Aalto University School of Science Degree Programme in Computer Science and Engineering

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Software Processes for Dummies: Re-inventing the Wheel

Master's Thesis Espoo, June 18, 2011

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Advisor: Olli Ohjaaja M.Sc. (Tech.)



Aalto University School of Science

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The thesis example file (thesis-example.tex), all the chapter content files (1introduction.tex and so on), and the Aalto style file (aalto-thesis.sty) are commented with explanations on how the Aalto thesis works. The files also contain some examples on how to customize various details of the thesis layout, and of course the example text works as an example in itself. Please read the comments and the example text; that should get you well on your way!

Keywords:
ocean, sea, marine, ocean mammal, marine mammal, whales, cetaceans, dolphins, porpoises

Language:
English

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I wish to thank all students who use LATEX for formatting their theses, because theses formatted with LATEX are just so nice.

Thank you, and keep up the good work!

Espoo, June 18, 2011

Stella Student

Abbreviations and Acronyms

2k/4k/8k mode COFDM operation modes

3GPP 3rd Generation Partnership Project

ESP Encapsulating Security Payload; An IPsec security

protocol

FLUTE The File Delivery over Unidirectional Transport pro-

tocol

e.g. for example (do not list here this kind of common

acronymbs or abbreviations, but only those that are essential for understanding the content of your thesis.

note Note also, that this list is not compulsory, and should

be omitted if you have only few abbreviations

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Introduction

This is my master's thesis, and I am very proud of it. Of course, when I write my real master's thesis, I will not use the singular pronoun I, but rather try to avoid referring to myself and speak of the research we have conducted—I rarely work alone, after all. Yet, both I and we are correct, and it depends on the instructor and the supervisor (of course from you, too), which one they would prefer. Anyway, the tense should be active, and passive sentenses should be avoided (especially, writing sentences where the subject is presented with by preposition), so often you cannot avoid choosing between the pronouns. Life is strange, but there you have it.

By the way, the preferred order of writing your master's thesis is about the same as the outline of the thesis: you first discover your problem and write about that, then you find out what methods you should use and write about that. Then you do your implementation, and document that, and so on. However, the abstract and introduction are often easiest to write last. This is because these really cover the entire thesis, and there is no way you could know what to put in your abstract before you have actually done your implementation and evaluation. Rarely anyone write the thesis from the beginning to the end just one time, but the writing is more like process, where every piece of text is written at least twice. Be also prepared to delete your own text. In the first phase, you can hide it into comments that are started with % but during the writing, the many comments should be visible for your helpers, the instructor and supervisor.

The introduction in itself is rarely very long; two to five pages often suffice.

1.1 Problem statement

Undergraduate students studying technical subjects do not consider typography very interesting these days, and therefore the typographical quality of many theses is unacceptably low. We plan to rectify this situation somewhat by providing a decent-quality example thesis outline for students. We expect that the typographical quality of the master's theses will dramatically increase as the new thesis outline is taken into use.

1.2 Helpful hints

Read the information from the university master's thesis pages [4] before starting the thesis. You should also go through the thesis grading instructions [1] together with your instructor and/or supervisor in the beginning of your work.

1.3 Structure of the Thesis

You should use transition in your text, meaning that you should help the reader follow the thesis outline. Here, you tell what will be in each chapter of your thesis.

Background

The problem must have some background, otherwise it is not interesting. You can explain the background here. Probably you should change the title to something that describes more the content of this chapter. Background consists of information that help other masters of the same degree program to understand the rest of the thesis.

Transitions mentioned in Section 1.3 are used also in the chapters and sections. For example, next in this chapter we tell how to use English language, how to find and refer to sources, and enlight different ways to include graphics in the thesis.

2.1 Language and Structure

Moreover, the transitions are also used in the paragraph and the sentence level meaning that all the text is linked together. For example, the word "moreover" here is one way, but of course you should use variation in the text. Examples of transitional devices (words) and their use can be found from writing guides, e.g. from the Online Writing Lab (OWL)¹ of Purdue University or Strunk's Elements of Style². Remember that footnotes are additional information, and they are seldom used. If you refer to a source, you do no not use footnote. The right command for the references is *cite*.

The language used in the thesis should be technical (or scientifical). For example, the abreviations aren't used but all them are written open (i.e. "are not"). Since the content itself is often hard to understand (and explain), the sentences should not be very long, use complex language with several examples embedded in the same sentence, and, also, seldom used words and

¹http://owl.english.purdue.edu/owl/resource/574/02/

²http://www.bartleby.com/141/

weird euphemism or paraphrases can make the sentence hard to follow and to read it with only one time, and making everything even harder to understand all this without any punctuation marks makes the instructor cry and finally after trying to correct the language, you will get boomerang, and everyone's time has just been wasted.

Please use proofreaders before sending even your unfinished version to the instructor and/or supervisor. You will get better comments when they do not need first proofread your text. Moreover, they can consentrate to the content better if the language and spelling mistakes are not distracting the reading. Several editors have their own proofreading tools, e.g. ispell in emacs. You can also use Microsoft Word to proofread your thesis: it can correct also some grammatical errors and not just misspelled words.

Note also that if you have a section or a subsection, you have to have at least two of them, or otherwise the section or subsection title is unnecessary. Same with the paragraphs an: you should not have sections with only one paragraphe, and single sentence paragraph. Furthermore, always write some text after the title before the next level title.

2.2 Finding and referring to sources

Never ever copy anything into your theses from somebody else's text (nor your own previously published text). Never. Not even for starting point to be rewritten later. The risk is that you forgot the copied text to your thesis and end up to be accused of plagiarism. Plagiarism is a serious crime in studies and science and can ruin your career even its beginning. To repeate: never cut and paste text into your thesis!

2.2.1 Finding sources

All work is based on someone else's work. You should find the relevant sources of your field and choose the best of them. Also, you should refer to the original source where a fact has been mentioned first time. Remember source evaluation (criticism) with all sources you find.

Good starting points for finding references in computer science are:

- Nelli Portal (Aalto Library): http://www.nelliportaali.fi
- ACM Digital library: http://portal.acm.org/
- IEEExplore: http://ieeexplore.ieee.org
- ScienceDirect: http://www.sciencedirect.com/

• ...although Google Scholar (http://scholar.google.com/) will find links to most of the articles from the abovementioned sources, if you search from within the university network

Some of the publishers do not offer all the text of the articles freely, but the library has agreed on the rights to use the whole text. Thus, you should sometimes use computers in the domain of the university in order to get the full text. Sometimes the Nelli Portal can also help getting the whole article instead of just the abstract. The library has also brief instrucions how to find information [2].

Instead of normal Google, use Google Scholar (http://scholar.google.fi/). It finds academic publications whereas normal Google find too much commercial advertisements or otherwise biased information. Wikipedia articles should be referred to in the master thesis only very, very seldomly. You can use Wikipedia for understanding some basics and finding more sources, but often you cannot be sure if the article is correct and unbiased.

One important part of the sources that you have found is the reference list. This way you can find the original sources that all the other research of the field refer. Often you can also find more information with the name of the researchers that are often referred in the articles.

2.2.2 Referring to sources

The main point in referring to sources is to separate your own thinking and text from that of others. Facts of the research area can be given without reference, but otherwise you should refer to sources. This means two things: marking the source in the text where it has been used, and listing the sources usually in the end of the thesis in a way that help the reader to find the original source.

There are several bibliography styles, meaning how to form the bibliography in the end of the thesis. Aalto's library has good instructions for many styles [3]. You should ask from your supervisor or instructors which style you should use. This thesis template uses the number style that is often used in software engineering. The other style also used in the CS field, e.g. usability, is the Harvard style where instead of numbers, the reference is marked into the text with author's name and publishing year. Other areas use also many other styles for making the lists and marking the references.

In addition to the list in the end of the thesis, you have to mark the source in the text where the source is used. There are three places for the reference: in a sentence before the period, in the end of a sentence after the period, or in the end of a paragraph. All of them have different meaning.

The main point is that first you paraphrase the source using your own words and then mark the source. Next, we give short examples that are marked with *emphasised text*.

Haapasalo [13] researched database algorithms that allows use of previous versions of the content stored in the database. This kind of marking means that this paragraph (or until the next reference is given) is based on the source mentioned in the beginning. Giving the source you should use only the family name of the first author of the article, and not give any hints about what is the type of the article that is referred.

B+-trees offers one way to index data that is stored in to a database. Multiversion B+-trees (MVBT) offer also a way to restore the data from previous versions of the database. Concurrent MVBT allows many simultaneous updates to the database that is was not possible with MVBT. [13] When the marking is after the period, the reference is retrospective: all the paragraph (or after previous reference marking) is based on the source given in its end. If the content is very broad, you can start with saying According to Haapasalo, then continue referring the source with several separate sentences, and in the end put the marking of your source that shows that CMVBT are the best. [13].

If your paragraph has several sources, the above mentioned styles are not proper. The reader of your thesis cannot know which of your sources give which of the statements. In this case, it is better to use more finegraded refering where the reference markings that are embedded in the sentences. For example, the multiversion B+-tree (MVBT) index of Becker et al. [6] allows database users to query old versions of the database, but the index is not transactional. It's successor, the transactional MBVT (TMVBT), allows a single transaction running in its own thread or process to update the database concurrently with other transactions that only read the database [14]. Further development, titled the concurrent MBVT (CMVBT), allows several transactions to perform updates to the database at the same time [13]. Here, the references are marked before the period in the sentences where they are used.

Finally, direct quotes are allowed. However, often you should avoid them since they do not usually fit in to your text very well. Using direct quotes has two tricks: quotation marks and the source. "Even though deletions in a multiversion index must not physically delete the history of the data items, queries and range scans can become more efficient, if the leaf pages of the index structure are merged to retain optimality." [13] Quotes are hard to make neatly since you should use only as much as needed without changing the text. Moreover, you often do not really understand what the author has mentioned with his wordings if you cannot write the same with your own words. Remember also that never cut and paste anything without marking

13

the quotation marks right away, and in general, never cut and paste anything at all!

Sometimes getting the original source can be almost impossible. In an extremely desperate situation, you can refer with structure $mr \ X \ [\dots]$ according to $ms \ Y \ [\dots]$ defined that, if you find a source that refers to the original source. Note also that the reference marking is never used as sentence element (example of how **not** to do it: [13] describes an optimal algorithm for indexing multiversiond databases.).

Clustering Methods

As described in Chapter XX, all patients data is retrieved from the database directly without any manual labeling. Due to lack of labels, unsupervised learning algorithms should be adopted. Clustering is a collection of unsupervised methods, which identifies groups of data points according to a defined similarity metric, such that objects in the same group posses higher similarities compared to objects in other groups. The clustering process does not rely on labels but the choice of similarity metrics. Variations in similarity metrics lead to different clustering methods.

Applying clustering methods in anomaly detection tasks has been studied numerously [15]. This chapter introduces two typical methods, K-Means [18] and DBSCAN [11]. Problem formulation, solutions, and potential issues are formally described using elaborated notations in following sections. However, analysis on the performance and constraints of these two methods are postponed to Chapter XXX, which reveals their practicality and infeasibility in the previously described anomaly detection problem. (Time, Memory consumption. For K-Means, definition of center.)

3.1 K-Means

K-Means is one of the simplest unsupervised algorithm which solves clustering problem. Despite its simplicity, K-Means has gained success in various situations, including anomaly detection [15] [8], image segmentation and compression [12], and preprocessing for more complicated algorithms. The method can be formally defined as follow: Given a data set $\{\mathbf{x}_1,...,\mathbf{x}_N\}$ consisting of N observations in D-dimensional space, the object is to partition the data into K groups, by defining a set of K centers $\{\boldsymbol{\mu}_1,...,\boldsymbol{\mu}_k\}$ in the same space, and assigning each observation to exactly one center point. Each

center point represents a prototype associated with the k^{th} cluster.

The assignments can be represented using 1-of-K scheme. Then, for each data point x_n , a corresponding K-dimensional variable consisting of K binary elements $r_{nk} \in \{0,1\}$ is introduced. Among these r_{nk} , exactly one of them equals 1, which means \mathbf{x}_n belongs to the k^{th} cluster. Using this notation, evaluation of the clustering quality can be defined using the object function as follow:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} D(\mathbf{x}_N - \boldsymbol{\mu}_k)$$
(3.1)

where D is the dissimilarity metric. Common choice of the metric is l_1 norm or l_2 -norm. Mahalanobis distance is also adopted while considering the
covariances between the K-dimensions [9]. In the following context, l_2 -norm
is adopted for discussion. Intuitively, this function can be considered as the
distance summation of each point to its corresponding cluster prototype μ_k .
The K-Means aims at finding a set of μ_k which minimizes the object function.
Finding the optimal solution for the above object function proves to be NPHard [5]. However, employing heuristic algorithms enables finding converged
local optimal solutions. Section 3.1.1 describes one iterative algorithm, EM.
Section 3.1.2 explores common issues related to K-Means and remedies.

3.1.1 EM Algorithm in K-Means

EM algorithm is an iterative algorithm to find local maximum. Each iteration consists of two phases, Expectation and Maximization, which corresponds to minimize the objective function J with respect to r_{nk} and μ_k respectively. In the E(expectation) step, the algorithm minimize J with respect to r_{nk} , while keeping the μ_k fixed. Then in the following M(maximization) step, the algorithm minimizes J with respect to μ_k , while keeping r_{nk} fixed.

Considering the optimization in E step, a critical observation of (3.1) is that \mathbf{r}_n 's are independent of each other. Thus, optimization on \mathbf{r}_n 's can be done seperately for each n. The solution is simply setting the r_{nk} corresponding to the minimum $\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$ to 1. Intuitively, the algorithm assigns \mathbf{x}_n to the closest cluster center. Formally, the solution can be written as

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_{j} \| \mathbf{x}_{n} - \mu_{j} \|^{2} \\ 0 & \text{otherwise} \end{cases}$$
(3.2)

In the following M step, the above determined r_{nk} is clamped. Then, μ_k appears only in a quadratic term in J. Setting derivatives of J with respect to μ_k to zero, solution formula for μ_k can be expressed in following closed

form

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \mathbf{x}_n}{\sum_n r_{nk}} \tag{3.3}$$

This step can be considered as recomputing the cluster prototype by setting μ_k to the mean of all points assigned to that cluster.

EM keeps executing these two steps alternatively, until a convergence happens or until number of iterations exceeded a predifined value. Since in each phase, one variable is fixed and updating another variable minimizes the cost function J, convergence is guaranteed. Formal proof on convergence has been studied by MacQueen [19].

The algorithm is illustrated using dataset generated independently from three gaussian distributions in Figure 3.1. In this demonstration, the algorithm takes K=3, which is the correct number of components. Before running the first iteration, initialized μ_k is required. This initialization is done by choosing three objects from the data set randomly.

3.1.2 Issues in K-Means

Despite the simplicity of K-Means, several underlying issues exists. The first potential is that, how to choose the value for K. In the above illustration, K was set to 3 which is the correct number of components. However, if K wasn't set to the correct value, unsatisfied clustering may be generated. Example of this issue is shown in Figure 3.2(a)-(c). To solve this problem, one practical way is drawing graph of the cost function versus value of K, as shown in Figure 3.2(d). Intuitively, when K is under smaller than the true number of clusters, increasing K will lead to a huge drop of cost function value. However, when K has reached or exceeded the correct value, incresing K leads only small cost function value drop. Thus, number of clusters corresponding to the 'elbow' point can be considered as the real number of clusters.

Another issues of K-Means relates to the initialization of μ_k . Since EM finds only local optimal solutions, a poor initialization could lead to worse clustering result. To avoid this problem, it is practical to run K-Means for several times and choose the best result according to the value of the cost function.

One more critical issue of K-Means lies in the choice of similarity metric. As mentioned at the beginning of this chapter, variations in similarity metric leads to different clustering methods. Choosing l-2 norm is convenient in terms of computation, but this choice limits the type of data variables to certain types. Using l-2 norm on categorical data is inappropriate since no ordering of categorical values exists. Also, this makes computing the mean

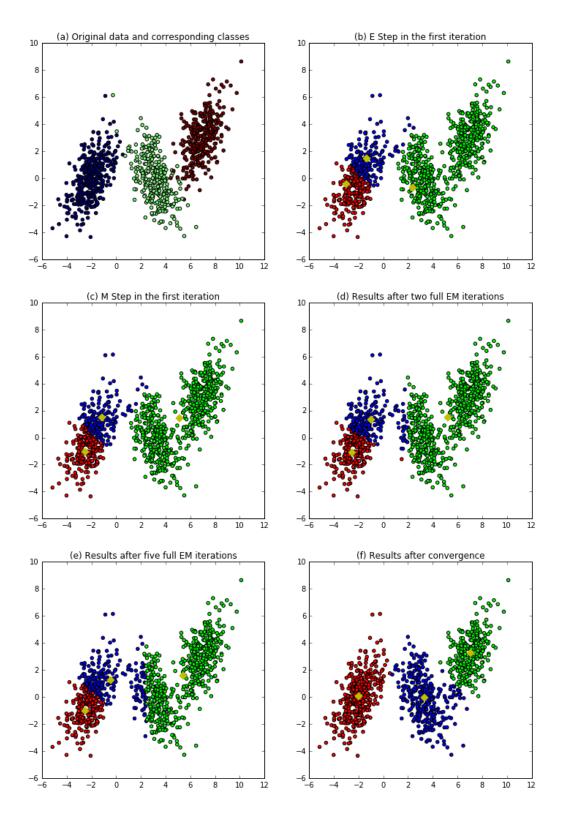


Figure 3.1: Illustraion of EM algorithm on K-Means using data generated independently from three gaussian distribution. (a) Original data and corresponding classes. Classes are denoted in different colors. (b) Assignments of each data after the first E step. The yellow diamonds represent the intialized μ_k . (c) Updated μ_k after the M step in the first iteration. (d)-(f) Clustering results after several successive full EM iterations until convergence is met.

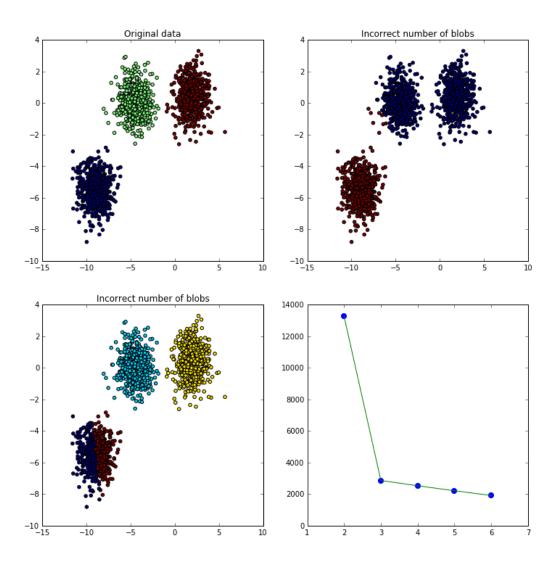


Figure 3.2: Issues of K-Means incurred by choosing inappropriate value for ${\cal K}$

value a hard problem. To use K-Means on other data types, the similarity metric should be elaborately designed.

Besides, K-Means tends to form clusters into a convex space. As shown in Figure 3.1(b)-(e), the boundary between two different clusters forms a line lying at the midway and is perpendicular to the line connecting two cluster prototypes. However, a cluster is not necessary to be convext. This also limits the application of K-Means.

Finally, K-Means is also sensitive to noises. As shown in formula 3.3, updating μ_k involves computing the mean of all data points assigned to that cluster. When noise objects with large deviation from other points in this cluster exist, update of μ_k will be strongly affected.

3.2 Density Based Clustering Methods

This section explores another type of clustering method which forms cluster from the view of density aspect. **Density-Based Spatial Clustering of Applications** with **Noise** (DBSCAN) [11] considers to be one of the most successful method from this category [17]. Compared to K-Means, DBSCAN posseses following advantages: 1). DBSCAN can detect clusters of arbitrary shape. 2). DBSCAN can determine the number of clusters automatically. 3). DBSCAN is robust to noises.

The following of this chapter is organized as follows. Section 3.2.1 compares and reveals the relation of DBSCAN to a basic graph traversal algorithm **D**epth **F**irst **S**earch(DFS). This section will introduce the critical concept used by DBSCAN which differentiate it with DFS. Section 3.2.2 describe this concept in more details. Section 3.2.3 compares DBSCAN and K-Means, and discusses practical issues of DBSCAN.

3.2.1 DBSCAN and DFS

Before introducing DBSCAN, it would be helpful to review a basic graph traversal algorithm, DFS, which is an algorithm which traverses or visits a graph. In the discussion of this context, the whole process is divided into two procedures DFS and DFS-VISIT. A typical recursive implementation is described as follow.

```
DFS(G)
1
   for each vertex u \in G
2
        u.visited = FALSE
3
   for each vertex u \in G
4
        if u.visited == FALSE
             DFS-VISIT(G, u)
5
DFS-VISIT(G, u)
   u.visited = TRUE
2
   for each vertex v \in G. Adj[u]
3
        if v.visited == FALSE
4
             DFS-VISIT(G, v)
```

The first two lines in DFS initializes the algorithm by setting all nodes to be unvisited. Then, the algorithm traverse vertices in the graph. Once an unvisited node is found, DFS-VISIT is called. In the procedure DFS-VISIT, the given node u is labled as visited. If an unvisited child v of u is found, this procedure goes one layer deeper by calling another DFS-VISIT on v. After finishing DFS-VISIT(G, u), the algorithm backtrack to visit other unvisited children of u, which are siblings of v.

Assume DFS executes on an undirected graph. Each call of DFS-VISIT on an unvisited node u explores u and all nodes reachable to it. These nodes form a component which disconnects with other components by other runs of DFS-VISIT. Thus, each component can be considered as a cluster. The criterion to form a cluster is that each pair of nodes can reache each other through a path consisting of nodes only in this cluster.

DBSCAN can be seen as an application of DFS. However, DBSCAN differs from standard DFS from its useage of DFS-VISIT. In standard DFS, the algorithm goes deeper by calling DFS-VISIT(G, v) on all unvisited children of node u. In DBSCAN, however, the algorithm goes deeper if and only if node u satisfies extra conditions, which are specified by two user given value Eps and MinPts. These extra conditions make the component generated from DBSCAN a meaningful cluster viewing from the density side. The pseudocode is shown below.

```
DBSCAN(S, Eps, MinPts)
    ClusterId = 1
2
    for each point u \in S
3
         if u.label \neq NIL
 4
             continue
5
         u.neighbor = Region-Query(u, Eps)
6
         if ||u.neighbor|| < MinPts
 7
             u.label = NOISE
8
         else
9
             EXPAND-CLUSTER(u, ClusterId, Eps, MinPts)
10
              ClusterId = ClusterId + 1
EXPAND-CLUSTER(u, ClusterId, Eps, MinPts)
   u.label = ClusterId
2
   for each point v \in u.neighbor
3
       if v.label == NIL
4
            v.label = ClusterId
5
            v.neighbor = Region-Query(v, Eps)
6
            if ||v.neighbor|| < MinPts
7
                 Expand-Cluster (v, Cluster Id, Eps, MinPts)
8
       elseif v. label == NOISE
9
            v.label = ClusterId
```

Similiar with DFS traverse, DBSCAN clustering is also divided into two procedures, DBSCAN and Expand-Cluster. DBSCAN functions as a wrapper function in the same way as DFS. This procedure goes through each point in the data set S. If the current point u has been visited, the procedure skips it. Otherwise, further process continues. However, unlike calling DFS-VISIT on every unvisited u unconditionally as DFS does, in DBSCAN, another procedure Expand-Cluster is called if and only if u has sufficient number of neighbors in a given range Eps. Region-Query(u, Eps) returns all the neighbors of u with a distance no further than Eps. This is the extra condition mentioned earlier. Similiarly, this condition is also checked in Expland-Cluster at line 6, as opposed to DFS-Visit. Besides these two places, the rest of the two algorithms are the same. Details of extra conditions are fully explained in next section.

3.2.2 Notions of Density in Clusters

From the view of density, points in a space can be classified into three categories: core points, border points, and outliers/noise. The classification

criterion on a point u bases on the size of its Eps-neighborhood, denoted as N(u; Eps). The N(u; Eps) represents the collection of all points whose distances to u are within Eps, which is specified by user. More formally, $N(u; Eps) = \{v \mid dist(u, v) < Eps\}.$

Based on above definition, a point u is a core point if and only if $||N(u; Eps)|| \ge MinPts$, where both Eps and MinPts are user specified. After defining core points, it is relatively easy to define the other two categories. A border point v is a neighbor point of a core point u, but v is not a core point itself. Formally, ||N(u; Eps)|| < MinPts, and $v \in N(u; Eps)$, where $||N(u; Eps)|| \ge MinPts$. For a outlier, it's a point v which is neither a core point itself nor a neighbor point of a core point. An example graph is showing in Fig 3.3.

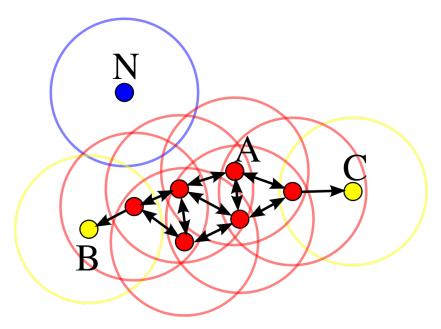


Figure 3.3: Illustration of core points(red), border points(yellow), and outlier(blue) [23]. In the illustration, MinPts = 4, Eps is the radius of those circles.

As show in the figure, red points are core points since in each red circle, there are at least 4 points(including the center point). While for the yellow point, they don't have enough points in their circles, but they embed in one of the red circles. Thus, they are border points. As for the blue point, it has neither enough point in the blue cirle nor is in any red circle. Thus, the blue point an outlier/noise.

These definitions reveal the assumption and theory of DBSCAN. DB-SCAN assumes that, each cluster consists of two types of points, core points

and border points. Core points form inner denser areas compared to spaces outside of clusters. Border points form a slightly sparser areas surrouding the inner core area, but still the density is higher than spaces between different clusters, possesed by noise. In DBSCAN, the density of an area is measured by the number of points centered at u within an area specified by the given radius Eps. If there are at least MinPts points, this area is considered to be a dense area. Thus, this area is part of a cluster. In the procedure Expand-Cluster, the algorithm will explore the whole dense area and less dense border area belonging to the same cluster. Each call of Expand-Cluster visits a different cluster. Thus, when the whole procedure DBSCAN finishes, different clusters are formed.

3.2.3 Analysis of DBSCAN

DBSCAN applies to a broader range of problems comapred to K-Means. In K-Means, one of the obstacle is to compute the mean value. DBSCAN doesn't have this problem as long as the distance between points is computable. This enables DBSCAN to use more compliated distance measurement, such as edit distance, which is very useful in dealing with strings. Another advantage of DBSCAN is its robustness to noises. As mentioned in section 3.1.2, the mean value will be heavily interfere by noises/outliers. In contrast, DBSCAN has a notion noises and it is able to spot these outliers, which is a core problem of this thesis. Finally, the most important advantage of DBSCAN is that it can find arbitrarily shaped clusters. It can even seperate a cluster completely surrounded by a different cluster. An example is shown in Fig 3.4.

Simliar to K-Means, DBSCAN also requires user specified parameters. To get the optimal result, a careful choice of these parameters is needed. Finding the appropriate parameter can be achieved in the similiar way by finding the elbow point as mentioned in section 3.1.2. The user can pick a number for MinPts first. Then, for each point, the distance from its kth nearest neighbor is computed. After sorting these distances in descending order and plot them, a graph called sortedk-distgraph can be obtained. This graph reveals insights about the density distribution of the whole dataset reflected in how the k-dist varies. Then the Eps can be set to the value corresponding to the elbow point. This heuristic works well as the graph won't differ too much for k > 4. An illustration of this approach is shown in Figure 3.5. [11]

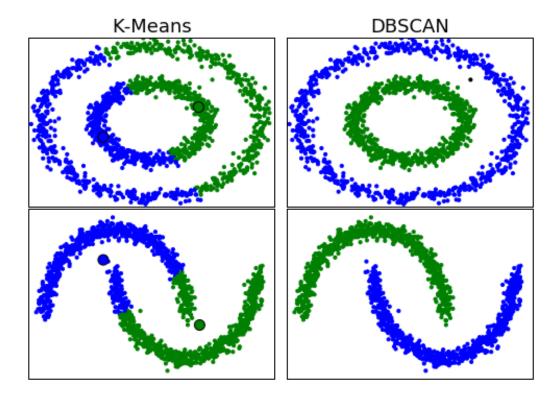


Figure 3.4: A Comparison of K-Means and DBSCAN. In the diagram, two datasets "circles" and "moons" are used. Compared to K-Means, DB-SCAN gives more reasonable clustering results on these two irregular shaped datasets.

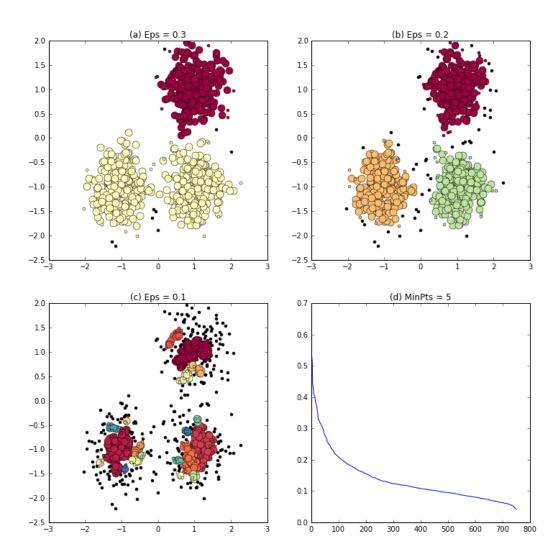


Figure 3.5: Illustration of the heuristic parameter choosing approach for DB-SCAN. (a)-(c) illustrates clustering results obtained by using different Eps. Each cluster is painted with a different color. Core points are represented using larger circles while border points are represented using smaller circles. Black small circles represent outliers. In figure (a), very few points are labeled as noise and the bottom two clusters are not distinguished. In figure (b), the result is more reasonable and can be considered as optimal. In figure (c), too many points are labeled as noise and more than 3 clusters are reported. According to the k-distgraph shown in (d), 0.2 should be the best value for Eps, which corresponds to the result in figure (b).

Generative Methods

This chapter is going to explore generative methods for anomaly detection. Generative methods are a collection of algorithms which try to build a model that explains the process of how the data generates. Then, based on information from the proposed model, anomalies are detected. A family of algorithms belonging to this category is the Markov models.

As described in Chapter 2, the patients visits can be seen as time sequential data consisting of a series of events. The events in one visit are not generated independently and randomly. Instead, past events have an effect on the type of the next possible event. To handle sequential data, Markov models are the correct choice since they consider the relation between consecutive observations. In the following context, Section 4.1 introduces the basic Markov chain model. Later, Section 4.2 expands the Markov chain to a more complicated Hidden Markov Model by introducing hidden variables.

4.1 Discrete Markov Process

Consider a system having N distinct states S_1, S_2, \dots, X_N . At any time, the system will be in one of these states. After a given time period t, a series observation x_1, x_2, \dots, x_t can be obtained. (Without loss of generality, the following discussion assumes the variables are all scalar. The assumption holds in the rest of the context unless explicitly stated otherwise) According to the product rule of probability, the joint probability distribution for this sequence of observations is

$$p(x_1, x_2, \dots, x_t) = \prod_{i=2}^{t} p(x_i \mid x_1, \dots, x_{i-1})$$
(4.1)

The conditional probability distribution of each observation x_i depends on

all observations having a smaller index than it. The above relations between the observations can be represented graphically in Fig 4.1(a). The graph is fully connected, and no independence property can be obtained from it. Now assume that each observation x_i only depends on one immediate previous observation x_{i-1} . Then the joint distribution becomes

$$p(x_1, x_2, \dots, x_t) = p(x_1) \prod_{i=2}^{t} p(x_i \mid x_{i-1})$$
 (4.2)

This newly obtained model is depicted in Fig 4.1(b), and is referred as first-order Markov chain. The term first-order indicates the dependence on only one previous observation. Suppose the system has only 3 states, as shown in Fig 4.1(c). Then, to fully represent the system, the only required information is the transition probabilities between different sates. The transition probabilities are usually referred as transition matrix, denoted as \mathbf{A} . Each element A_{ij} represents the probability of transfering from state s_i to state s_j . Learning the parameters of this model is very simple. Since the states are exactly the observations, A_{ij} can be simply obatained by compute the frequency of transfering to s_j starting from s_i . The number of free parameters in this model is K(K-1), where K represents the number of states in the system.

Sometimes, the observations can depend on more than one observations in the past. One simple way to achieve this is creating a higer order Markov chain. By allowing each observation to depend on previous two values, a second-order Markov chain is obtained, as shown in Fig 4.2. Then the joint distribution becomes

$$p(x_1, x_2, \dots, x_t) = p(x_1)p(x_2 \mid x_1) \prod_{i=3}^{t} p(x_i \mid x_{i-1}, x_{i-2})$$
(4.3)

Compared to first-order Markov chain, the second-order Markov chain has better capability of modelling complex relations between variables. In fact, the higher the order is, the more flexible the model is. However, the number of parameters grows as well, which makes the model difficult to train. For a M^{th} order markov chain, there will be $K^M(K-1)$ parameters. Because the exponential growth in number of parameters, the model gardually becomes impractial as M grows.

The markov chain model can be expanded in another way, by associating an emission distribution \mathbf{E}_k , $k=1,\dots,K$, to each state in the system. Thus, two observations x_i , y_i exist at any time, where y_i is generated depending on x_i . If the expansion is based on a first-order Markov chain, the joint

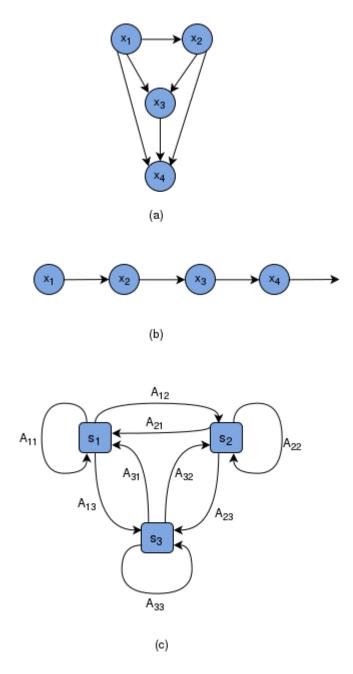


Figure 4.1: Illustration of a Markov Chain of 4 observations possessing 3 states. Variables are represented using filled circles, while states are represented using filled squares.

distribution becomes

$$p(x_1, y_1, \dots, x_t, y_t) = p(x_1) \Big(\prod_{i=2}^t p(x_i \mid x_{i-1}) \Big) \Big(\prod_{i=1}^t p(y_i \mid x_i) \Big)$$
(4.4)

The patient visits can be seen as an example of this expanded model. For each visit, the patient will go through a series of events, which can be considered as states. Each event will then last for a certain period of time. The duration can be seen as generated from a distribution, and the parameters of this distribution depend on the event. The example is shown in Fig 4.3.

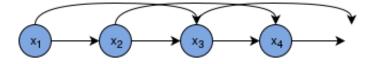


Figure 4.2: Illustration of a second-order Markov model.

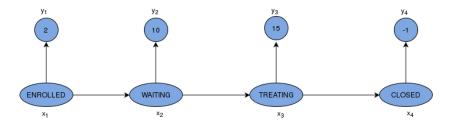


Figure 4.3: Modelling a patient visit as an expansion of first-order Markov model.

4.2 Hidden Markov Models

As mentioned in the last section, a tradeoff between flexibility and practicality exists in deciding the order number for a Markov chain model. In special situations, such as speech recognition, very high-order Markov chain is expected. But the computation resource requires as few number of parameters as possible. It would be ideal if a model is not limited to any specific given order, and still only limited number of parameters are required to specify the model. Luckily, these requirements can be satisfied by constructing a Hidden Markov Model using additional latent variables.

Suppose a sequence of observations $\mathbf{X} = \{x_1, \dots, x_N\}$ is obtained. In stead of assuming each observation depends directly on a specific number of previous observations, the new assumption is that, there is a latent variable

 z_i corresponding to each observation, and the latent variables form a Markov chain. The latent variables don't have to possess any physical meanings. They can even be of different type to the observations, in terms of distribution and dimensionality. A graphical representation of this model is shown in Fig 4.4. It's easy to get confused by comparing Fig 4.3 and Fig 4.4 since they share the same graphical structure. The difference is that, in Fig 4.4, the z_i 's are unobserved latent variables, which is depicted using unfilled circles. While in Fig 4.3, both events and duration are observed values. All observed variables are represented using filled circles. If the HMM is applied to the patient visits, one potential structure could be the one shown in Fig 4.5. In this model, the value of latent variable determines which event will generate, then the event determines how long the duration will be. Notice that the latent variables don't have any associated physical meaning or specific distribution form. One can explain them as indication of the functioning statu of the system by selecting them to be binary variables. When $z_i = 1$, it indicates the queue system in the hospital is working in normal mode. When $z_i = 0$, it means the system is working in a problametic way.

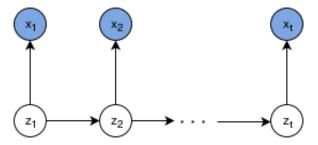


Figure 4.4: Graphical representation of a Hidden Markov Model. Observations are represented using filled circles, while latent variables are depicted using unfilled circles. The latent variables form a first-order Markov chain.

In the framework of HMM, the joint distribution over both observed and latent variables is given below

$$p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta}) = p(z_1 \mid \pi) \left(\prod_{n=2}^{N} p(z_n \mid z_{n-1}, \mathbf{A}) \right) \left(\prod_{m=1}^{N} p(x_m \mid z_m, \phi) \right)$$
(4.5)

where $\mathbf{X} = \{x_1, \dots, x_N\}$ represents all the observed variables, $\mathbf{Z} = \{z_1, \dots, z_N\}$ represents latent variables, and $\boldsymbol{\theta} = \{\pi, \mathbf{A}, \phi\}$ represents the parameters in this model. The π is a prior distribution for deciding the value of the first variable z_1 . The matrix \mathbf{A} is the transition matrix among the latent vari-

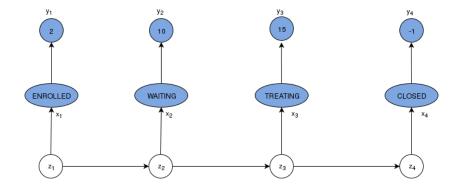


Figure 4.5: Modelling patient visit as Hidden Markov Model. Event types and event duration are represented using filled eclipses and circles respectively. Additional hidden variables are represented using unfilled circles. No specific physical meaning is associated with these latent variables.

ables. The ϕ are the parameters of the emission distribution associated with z_i and x_i .

4.2.1 Learning and Inference

There are three basic problems in HMM. [22] These problems are described below using above notations:

- Problem 1: Given a sequence of observations $\mathbf{X} = \{x_1, \dots, x_N\}$, what is the probability $p(\mathbf{X} \mid \boldsymbol{\theta})$ over the observations, under specific parameters $\boldsymbol{\theta} = \{\pi, \mathbf{A}, \phi\}$?
- Problem 2: What's the value of the parameters which maximizes $p(\mathbf{X} \mid \boldsymbol{\theta})$?
- Problem 3: Given a sequence of observations $\mathbf{X} = \{x_1, \dots, x_N\}$, what is the value of the corresponding latent variables?

The rest of the context focus on the first two questions. The reason is that, once the value of $p(\mathbf{X} \mid \boldsymbol{\theta})$ is computed, the decision on whether a given sequence is anomaly can be made by comparing $p(\mathbf{X} \mid \boldsymbol{\theta})$ to a threshould value.

Though it seems more intuitive that finding a way to evaluate $p(\mathbf{X} \mid \boldsymbol{\theta})$ should come before maximizing it with respect to the parameters, it would be more convenient to start at solving problem 2. After solving problem 2, the

solution to the first problem will appear naturally. The following discussion begins by introducing some new concepts and notations.

The distribution over only observed variables $p(\mathbf{X} \mid \boldsymbol{\theta})$ is usually referred as incomplete likelihood, while distribution over both observed and unobserved variables $p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$ is referred as complete likelihood. Using formula (4.5), the logarithm of incomplete likelihood can be represented as

$$\ln p(\mathbf{X} \mid \boldsymbol{\theta}) = \ln \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$$

$$= \ln p(z_1 \mid \pi) + \ln \sum_{\mathbf{Z}} \left(\left(\prod_{n=2}^{N} p(z_n \mid z_{n-1}, \mathbf{A}) \right) \left(\prod_{m=1}^{N} p(x_m \mid z_m, \phi) \right) \right)$$
(4.6)

The above formula is a generalization of the mixture distribution [7]. Maximizing this formula with respect to the parameters is very difficult since the derivatives don't have a closed form. An alternative practical working algorithm is the expectation-maximization(EM) algorithm [10][20]. The EM algorithm is very similiar to the K-Means algorithm mentioned in Chapter 3. The algorithm consists of two steps, E-step and M-step. In the E-step, the algorithm fixes the value of parameters and find the posterior distribution of the laten variables $p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{old})$. Here the notation is adopted from Bishop's [7]. The superscription old in θ^{old} means the parameter is fixed. Then the algorithm computes the expectation of the logarithm of the complete likelihood, with respect to the derived posterior distribution. The newly derived term becomes a function of $\boldsymbol{\theta}$, which is shown below

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{old}) \ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$$
(4.7)

Then in the M-step, the new value of $\boldsymbol{\theta}$ is updated by maximizing $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old})$. Compared to K-Means, the E-step corresponds to assign each point to a cluster prototype, and the M-step corresponds to update the value of the prototypes. These two steps are excecuted alternatively until convergence or maximum number of iteration is reached. In the rest context, $\gamma(\mathbf{z}_n)$ and $\gamma(\mathbf{z}_{n-1}, \mathbf{z}_n)$ are introduced which stands for the posterior distribution of a single latent variable and the joint posterior distribution over two consecutive latent variables, seperately. Instead of assuming the latent variables are scalar, here they are represented using 1-of-K coding. Namely, each latent variable is a length K vector, where one and only one of these K elements equals 1. When $z_{nk} = 1$, it means the nth latent variable is in the kth state.

update equation can be obtained

Using this representation schema, following equations are obtained

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X}, \boldsymbol{\theta}^{old}) \tag{4.8}$$

$$\gamma(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}, \boldsymbol{\theta}^{old})$$
(4.9)

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{old}) = \sum_{k=1}^{K} \gamma(z_{1k}) \ln \pi_k + \sum_{n=2}^{N} \sum_{j=1}^{K} \sum_{k=1}^{K} \gamma(\mathbf{z}_{n-1}, \mathbf{z}_n) \ln A_{jk}$$

$$+ \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \ln p(x_n | \phi_k)$$
(4.10)

Computation in the M-step is relatively easy. Assume the E-step has been done, so that $\gamma(\mathbf{z}_n)$ and $\gamma(\mathbf{z}_{n-1}, \mathbf{z}_n)$ are like constants now. Then following

$$\pi_k = \frac{\gamma(z_{1k})}{\sum_{j=1}^K \gamma(z_{1j})} \tag{4.11}$$

$$A_{jk} = \frac{\sum_{n=2}^{N} \gamma(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \gamma(z_{n-1,j}, z_{nl})}$$
(4.12)

Updation of ϕ_k is more tricky, since it depends on the specific choice of the emission distribution. One good observation is that, only the final term depends on ϕ_k , and different ϕ_k doesn't couple with each other. Thus, each ϕ_k can be updated separately. The term $\gamma(z_{nk})$ functions as a soft assignment, representing the probability of assigning a point x_n to each state.

Computation in E-step is more difficult which requires efficient algorithm. The most widely used algorithm is known as *alpha-beta* algorithm. This algorithm can be seen as an application of dynamic programming technique which takes advantage of the tree structure in HMM thus leading to efficiency. To start with the alpha-beta algorithm, following conditional independence properties should be obtained first [16]

$$p(\mathbf{X}|\mathbf{z}_n) = p(x_1, \dots, x_n|\mathbf{z}_n)$$
$$p(x_{n+1}, \dots, x_N|\mathbf{z}_n)$$
(4.13)

$$p(x_1, \dots, x_{n-1}|x_n, \mathbf{z}_n) = p(x_1, \dots, x_{n-1}|\mathbf{z}_n)$$
 (4.14)

$$p(x_1, \dots, x_{n-1}|z_{n-1}, \mathbf{z}_n) = p(x_1, \dots, x_{n-1}|\mathbf{z}_{n-1})$$
 (4.15)

These equations can be obtained by using d-seperation technique [21], or proved formally using sum and product rules of probability. Using the first

independence property and Bayes' theorem, following equations are obtained

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n | \mathbf{X}) = \frac{p(\mathbf{X} | \mathbf{z}_n) p(\mathbf{z}_n)}{p(\mathbf{X})} \\
= \frac{p(x_1, \dots, x_n, \mathbf{z}_n) p(x_{n+1}, \dots, x_N | \mathbf{z}_n)}{p(\mathbf{X})} \\
= \frac{\alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)}{p(\mathbf{X})} \tag{4.16}$$

where

$$\alpha(\mathbf{z}_n) = p(x_1, \cdots, x_n, \mathbf{z}_n) \tag{4.17}$$

$$\beta(\mathbf{z}_n) = p(x_{n+1}, \cdots, x_N | \mathbf{z}_n) \tag{4.18}$$

Using the other two conditional independence properties, $\alpha(\mathbf{z}_n)$ can be expressed recursively in terms of $\alpha(\mathbf{z}_{n-1})$

$$\alpha(\mathbf{z}_n) = p(x_n|\mathbf{z}_n) \sum_{\mathbf{z}_{n-1}} p(x_1, \dots, x_{n-1}, \mathbf{z}_{n-1}) p(\mathbf{z}_n|\mathbf{z}_{n-1})$$

$$= p(x_n|\mathbf{z}_n) \sum_{\mathbf{z}_{n-1}} \alpha(\mathbf{z}_{n-1}) p(\mathbf{z}_n|\mathbf{z}_{n-1})$$
(4.19)

Similarly, $\beta(\mathbf{z}_n)$ can also be expressed recursively as

$$\beta(\mathbf{z}_n) = \sum_{\mathbf{z}_{n+1}} \beta(\mathbf{z}_{n+1}) p(x_{n+1}|\mathbf{z}_{n+1}) p(\mathbf{z}_{n+1}|\mathbf{z}_n)$$
(4.20)

The term $\alpha(\mathbf{z}_n)$ can be seen as messages propagated from the beginning to the end. Each $\alpha(\mathbf{z}_n)$ receives messages passed from its predecessor, combines these information with its own information and then pass them to its successor. The logical also applies to the term $\beta(\mathbf{z}_n)$, but the messages are from the end to the beginning. Due to the tree strucutre in HMM, computing each term only depends on one adjacent term, instead of all terms before/after it. Thus, the computation reduces dramatically which makes the algorithm efficient. To start the whole computation, initial conditions $\alpha(\mathbf{z}_1)$ and $\beta(\mathbf{z}_n)$ are required. The initial conditions are given below

$$\alpha(\mathbf{z}_1) = \prod_{k=1}^{K} \{ \pi_k p(x_1 | \phi_k) \}^{z_{1k}}$$
 (4.21)

$$\beta(\mathbf{z}_N) = 1 \tag{4.22}$$

Having obtained $\alpha(\mathbf{z}_n)$ and $\beta(\mathbf{z}_n)$, the posterior distribution $\gamma(\mathbf{z}_n)$ can be computed as in equation (4.16). As for $\gamma(\mathbf{z}_{n-1}, \mathbf{z}_n)$, it can be computed as following

$$\gamma(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X})
= \frac{p(\mathbf{X} | \mathbf{z}_{n-1}, \mathbf{z}_n) p(\mathbf{z}_{n-1}, \mathbf{z}_n)}{p(\mathbf{X})}
= \frac{p(\mathbf{x}_1, \dots, \mathbf{x}_{n-1} | \mathbf{z}_{n-1}) p(\mathbf{x}_n | \mathbf{z}_n) p(\mathbf{x}_{n+1}, \dots, \mathbf{x}_N | \mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) p(\mathbf{z}_{n-1})}{p(\mathbf{X})}
= \frac{\alpha(\mathbf{z}_{n-1} p(\mathbf{x}_n | \mathbf{z}_n) p(\mathbf{z}_n | \mathbf{z}_{n-1}) \beta(\mathbf{z}_n)}{p(\mathbf{X})}$$
(4.23)

Up till now, both steps in EM algorithm are introduced, and the problem 2 can be solved efficiently. The left question is how to solve problem 1, computing the likelihood over the incomplete data. The solution comes from equation (4.16). Notice that $\gamma(\mathbf{z}_n)$ is a posterior distribution. Integrating both sides of equation (4.16) over \mathbf{z}_n gives

$$p(\mathbf{X}) = \sum_{\mathbf{z}_n} \alpha(\mathbf{z}_n) \beta(\mathbf{z}_n)$$
 (4.24)

where \mathbf{z}_n is an arbitrary latent variable. If n = N, then $\beta(\mathbf{z}_n) = 1$, which makes the above equation simpler

$$p(\mathbf{X}) = \sum_{\mathbf{z}_N} \alpha(\mathbf{z}_N) \tag{4.25}$$

Then, both problem 1 and problem 2 are solved.

Experiment

This chapter describes the detailed experimental implementation. Following topics will be discussed:

- Which specific data are used? How to represent the data?
- What preprocess has been done? What related functions are defined?
- Which methods are used? What's the reason to use such methods?

The three topics will be discussed in three sections, respectively. Analysis of the result will be postponed to Chapter 6.

5.1 Data Details

Since the akseli system has gone through several updation after its first release, many features have changed, including how the visit log is reocrded. Considering this aspect, only data generated after year 2014 is retrieved. 243K unique visits with 1.93 million entries are retrieved, which spans from January to July. The retrieved data consists of three columns: visit id, event type, and recorded time of the event. Other information, such as which resource generated the data, is not retrieved. Among the retrieved data, 7 event types are adopted. The used event types are: ENROLLING, WAITING, IN_TREATMENT_ROOM, PAUSED, IN_TREATMENT_ROOM_FROM_PAUSED, CLOSED, and CANCELLED.

Evaluation

You have done your work, but that's not enough.

You also need to evaluate how well your implementation works. The nature of the evaluation depends on your problem, your method, and your implementation that are all described in the thesis before this chapter. If you have created a program for exact-text matching, then you measure how long it takes for your implementation to search for different patterns, and compare it against the implementation that was used before. If you have designed a process for managing software projects, you perhaps interview people working with a waterfall-style management process, have them adapt your management process, and interview them again after they have worked with your process for some time. See what's changed.

The important thing is that you can evaluate your success somehow. Remember that you do not have to succeed in making something spectacular; a total implementation failure may still give grounds for a very good master's thesis—if you can analyze what went wrong and what should have been done.

 $^{^{1}}$ By the way, do *not* use shorthands like this in your text! It is not professional! Always write out all the words: "that is".

Discussion

At this point, you will have some insightful thoughts on your implementation and you may have ideas on what could be done in the future. This chapter is a good place to discuss your thesis as a whole and to show your professor that you have really understood some non-trivial aspects of the methods you used...

Conclusions

Time to wrap it up! Write down the most important findings from your work. Like the introduction, this chapter is not very long. Two to four pages might be a good limit.

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Appendix A

First appendix

This is the first appendix. You could put some test images or verbose data in an appendix, if there is too much data to fit in the actual text nicely. For now, the Aalto logo variants are shown in Figure A.1.



(a) In English



(b) Suomeksi



(c) På svenska

Figure A.1: Aalto logo variants