g., e=(ab)
- Sequence
- An ordered list of events, e.g., $s=<e_{1} e_{2} \ldots e_{l}>$
- Length of a sequence
- The number of instances of items in a sequence - The length of < (ef) (ab) (df) c b > is 8 (Not 5!)


## Subsequence

## - Subsequence

- For two sequences $\alpha=<a_{1} a_{2} \ldots a_{n}>$ and $\beta=<b_{1} b_{2} \ldots b_{m}>, \alpha$ is called a subsequence of $\beta$ if there exists integers $1 \leq j_{1}<j_{2}<\cdots<$ $j_{n} \leq m$, such that $a_{1} \subseteq b_{j_{1}}, \ldots, a_{n} \subseteq b_{j_{n}}$
- Supersequence
- If $\alpha$ is a subsequence of $\beta, \beta$ is a supersequence of $\alpha$

$$
\begin{aligned}
& \text { <a(bc)dc> is a subsequence of } \\
& \text { <a(abc)(ac)d(cf)>> }
\end{aligned}
$$

## Sequential Pattern

- Support of a sequence $\alpha$
- Number of sequences in the database that are supersequence of $\alpha$
- Support $_{S}(\alpha)$
- $\alpha$ is frequent if $\operatorname{Suppor}_{S}(\alpha) \geq$ min_support
- A frequent sequence is called sequential pattern
$\cdot 1$-pattern if the length of the sequence is 1


## EM?

## A sequence database

| SID | sequence |
| :---: | :---: |
| 10 | $<a(\underline{a b c})(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |
| 20 | $<(\mathrm{ad}) \mathrm{c}(\mathrm{bc})(\mathrm{ae})>$ |
| 30 | $<(\mathrm{ef})(\mathrm{ab})(\mathrm{df}) \mathrm{cb}>$ |
| 40 | $<\mathrm{eg}(\mathrm{af}) \mathrm{cbc}>$ |

Given support threshold min_sup $=2,<(\mathrm{ab}) \mathrm{c}>$ is a sequential pattern

## 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 $<(a h) b>$

| Seq. ID | Sequence |
| :---: | :---: |
| Given support threshold |  |
|  | $<(\mathrm{bd}) \mathrm{cb}(\mathrm{ac})>$ |
| 20 | $<(\mathrm{bf})(\mathrm{ce}) \mathrm{b}(\mathrm{fg})>$ |
| 30 | $<(\mathrm{ah})(\mathrm{bf}) \mathrm{abf}>$ |
| 40 |  |
| 40 | $<(\mathrm{be})(\mathrm{ce}) \mathrm{d}>$ |
| 50 | $<\mathrm{a}(\mathrm{bd}) \mathrm{bcb}=2$ |

## 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
$-\quad\langle\mathrm{d}\rangle,\langle\mathrm{b}\rangle,\langle\mathrm{c}\rangle,\langle\mathrm{d}\rangle,\langle\mathrm{e}\rangle,\langle\mathrm{f}\rangle,\langle\mathrm{g}\rangle$,

$\langle\mathrm{h}\rangle$

- Scan database once, count support for candidates
min_sup $=2$

| Seq. ID | Sequence |
| :---: | :---: |
| 10 | $<(\mathrm{bd}) \mathrm{cb}(\mathrm{ac})>$ |
| 20 | $<(\mathrm{bf})(\mathrm{ce}) \mathrm{b}(\mathrm{fg})>$ |
| 30 | $<(\mathrm{ah})(\mathrm{bf}) \mathrm{abf}>$ |
| 40 | <(be)(ce)d> |
| 50 | <a(bd)bcb(ade)> |


| Cand | Sup |
| :---: | :---: |
| $\langle\mathrm{a}\rangle$ | 3 |
| $\langle\mathrm{~b}\rangle$ | 5 |
| $\langle\mathrm{c}\rangle$ | 4 |
| $\langle\mathrm{~d}\rangle$ | 3 |
| $\langle\mathrm{e}\rangle$ | 3 |
| $\langle\mathrm{f}\rangle$ | 2 |
| $\langle\mathrm{~g}\rangle$ | 1 |
| $\langle\mathrm{~h}\rangle$ | 1 |

## GSP: Generating Length-2 Candidates

## 51 length-2 Candidates

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


|  | $<\mathrm{a}>$ | $<\mathrm{b}>$ | $<\mathrm{c}>$ | $<\mathrm{d}>$ | $<\mathrm{e}>$ | $<\mathrm{f}>$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| <a> |  | $<(\mathrm{ab})>$ | $<(\mathrm{ac})>$ | $<(\mathrm{ad})>$ | $<(\mathrm{ae})>$ | $<(\mathrm{af})>$ |
| <b> |  |  | $<(\mathrm{bc})>$ | $<(\mathrm{bd})>$ | $<(\mathrm{be})>$ | $<(\mathrm{bf})>$ |
| <c> |  |  |  | $<(\mathrm{cd})>$ | $<(\mathrm{ce})>$ | $<(\mathrm{cf})>$ |
| <d> |  |  |  |  | $<(\mathrm{de})>$ | $<(\mathrm{df})>$ |
| <e> |  |  |  |  |  | $<(\mathrm{ef})>$ |
| <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 $\mathrm{k}-1$ subsequences of a candidate is contained in $L_{k-1}$


## The GSP Mining Process

$5^{\text {th }}$ scan: 1 cand. 1 length- 5 seq. pat.
$4^{\text {th }}$ scan: 8 cand. 7 length- 4 seq. pat. $3^{\text {rd }}$ scan: 46 cand. 20 length-3 seq pat. 20 cand. not in DB at all $2^{\text {nd }}$ scan: 51 cand. 19 length-2 seq. pat. 10 cand. not in DB at all $1^{\text {st }}$ scan: 8 cand. 6 length- 1 seq. pat.


| min_sup $=2$ | 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)> |

## 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 (S_ 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 | c |
| 2 | 3 | bc |
| 2 | 4 | ae |
| 3 | 1 | ef |
| 3 | 2 | ab |
| 3 | 3 | df |
| 3 | 4 | c |
| 3 | 5 | b |
| 4 | 1 | e |
| 4 | 2 | g |
| 4 | 3 | af |
| 4 | 4 | c |
| 4 | 5 | b |
| 4 | 6 | c |


| a |  | b |  | $\cdots$ |
| :---: | :---: | :---: | :---: | :---: |
| SID | EID | SID | EID | $\cdots$ |
| 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

| ab |  |  |  | ba |  |  |  | $\cdots$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| SID | EID (a) | EID(b) | SID | EID (b) | EID(a) | $\cdots$ |  |  |
| 1 | 1 | 2 | 1 | 2 | 3 |  |  |  |
| 2 | 1 | 3 | 2 | 3 | 4 |  |  |  |
| 3 | 2 | 5 |  |  |  |  |  |  |
| 4 | 3 | 5 |  |  |  |  |  |  |


| aba |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| SID | EID (a) | EID(b) | EID(a) | $\cdots$ |
| 1 | 1 | 2 | 3 |  |
| 2 | 1 | 3 | 4 |  |

## 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 $10^{30}$ candidate sequences!

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

## Prefix and Suffix (Projection)

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

- <a>, <aa>, <a(ab)> and <a(abc)> are prefixes of sequence <a(abc)(ac)d(cf)>
- Note $\langle\mathrm{a}(\mathrm{ac})>$ is not a prefix of $\langle\mathrm{a}(\mathrm{abc})(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$
- Given sequence <a(abc)(ac)d(cf)>

| Prefix | Suffix (Prefix-Based Projection) |
| :---: | :---: |
| $<\mathrm{a}>$ | $<(\mathrm{abc})(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |
| $<\mathrm{aa}>$ | $<\left(\_\mathrm{bc}\right)(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |
| $<\mathrm{a}(\mathrm{ab})>$ | $<\left(\_\mathrm{c}\right)(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |

## Mining Sequential Patterns by Prefix Projections

- Step 1: find length-1 sequential patterns
$\cdot\langle\mathrm{a}\rangle,\langle\mathrm{b}\rangle,\langle\mathrm{c}\rangle,\langle\mathrm{d}\rangle,\langle\mathrm{e}\rangle,\langle\mathrm{f}\rangle$
- 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 <b>;
- The ones having prefix $<\mathfrak{f}>$

| SID | sequence |
| :---: | :---: |
| 10 | $<a(\mathrm{abc})(\mathrm{ac}) \mathrm{d}(\mathrm{cf})>$ |
| 20 | $<(\mathrm{ad}) \mathrm{c}(\mathrm{bc})(\mathrm{ae})>$ |
| 30 | $<(\mathrm{ef})(\mathrm{ab})(\mathrm{df}) \mathrm{cb}>$ |
| 40 | $<e g(\mathrm{af}) \mathrm{cbc}>$ |

## Finding Seq. Patterns with Prefix <a>

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

| SID | sequence |
| :---: | :---: |
| 10 | $<a(a b c)(a c) d(c f)>$ |
| 20 | $<(a d) c(b c)(a e)>$ |
| 30 | $<(e f)(a b)(d f) c b>$ |
| 40 | $<e g(a f) c b c>$ |

- 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>


## Why are those 6 subsets?

- By scanning the <a>-projected database once, its locally frequent items are identified as
$\cdot a: 2, b: 4, \_b: 2, c: 4, d: 2$, and $f: 2$.
-Thus all the length-2 sequential patterns prefixed with $\langle a\rangle$ are found, and they are:

```
-〈aa> : 2, <ab> : 4, <(ab)> : 2, <ac> :4,<ad> : 2,
and <af> : 2.
```


## Completeness of PrefixSpan

SDB

| SID | sequence |
| :---: | :---: |
| 10 | $<a(a b c)(a c) d(c f)>$ |
| 20 | $<(a d) c(b c)(a e)>$ |
| 30 | $<(e f)(a b)(d f) c b>$ |
| 40 | $<e g(a f) c b c>$ |

Length-1 sequential patterns <a>, <b>, <c>, <d>, <e>, <f>

Having prefix <a>
<a>-projected database <(abc)(ac)d(cf)>
<(_d)c(bc)(ae)>
<(_b)(df)cb>
<(_f)cbc> Having prefix <b>

Having prefix <c>, ..., <f>
Length -2 sequential $\begin{aligned} & \text { <b>-projected database } \\ & \text { patterns } \\ & <\text { aa> }>,<a b>,<(a b)>, \\ & \text { <ac>, }<a d>,<a f>\end{aligned}$

Having prefix <aa> Having prefix <af>
<aa>-proj. db
<af>-proj. db

## 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 $\quad s=<a(a b c)(a c) d(c f)>$
- Pointer to the sequence

$$
\mathrm{s} \mid<a>:(, 2)<(a b c)(a c) d(c f)>
$$

- Offset of the postfix


## 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 C10T8S818



Support threshold (in \%)

## Performance on Data Set Gazelle



## 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
- $\operatorname{Pr}\left(\mathrm{x}_{\mathrm{i}}=\mathrm{a} \mid \mathrm{x}_{\mathrm{i}-1}=\mathrm{g}\right)=0.16$
- $\operatorname{Pr}\left(\mathrm{x}_{\mathrm{i}}=\mathrm{c} \mid \mathrm{x}_{\mathrm{i}-1}=\mathrm{g}\right)=0.34$
- $\operatorname{Pr}\left(\mathrm{x}_{\mathrm{i}}=\mathrm{g} \mid \mathrm{x}_{\mathrm{i}-1}=\mathrm{g}\right)=0.38$
- $\operatorname{Pr}\left(\mathrm{x}_{\mathrm{i}}=\mathrm{t} \mid \mathrm{x}_{\mathrm{i}-1}=\mathrm{g}\right)=0.12$
$\sum \operatorname{Pr}\left(x_{i} \mid x_{i-1}=g\right)=1$
Data Mining: Principles and
Algorithms


## Definition of Markov Chain Model

- 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

$$
\begin{aligned}
& \operatorname{Pr}(x)=\operatorname{Pr}\left(x_{L}, x_{L-1}, \ldots, x_{1}\right) \\
& =\operatorname{Pr}\left(x_{L} \mid x_{L-1}, \ldots, x_{1}\right) \operatorname{Pr}\left(x_{L-1} \mid x_{L-2}, \ldots, x_{1}\right) \ldots \operatorname{Pr}\left(x_{1}\right)
\end{aligned}
$$

- key property of a (1st order) Markov chain: the probability of each $\mathrm{x}_{\mathrm{i}}$ depends only on the value of $\mathrm{x}_{\mathrm{i}-1}$

$$
\begin{aligned}
& \operatorname{Pr}(x)=\operatorname{Pr}\left(x_{L} \mid x_{L-1}\right) \operatorname{Pr}\left(x_{L-1} \mid x_{L-2}\right) \ldots \operatorname{Pr}\left(x_{2} \mid x_{1}\right) \operatorname{Pr}\left(x_{1}\right) \\
& =\operatorname{Pr}\left(x_{1}\right) \prod_{i=2}^{L} \operatorname{Pr}\left(x_{i} \mid x_{i-1}\right)
\end{aligned}
$$

## The Probability of a Sequence for a Markov Chain Model



## 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:

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

## Markov Chains for Discrimination

- Why use

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

- According to Bayes' rule

$$
\begin{aligned}
\operatorname{Pr}(C p G \mid x) & =\frac{\operatorname{Pr}(x \mid C p G) \operatorname{Pr}(C p G)}{\operatorname{Pr}(x)} \\
\operatorname{Pr}(\text { null } \mid x) & =\frac{\operatorname{Pr}(x \mid \text { null }) \operatorname{Pr}(\text { null })}{\operatorname{Pr}(x)}
\end{aligned}
$$

- If we are not taking into account of prior probabilities of two classes, we just need to compare $\operatorname{Pr}(x \mid C p G)$ and $\operatorname{Pr}(x \mid$ null $)$


## 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

$$
\operatorname{Pr}\left(x_{i} \mid x_{i-1}, x_{i-2}, \ldots, x_{1}\right)=\operatorname{Pr}\left(x_{i} \mid x_{i-1}, \ldots, x_{i-n}\right)
$$

## 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: $\mathrm{A}^{\mathrm{n}}$
- 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



$$
\begin{gathered}
\text { TTTTT } \\
\operatorname{Pr}(g c+a c a)=\operatorname{Pr}(g c+a c) \operatorname{Pr}(a \mid g c t a c)
\end{gathered}
$$

Data Mining: Principles and Algorithms

## Hidden Markov Model



Given observed sequence AGGCT, which state emits every item?

## 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

$$
a_{k l}=\operatorname{Pr}\left(\pi_{i}=l \mid \pi_{i-1}=k\right)
$$

- Probability of transition from state $k$ to state I
- Emission Probabilities

$$
e_{k}(b)=\operatorname{Pr}\left(x_{i}=b \mid \pi_{i}=k\right)
$$

- Probability of emitting character bin state $k$


## An HMM Example


vata ivınıng: rrıncıpıes ana Algorithms

## 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


## How Likely is a Given Sequence?

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

$$
\operatorname{Pr}\left(x_{1} \ldots x_{L}, \pi_{0} \ldots \pi_{N}\right)=a_{0 \pi_{1}} \prod_{i=1} e_{\pi_{i}}\left(x_{i}\right) a_{\pi_{i} \pi_{i+1}}
$$



## How Likely is a Given Sequence?

- The probability over all paths is

$$
\operatorname{Pr}\left(x_{1} \ldots x_{L}\right)=\sum_{\pi} \operatorname{Pr}(x_{1} \ldots x_{L}, \underbrace{\left.\pi_{0} \ldots \pi_{N}\right)}_{\pi}
$$

- 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 $\operatorname{Pr}(x)$, the probability of being in the end state having observed all of sequence $x$
- Can define this recursively
- use dynamic programming


## The Forward Algorithm

- Initialization
- $f_{0}(0)=1$ for start state; $f_{i}(0)=0$ for other state
- Recursion
- For emitting state ( $\mathrm{i}=1, \ldots \mathrm{~L}$ )

$$
f_{l}(i)=e_{l}(x i) \sum_{k} f_{k}(i-1) a_{k l}
$$

- Termination

$$
\operatorname{Pr}(x)=\operatorname{Pr}\left(x_{1} \ldots x_{L}\right)=\sum_{k} f_{k}(L) a_{k N}
$$

N : ending state;
denoted as 0 in textbook

## Forward Algorithm Example



Given the sequence $x=T A G A$

Data Mining: Principles and Algorithms

## Forward Algorithm Example

## - Initialization

$$
\bullet \mathrm{f}_{0}(0)=1, \mathrm{f}_{1}(0)=0 . . . \mathrm{f}_{5}(0)=0
$$

- Computing other values

$$
\begin{aligned}
-\mathrm{f}_{1}(1) & =\mathrm{e}_{1}(\mathrm{~T})^{*}\left(\mathrm{f}_{0}(0) \mathrm{a}_{01}+\mathrm{f}_{1}(0) \mathrm{a}_{11}\right) \\
& =0.3^{*}\left(1^{*} 0.5+0^{*} 0.2\right)=0.15 \\
-\mathrm{f}_{2}(1) & =0.4^{*}\left(1^{*} 0.5+0 * 0.8\right) \\
-\mathrm{f}_{1}(2) & =\mathrm{e}_{1}(\mathrm{~A})^{*}\left(\mathrm{f}_{0}(1) \mathrm{a}_{01}+\mathrm{f}_{1}(1) \mathrm{a}_{11}\right) \\
& =0.4^{*}\left(0^{*}\left(0.5+0.15^{*} 0.2\right)\right.
\end{aligned}
$$

- $\operatorname{Pr}(\mathrm{TAGA})=\mathrm{f}_{5}(4)=\mathrm{f}_{3}(4) \mathrm{a}_{35}+\mathrm{f}_{4}(4) \mathrm{a}_{45}$


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

Finding the Most Probable Path: The Viterbi Algorithm

- Define $\mathrm{v}_{\mathrm{k}}(\mathrm{i})$ 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 $\mathrm{v}_{\mathrm{N}}(\mathrm{L})$ efficiently


## Algorithm

## Method:

(1) Initialization $(i=0): \quad v_{0}(0)=1, v_{k}(0)=0$ for $k>0$
(2) Recursion $(i=1 \ldots L): \quad v_{l}(i)=e_{l}\left(x_{i}\right) \max _{k}\left(v_{k}(i-1) a_{k l}\right)$

$$
\operatorname{ptr}_{i}(l)=\operatorname{argmax}_{k}\left(v_{k}(i-1) a_{k l}\right)
$$

(3) Termination:

$$
\begin{aligned}
& P\left(x, \pi^{*}\right)=\max _{k}\left(v_{k}(L) a_{k 0}\right) \\
& \pi_{L}^{*}=\operatorname{argmax}_{k}\left(v_{k}(L) a_{k 0}\right)
\end{aligned}
$$

## 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


## *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 $O\left(S^{2} L\right)$
- This assumes that the states are densely interconnected
- Given $M$ sequences of length $L$, the complexity of Baum Welch on each iteration is $O\left(M S^{2} L\right)$


## Sequence Data

-What is sequence data?

- Sequential pattern mining
- Hidden Markov Model
- Summary



## Summary

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

