Inferring Informed Clustering Problems with Minimum Description Length Principle

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January 2007

Dissertation submitted in partial fulfilment for the degree of

Doctor of Philosophy in Computer Science

Department of Computing Science

University at Albany

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Abstract

Clustering, one of the most commonly practiced tasks in machine learning and data mining, partitions unlabeled patterns into structured subsets, known as clusters, by maximizing similarities among patterns within the same cluster and minimizing the similarities across distinct clusters according to a pre-defined similarity function. Learning clusters from patterns can often be complicated by additional background knowledge. Ad hoc clustering algorithms are commonly introduced for various types of background knowledge to accommodate them into the clustering process.

The dissertation proposes a unified framework on clustering with background information by utilizing the Minimum Description Length (MDL) principle. With MDL as a tool, all information is encoded into binary string and code length becomes the ubiquitous measure on information and complexity. The optimal clustering solution corresponds to the partition that leads to the shortest overall encoding length.

The dissertation explores three clustering problems with different types of background information, namely multi-view clustering, semi-supervised clustering and constrained clustering. For each type of clustering problem, we illustrate efficient encoding of the patterns into binary strings and appropriate optimization approaches to searching for the shortest encoding length solution. Empirical results indicate that the proposed MDL framework on informed clustering offers automatic information weighing and improved predictive performance.

Acknowledgements

The course of writing this dissertation is an arduous one, yet not lonely, because of the support and encouragement I have been constantly receiving from different groups of people, without whom the work would be completely impossible.

First and foremost, I am most deeply indebt with my ph.D advisor, Professor Davidson, who originally motivated me in pursuing a doctoral degree in computer science. During years of doing research work with him, he has not only imparted the fascinating knowledge in machine learning and data mining, but also the skill of approaching problems in a strategic manner. I am also especially grateful that he sacrifices his off-working hours to advise me on the dissertation, to accommodate my own inflexible schedule.

I am also fortunate to have the most resourceful committee that I could have asked. The dissertation involves a spectrum of different fields, including machine learning, statistics and algorithms. Each of the committee members, Professor Davidson, Professor Stratton and Professor Ravi brings expertise in the areas and provides precious opinions and suggestions in shaping the dissertation.

I also owe my thanks to Pat Keller, who has always been so helpful in rescuing me from administrative problems, when I am on campus and away from campus.

Finally I cannot express enough gratitude towards my parents, who has always been my endless source of encouragement and enlightenment, and my beautiful wife Ruowen, for her considerate understanding and constant supportiveness during the course.

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1 Introduction

1.1 Data Clustering

Clustering [Har75] [JD88] [JMF99] is one of the most frequently practiced tasks in machine learning and data mining field. The goal of clustering is to partition a set of patterns, into finite groups known as clusters, such that the similarity of the patterns are maximized within the same cluster and minimized across clusters. The importance of clustering lies in the constructed structure from the otherwise unstructured data, offering both an explanation on the data generating mechanisms and a predictive device. For example, a set of mortgage loan borrowers can be partitioned into two clusters based on their credit score, income, housing value and other information, with one cluster representing borrowers with high propensity for delinquency and the other for punctual payments. The structure learnt through clustering process can subsequently predict the payment behavior of a considered mortgage borrower by comparing profile similarity between the borrower and each of the learnt clusters. Clustering belongs to the category of unsupervised learning in the sense that the learner is not coached by the training

patterns with explicit labels, rather, the learner has the freedom of partitioning the patterns into clusters, each corresponding to an implicit label, hence the name, unsupervised.

From the perspective of partitioning methodology, clustering falls into two categories, hierarchical and nonhierarchical. Hierarchical clustering finds the clusters progressively. It either starts with the entire population as a single cluster, repetitively cleaving larger clusters into smaller ones, known as the top down approach, or begins with each pattern as a cluster and incrementally merges them, known as bottom up approach. In contrast, nonhierarchical clustering partitions all the patterns in a parallel fashion. In this work, unless explicitly specified, clustering refers to nonhierarchical clustering. Some most well known nonhierarchical clustering algorithms are K-means clustering and expectation maximization (EM) on mixture Gaussian models [JD88]. The goal of K-means clustering is to find partition such that the distortion function, which is the sum of the squared Euclidean distances of the patterns from the corresponding cluster centers, is minimized. This is achieved by iteratively assigning each pattern to its closest cluster center via a greedy algorithm. The algorithm halts when local minimum is achieved and further iteration does not alter the partition or partition solutions from adjacent iterations are notably small. Figure 1.1 demonstrates an example of K-means clustering that partitions 150 patterns from X-Y space into three non overlapping clusters.

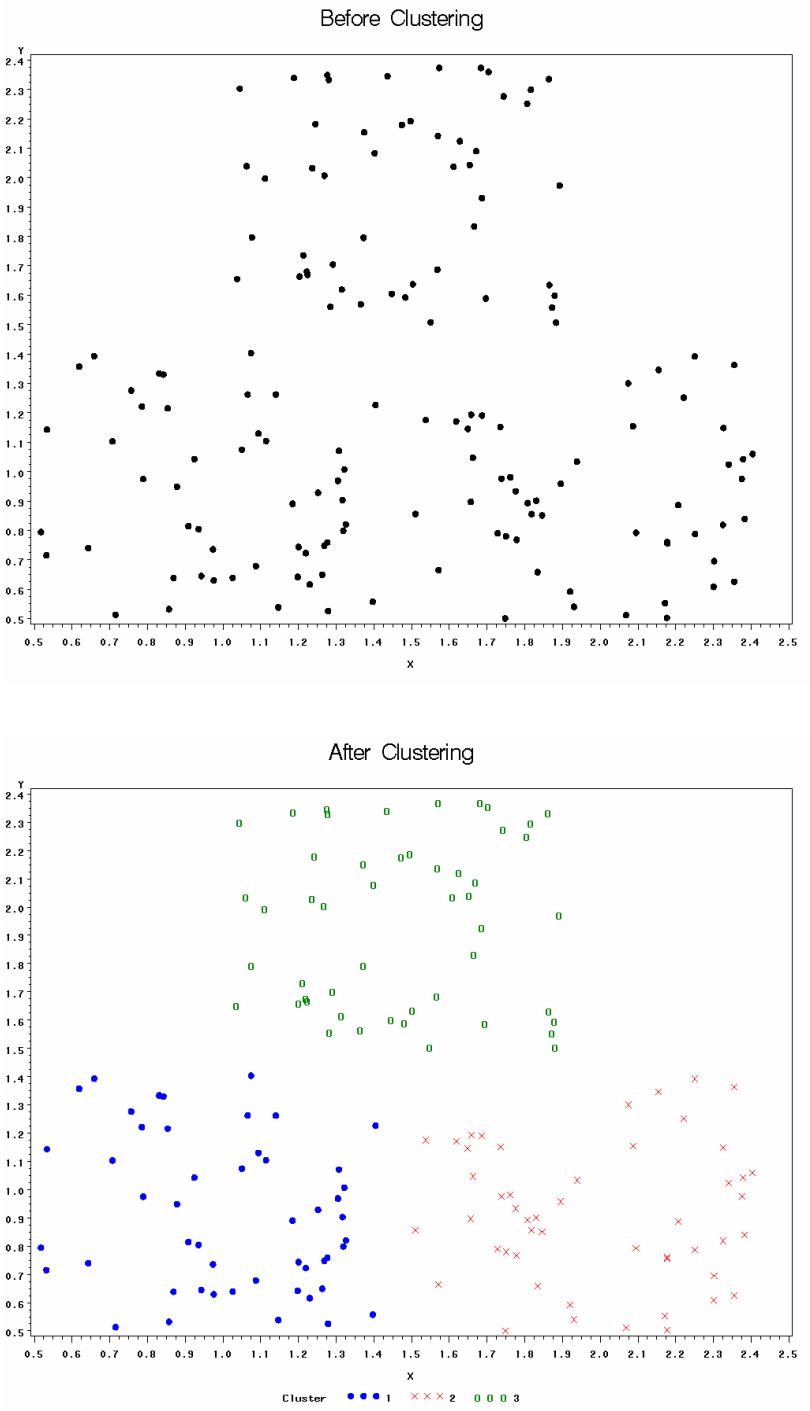


Figure 1.1 An example of K-means clustering on X-Y plane

1.2 Informed Clustering Problems

Pragmatic clustering problems, however, sometimes involve more complicated situation than having a set of unlabeled patterns assigned into a fixed number of clusters. Instead, the learner may have background knowledge on the patterns, which should be considered into the clustering process. The type of background knowledge can vary by source and nature. For example, in some problem, partial exterior label may be present for a small proportion of the patterns to be clustered. A partition of the patterns into clusters must be consistent with the existing information implied by the labels. While background knowledge is mostly beneficial in aiding the learner to find more meaningful clusters, it complicates the clustering process because the additional information it provides does not automatically falls into the existing clustering framework. In this dissertation, the name **informed clustering** is used for all the clustering problems where background knowledge is imposed. We use a few pragmatic clustering applications to illustrate the necessity of investigating informed clustering problems.

1.2.1 Multi-View Clustering

A set of patterns sometimes can be described by multiple data sources which constitute multiple views of the patterns. For example, a database in a commercial bank can have a table that stores all the demographic information about the mortgage loan borrowers, including gender, income, credit score, loan purpose, etc. A separate table stores the monthly payment information such as paid amount and delinquency. Each table is a view of the patterns (loan borrowers) and can be used to cluster the patterns. Clustering a set of patterns with more than one view (typically two) is called multi-view clustering [BS04].

The approach to clustering each view independently is insufficient because it does not utilize the information that the views are describing the **same** set of patterns. The independently clustered results would be identical to a problem without the knowledge that the two views are describing same set of patterns thus the learner has not used all the information provided. Because the views can potentially be dependent, each view provides additional information in clustering other views. For this reason, clustering should be carried simultaneously across the views. Kaski et al. proposed associative clustering algorithm [KNS+05], with the above stated strategy behind. The algorithm maximizes the mutual information of the cluster assignments between the views, under the constraint that each cluster is of Voronoi type, that is, each pattern belongs to its nearest cluster according to the distance function. The approach is successfully applied in identifying the dependency between gene expression and regulator binding.

1.2.2 Semi-Supervised Clustering

A second type of informed clustering is semi-supervised clustering. As implied by name, the problem is the middle ground between supervised and unsupervised learning, such that the patterns are partially labeled. Partial labeling arises when labeling the entire set of patterns is too expensive or simply impossible. In some semi-supervised clustering work, the partial labels are treated as constraints so that patterns with the same class label form must link constraints and patterns of distinguished class label form cannot link constraints [BBM02][CCM03]. In other works, the clustering algorithm only have a preference on assigning patterns with the same explicit labels into the same cluster but does not enforce it. Instead, a penalty is imposed for heterogeneity of class labels within

the same cluster [GH04].

1.2.3 Constrained Clustering

A third type of informed clustering is constrained clustering. In constrained clustering, Cluster solutions are bound by a set of rules specified in advance based on either prior knowledge or problem requirement. The constraints fall into three categories, instance-level constraint, cluster-level constraint and model-level constraint. The instance level constraints include must-link and cannot-link constraints. Must-link constraints require two patterns be assigned to the same cluster; Cannot-link constraints enforce two patterns not be assigned to the same cluster. Cluster-level constraints enforce the similarity of patterns within a cluster and dissimilarity of patterns across clusters. Two types of cluster-level constraints are proposed in [DR05]: the δ-constraint specifies the minimum distance between any given two patterns from different clusters; the ε-constraint enforces the maximum distance between any two patterns within a cluster. Model-level constraints are concerned with clustering solution as a whole, targeting at eliminating dominating clusters and attributes. The computational complexity of clustering optimization under constraints may increase significantly with the quantity and complexity of constraints. Davidson and Ravi investigated the computational complexity of deciding cluster feasibility under instance-level and cluster-level constraints [DR05].

In addition to the challenges imposed on each informed clustering problem introduced above, they also inherit some of the challenges from the original clustering problems such as deciding the number of clusters. Most clustering algorithms assume known cluster

numbers, which is justified when the learner has that prior knowledge. However, under certain circumstances, it is desirable to allow the patterns themselves to inform the learner about the number of clusters. Choosing number of clusters is even more demanding in informed clustering, where the solution must accommodate the background knowledge in the problem.

The key approach to solving the informed clustering problem is to combine information from different types and reach a clustering solution that comprehensively summarizes all the information. This involves deciding the importance and relevance of information, and the tradeoff among them. For example, in semi-supervised clustering, although it is desirable to have patterns with the same class labels assigned to the same cluster, it should not be achieved by sacrificing too much on the cluster qualities, which can be measured by the similarity of patterns within a cluster. The same rationale applies in deciding the number of clusters: while incrementing the cluster number always improves the similarity among the clusters, the dissimilarity across the clusters will be reduced thus lead to potentially worsened clustering partition. As a consequence, various type of information needs to be computed, combined and optimized simultaneously in informed clustering. However, the various types of information are not immediately combinable, as the scale and unit measuring them are not directly comparable.

1.3 Minimum Description Length Principle

The learning by compact encoding theories [WF87] [Ris87] avail themselves as tools to measure information in a ubiquitous way. In the theories, all types of information, of

patterns, of clusters, of secondary view, of partial labels or of constraints, are measured in the same unit by encoding the information into binary strings, the lengths of which are the sole measurement on the information amount. There are two branches in the learning by compact encoding theories, namely minimum message length (MML) and minimum description length (MDL). The two theories share the same philosophical insights but with subtle nuances. MML constructs a code with two steps: the first step encodes a theory from a countable set of theories, which is similar to the subjective prior in Bayesian with discretization; the second step constructs a code for the data with the presence of knowledge from the already encoded theory. The inferred theory in MML is the one that minimizes expected total code length within a theory. In contrasts, MDL allows one part message encoding and the complexity of a theory is represented by the entire theory set rather than individual theories. In addition, the MDL inference is the one that minimize the expected code length over all possible data. In this work, we choose MDL as the inference tool for the convenience of one part code.

1.4 Dissertation Contribution

The dissertation establishes a unified framework for informed clustering with MDL as a tool. It makes the following contributions into the current research on informed clustering:

1. It provides a unified framework for informed clustering problems which optimize information weighing and complexity tradeoff, offering inference methodology on informed clustering problems with improved empirical predictive capability.
2. The work develops efficient encoding for the three informed clustering problems

mentioned. For each of the three informed clustering problems, the work derives the description length function and applies different optimization techniques in searching for the solution.

3. As the framework utilizes MDL, it automatically addresses the model selection problem in informed clustering, which is otherwise not frequently addressed.

1.5 Dissertation Overview

The chapters of the dissertation are to be organized in the following manner: Chapter 2 provides a brief introduction to the MDL principle and related literature. It discusses the relationship between probability and codes, encoding discrete and continuous data, two parts and one part MDL encoding, and encodings for some commonly encountered distributions, which serve as building blocks for subsequent chapters. Chapter 3 focuses on multi-view clustering problem. The chapter explores the encoding, optimization of the multi-view clustering problem with MDL principle. Dependency information among the views can be captured by encoding the views simultaneously, which offers superior clustering solutions to clustering the views independently, as indicated by various empirical results. Chapter 4 addresses semi-supervised clustering problem, where the patterns are partially labeled. The chapter explores mixture Gaussian model and establish the MDL encoding method. MDL coupled Markov chain Monte Carlo (MCMC) sampling is introduced and applied in searching for the clustering solutions. Chapter 5 concentrates on clustering problems under constraints. The chapter discusses how constraints as background knowledge can be exploited in shortening the overall encoding length. Also the chapter develops criteria in identifying “good” constraints that improves

the learning and “bad constraints” that deteriorates the learning. Chapter 6 summarizes preceding chapters and overviews informed clustering problems from a high level to yield a unified framework. The chapter concludes the dissertation and state further investigation directions.

2 Minimum Description Length

2.1 Introduction

In machine learning, a problem that often confronts the learner is to choose among multiple theories that seemingly consistent with the observed data, known as the model selection problem. Deciding the number of clusters is an example of model selection problem in the clustering context. A model that provides the best fitting is not necessarily the best model that captures most insight from the data. For example, in K-means clustering, model fitting is typically measured by the quantization error, the sum of the squared distances of all patterns from their allocated cluster centers. A smaller quantization error represents greater homogeneity within clusters and indicate better fitting. However, a trivial clustering solution that assigns each pattern into its own cluster has zero quantization error, yet it is obvious that no insight is gained from the model. Because a complicated model typically provides more flexibility and allows better fitting to the data, the improvement in fitting should be penalized with increased model

complexity, as stated by the famous Occam's razor, that "entities should not be multiplied beyond necessity".

How does one achieve the optimal trade-off between better data fitting and controlled model complexity? If the two are measured in the same unit, then a single objective function can be computed by combining the two and the best model minimizes the function. One method to realize the idea is by encoding both the model and data into binary strings, and measuring the total complexity as the lengths of the encoded strings. The encoded strings should be lossless compressions of the original data by exploiting the regularities. If the description length of the data with the aid of a model is shorter than that without, then the model has offered new knowledge in the data. Two similar theories have been derived from this philosophy, the minimum message length (MML) principle and the minimum description length (MDL) principle. While the concepts are similar, the two theories have some subtle and important differences.

The MML principle [WB68] [WF87] is first proposed by Wallace and Boulton in 1968. MML divides the model parameter space into discrete cells and place a prior distribution upon them. From the distribution, the parameters can be encoded up to a precision defined by the dimension of the cell. The data is then encoded with the knowledge of model. An optimal precision can be derived by minimizing the expected two parts message length over the parameter cell: if the precision is high, it takes longer message to encode the model parameters but the message length encoding the data can be reduced; on the other hand, a low precision enables shorter message encoding the model

parameters but lengthening the second part of the code. If the model parameter set is countable where no discretization is necessary, the actual message length rather than the expected message length is minimized. MML principle has been applied widely in machine learning problems. Wallace et al used MML to prevent over-fitting in decision tree classifier [WP93]; Oliver and Baxter developed a MML-based unsupervised learning framework [BO00]; Davidson proposed Markov chain Monte Carlo sampling in clustering problem where the full conditional probability is derived from the MML computation [Dav00]. Fitzgibbon, Allison and Dowe suggest the usage of MML in clustering ordered data [Fad00].

The MDL principle is developed by Rissanen independently in a series of papers [Ris78] [Ris87] [Ris01]. The early stage MDL is similar to MML, adopting a two part encoding method. The major difference between the two part MDL and MML is that MDL does not acknowledge a subjective prior, rather, it advocates non informative prior such as Jeffery's prior on the model parameters. However, different priors still lead to different encoding on the models and thus possibly different model selection outcomes. The two part MDL, also referred as the crude MDL, is refined into one part MDL when the normalized maximum likelihood (NML) distribution is introduced to encode the data. The NML encoding is a universal code where the encoding for any encountered data is almost as short as can be achieved by the maximum likelihood code. Furthermore, the code length representing the model complexity does not depends on particular model parameters anymore; instead it is a fixed encoding cost that is only pertinent to the "richness" of model. Both crude MDL and refined MDL have received numerous

applications. It has been used in efficient decision tree pruning which yields in improved predictive accuracy [QR89] [MRA95]. In unsupervised learning, Kontkanen et al has developed efficient recursive computation of one part MDL for multinomial distribution [KMB+03] and apply it in the clustering framework [KMB+05].

This chapter introduces minimum description length principle and its applications in plain clustering, which serves as the basics for the subsequent chapters.

2.2 Code

We define a *code* as a mapping from a countable set S to a set of finite binary strings, with each mapped binary strings called a code word. A *prefix code* is a code where no code word is a prefix of another. For example, {A, B, C, D}→{00, 01, 10,11} constitutes a prefix code while {A, B, C, D}→{1, 10, 110, 111} does not. The significance of prefix code is that the decoding process requires no additional delimiter and can be done unambiguously.

In MDL principle, one is only concerned with the length of the codes rather than the contents themselves. For prefix code, the code word lengths must satisfy certain mathematical properties. Let L_C: $S \rightarrow R^+$ denotes the function computes to code length for $s \in S$ with prefix code C. In the above prefix example, the code lengths are the same for all four symbols in the set, L_C(A)= L_C(B)= L_C(C)= L_C(D)=2. As the goal in MDL is to shorten the message length, a natural question to ask is how short L_C can be while the code is still decodable, which is answered by Kraft's inequality.

Kraft's Inequality: For a prefix code C that encodes a finite set S with an alphabet of size r with encoding length function L_C, the following inequality holds:

$$\sum_{s \in S} r^{-L_C(s)} \leq 1 \tag{2.1}$$

Conversely, for any encoding length function L_C that satisfies the inequality, a prefix code mapping from S to an alphabet of size r can be constructed.

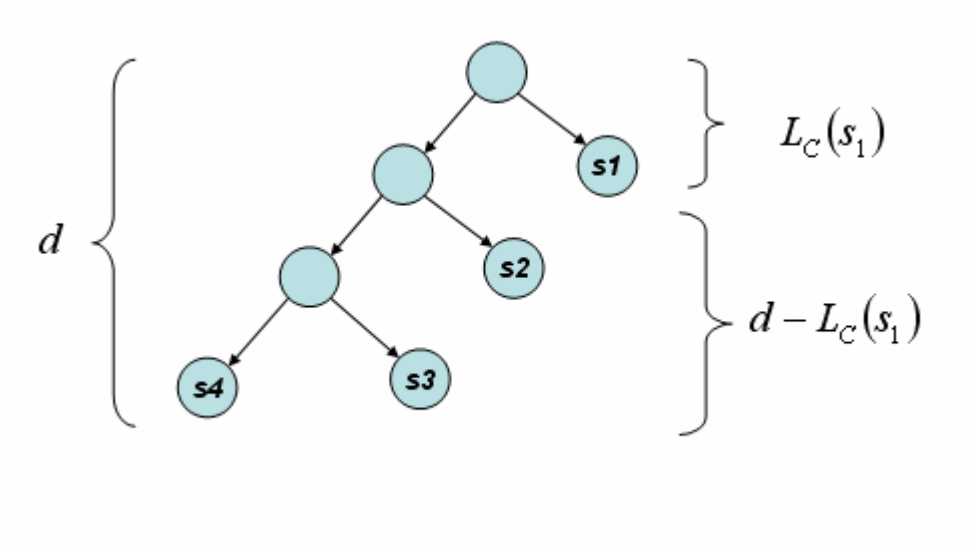


Figure 2.1 Kraft's Inequality

The correctness of Kraft's inequality can be illustrated by explicitly constructing an r-ary tree as illustrated in Figure 2.1 for code C, where each node represents a symbol in the alphabet thus each path from root to leaf represents a code word. By the nature of the construction, the code is prefix. Let d be the depth of the tree. For a code word $s1$ with length $L_C(s_1)$, the leaf node can be potentially expand into a sub-tree with $r^{d-L_C(s_1)}$ leaf nodes. However the sum of all the leaf nodes expanded from the current tree should not exceed to maximum number of leaf nodes for a tree with depth of d,

$$\sum_{s_1 \in S} r^{d - L_C(s_1)} \leq r^d \tag{2.2}$$

The Kraft's inequality follows. Conversely, given a description length function L_C that satisfies Kraft's inequality, one can always construct a tree in the same manner such that the number of leaf nodes equals the size of the alphabet and the depth of the nodes corresponds to the lengths of the descriptions.

An immediate implication of Kraft's inequality is that a code that used by MDL which yields the shortest description length must satisfy the equality condition. If not, the code length of certain symbol in set *S* can be shortened so that the equality is established. Thus, only efficient prefix code that satisfies the equality condition is the candidate code that corresponds to the shortest description length. For an efficient prefix code,

$$\sum_{s \in S} r^{-L_C(s)} = 1 \tag{2.3}$$

Equation (2.3) states that an efficient prefix code corresponds to a probability measure on set *S*. It is easy to verify that

$$P(s) = r^{-L_C(s)} \tag{2.4}$$

satisfies the three conditions for probability measure: non-negativity, unity and countable additivity. A probability distribution implies a code length function and vice versa. For a probability measure *P* on *S*, a unique efficient code length function can be constructed,

$$L_C(s) = -\log_r P(s) \tag{2.5}$$

Although the code length function L_C is unique, potentially more than one efficient prefix code can be constructed to satisfy the function. However, as MDL is only concerned with code length, they are considered indistinguishable and yield the same inference.

2.3 Crude MDL

With a known probability measure on a finite symbol set *S* of size *r*, the one-to-one correspondence between probability measure *P* and efficient prefix code in section 2.2 offers a straightforward computation of the description length required to encode data *D* of length *N* composed with symbols from *S*. Let $n_D(s)$ be the number of times a symbol appeared in data, the description length is

$$L(P) = -\sum_{s \in S} n_D(s) \log_r P(s) \tag{2.6}$$

We want to minimize *L (P)* regarding to *P* subject to the constraints

$$P : \sum_{s \in S} P(s) = 1, P(s) > 0 \tag{2.7}$$

The Lagrange multiplier here is

$$\frac{\partial}{\partial P(s)} \left(-\sum_{s \in S} n_D(s) \log_r P(s) + \lambda \left(\sum_{s \in S} P(s) - 1 \right) \right) = 0 \tag{2.8}$$

This gives

$$-n_D(s) \frac{\ln r}{P(s)} + \lambda = 0 \tag{2.9}$$

Substituting to the constraint that probability sum up to one,

$$\sum_{s \in S} P(s) = \frac{1}{\lambda} \sum_{s \in S} n(s) \ln r = \frac{N \ln r}{\lambda} = 1, \quad \text{where } N = \sum_{s \in S} n(s) \tag{2.10}$$

Solving λ and substituting back to the Lagrange equation, the probability that minimizes the description length function is

$$P_D^*(s) = \frac{n(s)}{N} \tag{2.11}$$

and the corresponding shortest description length is

$$L_D^*(P) = -\ln r \sum_{s \in S} n_D(s) \ln \frac{n_D(s)}{N} \tag{2.12}$$

Two observations can be made from the results. First, the size of the set *r* plays the role of regulating the description length unit, which does not affect the minimization process. For mathematical convenience, *e* will be used for the rest of the dissertation. Second, the probability measure that leads to the shortest description length of the data is the relative frequency of each symbol within the data. Shorter code words are reserved for more frequently appeared symbols.

The above computation defines a code on all possible data with length *N*. For any data string *D* of length *N*, we first compute the probability measure that leads to the shortest description length, which is defined by the relative frequency of symbols in *D*. From the probability measure, we construct an efficient code on set *S* and use it to encode each symbol in *D*. Unfortunately such a code is not decodable by the receiver to recover *D* as the decoding the probability measure that encodes *D* depends on *D* itself. This is revealed by computing the left hand side of Kraft's inequality on all possible data with length *N*

$$\sum_{D \in S^N} \prod_{s=D_1}^{D_N} P_D^*(s) > \sum_{D \in S^N} \prod_{s=D_1}^{D_N} P_A(s) = \left(\sum_{s \in S} P_A(s) \right)^N = 1 \tag{2.13}$$

P_A here is an arbitrary prefix code on *S* that is fixed to encode all possible data *D* from S^N. The first inequality set holds strictly for all *N* greater than 1. The second equality sign comes from the multinomial theorem. The violation of Kraft's inequality states that relative frequency code is not a prefix code S^N.

The situation is mended by constructing a two part code: the first part of the code encodes the probability measure used to encode the subsequent data. The encoded probability measure can be regarded as theory *H*. The second part encodes the data S^N with the knowledge of theory *H*. To construct each part of code, one only needs to construct the corresponding marginal probability distribution on *H* and the conditional probability of S^N given *H*. The model of choice in MDL inference is the one that minimizes the total two parts description length

$$\begin{aligned} L(h) &= -\ln P(h) - \ln P(S^N \mid h) \\ h_{MDL} &= \arg\min_{h \in H} L(h) \end{aligned} \tag{2.14}$$

Example 2.1 (Binomial Sequence): Let $S = \{0, 1\}$. The data is a binary string with length *N* that may contain certain regularities. Let $h_p : S \to (0, 1)$ be a probability measure on S with $h(0) = p, h(1) = 1 - p$. Further let H be a set of h such that $p = \left\{0, \frac{1}{10}, \frac{2}{10}, ..., 1\right\}$. The agreed marginal probability distribution on *H* between the sender and receiver is $P(h_p) = \frac{2}{11} p$. For any particular given data string S^N, the sender chooses the theory that minimizes the two parts description length. The total description length is computed as

$$L(h_p) = -\ln \frac{2p}{11} - n(0) \ln p - n(1) \ln(1 - p) \tag{2.15}$$

Following table illustrates the description lengths of various probability measures for data with length 10 and length 100.

Table 2.1 Description Lengths of Binomial Sequence with Different Parameters

p	0	0.1	0.2	0.3	0.4	0.5
n(0)=4,n(1)=6	Inf	13.85	11.09	9.86	9.35	9.33
n(0)=40,n(1)=60	Inf	102.4	81.08	72.47	69.92	71.71
p	0.6	0.7	0.8	0.9	1	
n(0)=4,n(1)=6	9.76	10.71	12.48	16.05	Inf	
n(0)=40,n(1)=60	77.63	88.57	107.4	144.2	Inf	

The MDL inference on the first data is p=0.5 and inference on the second data is p=0.4. When the observed data is short, MDL prefers "simpler" model that requires less description length but for longer data, the fitness of the model on the data starts to dominate. More complex model is only used until enough data makes it necessary, which is consistent with Occam's razor philosophy.

While the conditional probability of the data given the model, which decides the second part of the description, is usually unambiguous and defined by the set of probability measure under consideration, the marginal probability which corresponds to the first part of the description is more subjective. With extreme specification of the marginal probability distribution on the model class *H*, one may infer any model desired, by concentrating probability mass on certain model. Even if one only restrict to objective priors such as Jeffery prior, it is not immediately clear whether a prior represents a model complexity well. A prior that encodes some data efficiently could potentially be very redundant in encoding some other data. This drawback on the crude MDL calls for universal coding where the code should perform close to optimal for different possible data.

2.4 Refined MDL

As mentioned above, the major difficulty in crude MDL approach is to encode the model so that the code performs well on all data. The maximum likelihood code, although always leads to the shortest possible second part description length, does not constitute a prefix code over all possible data. A natural question becomes, does a prefix code exist that is only slightly longer than the maximum likelihood code over all possible data. Such a prefix code is called a universal code. The increase in code length compared to the maximum likelihood code is called *regret*.

Definition 2.1(**Regret**): Given a class of codes *C*, the regret of a prefix code *Q* relative to *C* for data $D \in S^N$ is defined as

$$R(Q,D) = -\ln Q(D) - \max_{P \in \mathbf{C}} \{\ln P(D)\} = -\ln Q(D) + \ln P_D^*(D) \tag{2.16}$$

P_D^* is the non prefix maximum likelihood code on S^N. The regret is the extra description required for *Q* to encode *D* to make *Q* decodable. The regret is a function of both the code *Q* and the encountered data *D*. For a given code *Q* and data *D*, the regret can be large or small. A good code *Q* optimizes the worst case scenario, minimizing the largest regret over all possible data,

$$Q^*(D) = \arg\min_Q R_{\max}(Q) = \arg\min_Q \max_{D \in S^N} R(Q,D) \tag{2.17}$$

Theorem 2.1 (**Normalized Maximum Likelihood Code**) The code that minimizes the maximum regret is

$$Q^*(D) = \frac{P_D^*(D)}{\sum_{s^N \in S^N} P_{s^N}^*(s^N)} \tag{2.18}$$

Proof: The max regret for Q^* is a constant that does not depend on D

$$\max_D R(Q^*, D) = -\ln P_D^*(D) + \ln \sum_{s^N \in S^N} P_{s^N}^*(s^N) + \ln P_D^*(D) = \ln \sum_{s^N \in S^N} P_{s^N}^*(s^N)$$

For an arbitary code $Q \neq Q^*$, there must exist a data sequence that $Q(s^N) < Q^*(s^N)$, the regret difference on s^N is

$$R(Q^*, s^N) - R(Q, s^N) = -\ln Q^*(s^N) - \{-\ln Q(s^N)\} = \ln \frac{Q(s^N)}{Q^*(s^N)} < 0$$

Thus $$\max_D R(Q^*, D) < \max_D R(Q, D)$$

Q.E.D.

$Q^*(D)$ is known as the normalized maximum likelihood (NML) distribution on D. Thus the code derived from it is a prefix code on D that allows encoding all possible data efficiently. The description length of data D with the NML code is

$$L_{NML}(D) = \ln \sum_{s^N \in S^N} P_{s^N}^*(s^N) - \ln P_D^*(D) \qquad (2.19)$$

The second term is the maximum likelihood code that represents the fitness of the code on the data. The first term is a constant across all data for a given code class $\boldsymbol{C}$ and represents the complexity of the code class, known as the *Parametric Complexity* (PC) of the class. The total encoding length, the parametric complexity plus the likelihood code cost, is known as the *Stochastic Complexity* (SC).

The computation of parametric complexity can be a tedious and difficult task. When the code class $\boldsymbol{C}$ is parametric, if the stochastic complexity is finite and $\boldsymbol{C}$ belongs to an

exponential family, the parametric complexity can be approximated by its asymptotic form [Ris96],

$$PC(\mathbf{C}, N) = \frac{k}{2}\ln\frac{N}{2\pi} + \ln\int_{\theta\in\Theta}\sqrt{|I(\theta)|}d\theta + o(1) \tag{2.20}$$

Where k is the number of parameters and $I(\theta)$ is the Fisher information matrix where the (i, j) entry is computed as

$$I_{i,j}(\theta) = -E_D\left[\frac{\partial^2}{\partial\theta_i\partial\theta_j}\ln P(D \mid \theta)\right] \tag{2.21}$$

The first term of the asymptotic form of stochastic complexity computes the complexity contributed by the number of parameters, the form of which is consistent with *Bayesian Information Criterion* (BIC). However, measuring complexity by number of parameters alone is not sufficient. Both a Gaussian model and a uniform model have two parameters but the data representation capacities are different. This "richness" of a model space is captured by the second term derived from Fisher information matrix.

The one part MDL offers immediate guide on the model selection problem. Given two model classes, parametric complexity represents the complexity term of a model class and maximum likelihood code captures the goodness of the fit to the data. The sum of the two, stochastic complexity, offers the yardstick in the model selection problem. The model of choice is the one that minimizes the stochastic complexity.

2.5 Encoding Continuous Data

If data to be encoded is continuous, where the probability for a particular member is zero, the corresponding encoding length becomes infinity. Hence continuous data can only be encoded to a certain precision. Let x be a real number and let f be a continuous probability measure on the real numbers. The probability of x with precision ε is

$$\Pr(x) = \int_{x-\frac{\varepsilon}{2}}^{x+\frac{\varepsilon}{2}} f(x)dx \approx \varepsilon f(x) \tag{2.22}$$

The corresponding description length becomes

$$L_{f,\varepsilon}(x) = -\ln f(x) - \ln \varepsilon \tag{2.23}$$

In minimizing the description length regarding to f, the choice of precision becomes irrelevant. By assuming all codes use the same infinitesimal precision, the relative description length is simply $L_f(x) = -\ln f(x)$ by dropping the precision term. The relative description length can potentially be negative if the probability density of x is larger than one. In this scenario, it is sufficient to remember that the actual description length is always positive and the negative description function is the original description length less a constant where they share the same MDL estimators.

2.6 Computation of Stochastic Complexity

The computation of stochastic complexity involves integrating maximum likelihood over the entire data space and can be a tedious and time consuming task. When the asymptotic form applies, it facilitates the computation significantly. For large data size N and fixed number of parameters, the term contributed by Fisher information matrix becomes

insignificant and stochastic complexity reduces to Bayesian information criterion. However, MDL is significantly different from BIC when k and N are of comparable magnitude.

Example2.2 (Binomial Sequence): The probability mass function for a binomial distribution is given by

$$f(n;p)=\frac{N!}{n!(N-n)!}p^{n}(1-p)^{N-n} \tag{2.24}$$

The determinant of the Fisher information matrix is

$$|I(p)|=\frac{1}{p(1-p)} \tag{2.25}$$

The asymptotic form of the parametric complexity can thus be computed as

$$PC(\mathbf{P},N)=\frac{1}{2}\ln\frac{N}{2\pi}+\ln\int_{0}^{1}\sqrt{\frac{1}{p(1-p)}}dp+o(1)=\frac{1}{2}\ln N+\frac{1}{2}\ln\frac{\pi}{2}+o(1) \tag{2.26}$$

It is also impossible to compute the stochastic complexity exactly by exhaustively summing up the maximum likelihood over all possible data. Kontkanen et al [KMB+03] proposed an efficient recursive method that allows computing the parametric complexity at $O\left(N^{2}\ln|S|\right)$. For the binomial example, the exact parametric complexity and the asymptotic parametric complexity are compared in Figure 2.2. For practical purposes, the asymptotic form is good approximation of the exact form.

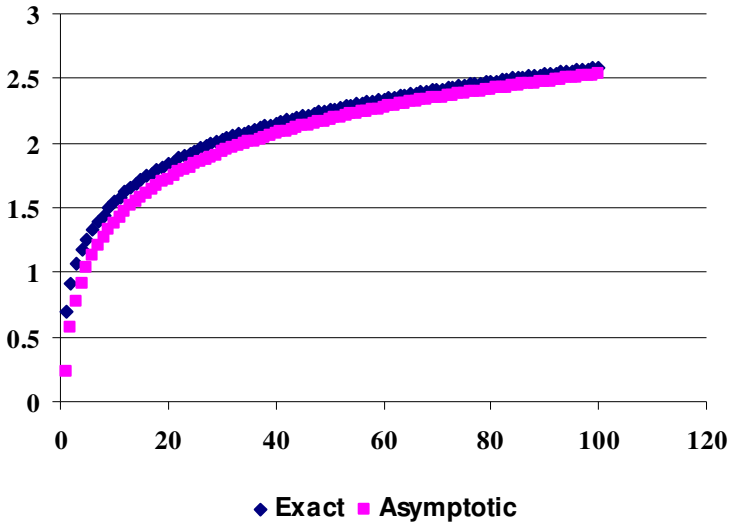


Figure 2.2 Exact and Asymptotic Parametric Complexity of Binomial Distribution

2.7 Encoding Clustering Data

For parameterized clustering algorithms such as K-means clustering, the MDL principle introduced above is immediately applicable once a prefix code on the data is designed within the clustering framework. For example, in K-means clustering, a pattern can be encoded with three parts of description indicated below.

The first part describes the cluster assignment of the pattern. This part combined with the cluster parameters constitutes the basis for subsequent descriptions. The second part and third part describes the direction and distance of the vector from the pattern to the cluster center. Three parts descriptions together fully encode a pattern in the data space.

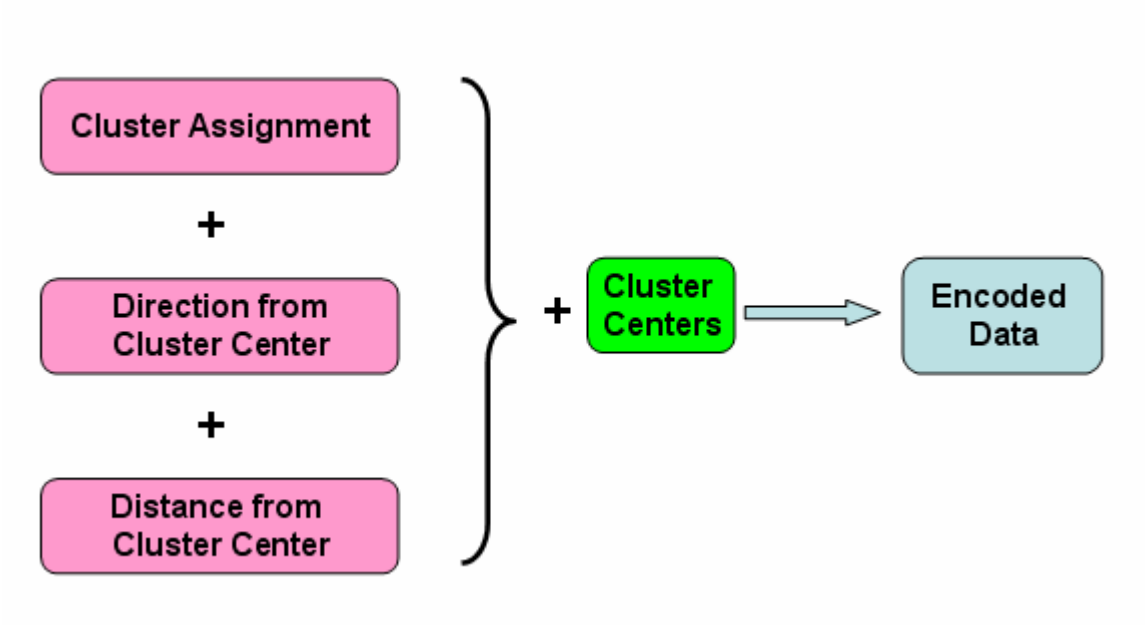


Figure 2.3 Encoding Clustering Data

2.7.1 Encoding Cluster Assignment

To encode the assignment of a pattern to K possible clusters is to encode a symbol from a finite alphabet with size K. The description length for encoding the cluster assignment for N patterns is,

$$L_1 = PC(N, \mathbf{C_K}) - \sum_{i=1}^{K} n(i) \ln \frac{n(i)}{N} \tag{2.27}$$

The parametric complexity can be either computed from with recursive method or from its asymptotic form. For fixed cluster number K, however, the parametric complexity is a constant that does not change with cluster parameters, thus can be excluded from the description length function without affecting inference. If the number of clusters is also a parameter, the parametric complexity must be included in the description length function to reflect the description length increase due to more complicated model.

2.7.2 Encoding Vector Direction

In K-means clustering, the Euclidean distances from the patterns to the cluster centers are treated equally regardless of the directions of the corresponding vectors they are computed from. This allows constant encoding length of the vector direction from the patterns to the cluster centers, which can be excluded from the description length function.

2.7.3 Encoding Vector Length

In K-means clustering, the Euclidean distance from a pattern $\boldsymbol{x}$ to its cluster center $\mathbf{C_x}$ is computed as

$$r = \left\| x - C_x \right\|^2 \tag{2.28}$$

The objective of K-means clustering is to minimize the sum of the Euclidean distances over all patterns. The prefix code to encode the distances must also reflect this preference, reserving succinct code words for short distances and redundant code words for large distances. One code of choice is the exponential distribution, whose probability density function is

$$f(r;\sigma) = \frac{1}{\sigma}\exp\left(-\frac{r}{\sigma}\right) \tag{2.29}$$

For N patterns with Euclidean distances $r_1,...,r_N$, the total length of the code as the function of the distances is,

$$L_\sigma(r_1,...,r_N) = \sum_{i=1}^{N}\frac{r_i}{\sigma} + N\ln\sigma + PC(\boldsymbol{\sigma}, N) \tag{2.30}$$

The maximum likelihood code is obtained by maximizing L_σ over σ,

$$\sigma^* = \frac{\sum_{i=1}^{n} r_i}{N} \tag{2.31}$$

Substitute the maximum likelihood estimator, the stochastic complexity the exponential distribution model is

$$L_{\sigma^*}(r_1,...,r_n) = N + N\ln\frac{\sum_{i=1}^{N} r_i}{N} + PC(\boldsymbol{\sigma}, N) \tag{2.32}$$

The Fisher information determinant of the model is,

$$I(\sigma) = \frac{1}{\sigma^2} \tag{2.33}$$

The asymptotic form of the parametric complexity suffers the infinity problem,

$$\int_0^{\infty} \sqrt{I(\sigma)}d\sigma = \infty \tag{2.34}$$

The problem can be solved by restricting our model space to $\sigma \in [\sigma_{\min}, \sigma_{\max}]$, the parametric complexity becomes,

$$PC(N,\boldsymbol{\sigma}) = \frac{k}{2}\ln\frac{N}{2\pi} + \ln\int_{\sigma_{\min}}^{\sigma_{\max}} \sqrt{I(\sigma)}d\sigma + o(1) = \frac{1}{2}\ln\frac{N}{2\pi} + \ln\ln\frac{\sigma_{\max}}{\sigma_{\min}} + o(1) \tag{2.35}$$

The total description length of K-means clustering is the sum of all three parts,

$$L_{K-means} = PC(N,\mathbf{C}_{\mathbf{K}}) - \sum_{i=1}^{K} n(i)\ln\frac{n(i)}{N} + N + N\ln\frac{\sum_{i=1}^{N} r_i}{N} + PC(\boldsymbol{\sigma}, N) \tag{2.36}$$

In the description length function, both the cluster frequencies $n(i)$ and the Euclidean distances r_i can be deterministically computed once the cluster partition is decided. The MDL solution to the cluster is to find the partition that minimizes the above description

length function. Various searching techniques can be applied in finding the optimal partition solution.

2.8 MDL and Informed Clustering

The MDL properties made it a superior inference method in the informed clustering problems to other alternatives such as maximum likelihood estimation.

- It measures information ubiquitously, facilitating combining and managing different types of background knowledge from various sources and formats.
- It automatically prevents model over-fitting, penalizing complex models via parametric complexity.
- It allows easy model selection and hypothesis testing, such as deciding the number of clusters of the relevance of cluster constraints.

Encoding patterns within clustering framework with MDL principle involves the three necessary steps

- Design efficient universal code to encode the data, which corresponds to a probability distribution on the data space.
- Derive the description length function regarding to the parameters.
- Find an efficient searching algorithm to minimize the description length function.

In the subsequent chapters, we explore different encoding and optimization approaches in solving three informed clustering problems introduced in chapter 1.

3 Multi-View Clustering with MDL

3.1 Introduction

A recent development on clustering is to cluster unsupervised data with multiple views. A view refers to a set of attributes that describes a class. In some practical problems, the attributes under investigation may naturally separate themselves into different groups. Take class STUDENT as an example, a set of attributes that describes the class include age, gender, nationality and other demographic related attributes. At the same time, STUDENT can also have attributes such as the grades for a list of courses she has completed. The attributes naturally fall into two categories, demographic and academic. Both views convey information about the STUDENT class so they can mutually inform each other in a learning problem. The multiple view learning problems first stemmed from supervised learning on web text classifications. A webpage can be described both by an intrinsic view, the contents of the webpage and an extrinsic view, the links related to the webpage. Blum and Mitchell [BM98] proposed co-training concept, allowing the

classified labels from one view be used as training examples of other views when the data is scarcely labelled, assuming conditional independence among the views.

If we view clustering as supervised learning but with no training labels at all, it is tempting to extent co-training framework into multiple view clustering. However, there is subtle and important difference. In Blum and Mitchell's co-training framework, the class labels from both views are from the same discrete set. In multiple views clustering, the latent labels are potentially from different sets: each view can have its own number of clusters thus even the cardinals of the latent labels are different. Nevertheless, such extension of co-training has been proposed, with a strong constraint that the views have the same number of cluster [BS04].

A natural approach to the multi-view clustering problems is to partition the patterns within each view independently and infer dependency information from the cluster assignments among the views. However, such type of inference is problematic, as the inference does not consider the fact that the views are observed from the same set of patterns. As a consequence, this approach usually underestimates the dependency among the views. The remedy is to factor in the dependent information among the views during the clustering process. As the views describe the same set of patterns, the cluster assignment among the views should be as similar as possible, while maintaining reasonable homogeneity of the patterns within the same clusters.

Kaski et al. proposed associative clustering algorithm [KNS+05], with the above stated philosophy behind. The algorithm clusters both views simultaneously, attempting to maximize the mutual information between the clustering latent labels, with constraints enforcing that each cluster is of Voronoi type, which states each pattern must be assigned to its closest cluster center. Associative clustering can be better understood from a Bayesian inference framework: A priori, the mutual information between the cluster latent labels from the two views should be maximized, with the prior knowledge that the views refer to the same set of objects. The prior is later adjusted with the observed attributes within the views. Thus associative clustering is a crude approximation of maximum a posteriori estimation.

Although associative clustering is a significant development towards the multi-view clustering problem, a number of challenges still remain. First, no bound is known for the quality of the approximation. It is desirable to have an exact method that quantitatively unifies the prior and the likelihood. Second, the number of clusters in most multiple view clustering methods, including associative clustering, is assumed to be known a priori. While it is reasonable to specify them a priori in some scenarios, one may prefer to allow the data to inform on the number of clusters when one is not equipped with sufficient prior knowledge or preference.

The MDL principle introduced in chapter 2 avail itself as an ideal tool to tackle the above mentioned challenges. By applying MDL principle, we have the following benefits in solving the multiple views problem:

1. Quantitatively define the dependency information between the latent labels of the clustering outcomes from both views, as well as the dissimilarity information within each cluster.
2. Quantitatively define model complexity based on the number of clusters from each view.
3. Unify all types of information to yield one global objective function to be minimized.

This chapter provides a framework on constructing encoding, deriving encoding length, optimizing encoding length for multiple views clustering problem.

3.2 Multiple Views Clustering with MDL

Let X and Y be two views of N patterns, and K_1 and K_2 be the number of clusters within each view. In this section, K_1 and K_2 are assumed to be given and fixed while we discuss how they can be informed by the patterns in later sections. Let P_i:$\{1,\ldots,N\}\rightarrow\{1,\ldots,K_i\}$ (i=1,2) be the partition mapping from the patterns to clusters. Let $L(P_1, P_2)$ be the description length function to encode both views with P_1 and P_2 as variables, the problem is to find the partitions P_1 and P_2 that minimizes L.

Encoding the patterns can be achieved by first encoding the partitions for both views and then encoding the patterns relative to the cluster centers which are deterministically defined by the partitions. For each pattern, the number of possible cluster assignment outcomes is K_1K_2, which we encode with a multinomial distribution. The one part complete MDL length is,

$$L_{DepL}(P_1, P_2) = -\sum_{\substack{i=1,\ldots,K_1 \\ j=1,\ldots,K_2}} n(i,j)\ln\frac{n(i,j)}{N} + PC(\mathbf{K}_{12}, N) \tag{3.1}$$

where $n(i, j)$ is the number of patterns that has been assigned to ith partition in view X and jth partition in view Y and $PC(\mathbf{K_{12}},N)$ is the parametric complexity. This syntactically simple joint encoding allows us to capture the dependently information between the partitions from the two views.

An alternative scheme to encode the partition information is to encode the partitions from both views independently with multinomial distribution of K_1 and K_2 possible outcomes respectively. The associated description length is

$$\begin{aligned} L_{Indep}(P_1, P_2) = &-\sum_{i=1,\ldots,K_1} n(i,.)\ln\frac{n(i,.)}{N} + PC(\mathbf{K}_1, N) + \\ &-\sum_{j=1,\ldots,K_2} n(.,j)\ln\frac{n(.,j)}{N} + PC(\mathbf{K}_2, N) \end{aligned} \tag{3.2}$$

The dependent encoding results in shortened description length when the cluster partitions between the views are correlated. The difference of encoding length between dependent encoding and independent encoding is,

$$L_{DepL}(P_1, P_2) - L_{Indep}(P_1, P_2) = -N\hat{I}(I\|J) + \Delta PC \tag{3.3}$$

$$\hat{I}(I\|J) = \sum_{\substack{i=1,\ldots,K_1 \\ j=1,\ldots,K_2}} \frac{n(i,j)}{N}\ln\frac{\frac{n(i,j)}{N}}{\frac{n(i,.)}{N}\frac{n(.,j)}{N}} \tag{3.4}$$

is the empirical mutual information between the two views and

$$\Delta PC = PC(\mathbf{K}_{12}, N) - PC(\mathbf{K}_1, N) - PC(\mathbf{K}_2, N) \tag{3.5}$$

is the extra parametric complexity of the dependent encoding over the independent encoding.

Equation (3.3) captures the essentials in multi-view clustering: If the mutual information between the assignments of the two views are large enough to overcome the increase of parametric complexity by adopting joint encoding, dependent encoding leads to shorter overall description length. Otherwise if the mutual information is not sufficient to compensate the increased parametric complexity, then independent encoding should be chosen.

After the partition information is encoded, with either independent or dependent encoding mentioned above, the patterns are encoded relative to their assigned cluster centers. We use the following assumptions in the code:

1. A priori, the pattern density distribution is uniform across all different angles.

2. The pattern density is larger when nearer to the cluster center.

These two assumptions are based on the fact we consider quantization error as a measure on the quality of the clusters. All the Euclidean distances from the patterns to the cluster centers are treated equally regardless of the directions of the corresponding vectors they are computed from. This allows constant encoding length of the vector direction from the patterns to the cluster centers, which can be excluded from the description length function. Assumption 2 reflects the fact we prefer smaller quantization errors. That is, if the probability density is larger near to the cluster centers, it in turn requires less number of bits to describe a pattern that is close to its corresponding cluster center than a pattern

that is far from its cluster center. For each pattern, there are two Euclidean distances (squared) to be encoded,

$$r_n = \left\| \mathbf{x}_n - \mathbf{C}_X\left(P_1(n)\right) \right\|^2, s_i = \left\| \mathbf{y}_n - \mathbf{C}_Y\left(P_2(n)\right) \right\|^2 \tag{3.6}$$

with $\mathbf{C}_X(i)$ representing the cluster center for the ith pattern in view X and likewise for Y. We encode the distances with the code introduced in (2.36),

$$\Pr(r) = \frac{1}{\sigma} \exp\left(-\frac{r}{\sigma} \right) \quad \sigma > 0 \tag{3.7}$$

While the exponential distribution is just one of the possible distributions that embodies the preference over smaller quantization errors, it provides attractive properties to the message length function, as we see later. The description length of the Euclidean distances for all the patterns is simply a sum of the individual description lengths,

$$L(\sigma) = N \ln \sigma + \frac{\sum_{i=1}^{N} r_i}{\sigma} + PC(\mathbf{\Sigma}, N) \tag{3.8}$$

The parametric complexity only depends on the choice of code set and the data length, thus does not affect the minimization solution. Minimizing L with σ yields the shortest description length function.

$$L_{NML}(r_1, ..., r_N) = N \ln \frac{\sum_{i=1}^{N} r_i}{N} + N + PC(\mathbf{\Sigma}, N) \tag{3.9}$$

Both equation (3.2) and equation (3.6) are functions of the partitions P_1 and P_2. The problem thus becomes minimizing the sum of the two in regard to the partitions. The total description length function after truncating constants becomes,

$$L = -\sum_{i,j} n(i,j) \ln \frac{n(i,j)}{N} + N \left(\ln \frac{\sum_{i=1}^{N} r_i}{N} + \ln \frac{\sum_{i=1}^{N} s_i}{N} \right) \tag{3.10}$$

Theorem 3.1 (Invariance) The MDL estimation on multi-view clustering with objective (3.10) is invariant to translation, rotation and scaling on each view.

Proof: As the encoding uses the polar coordinate and the description length function only depends on the distances between the patterns to the assigned cluster centers, translation and rotation will not change the objective function thus the estimation is invariant to both translation and rotation.

It is also easy to see that the estimation is invariant to view scaling: Let α, β be two scalars to be applied to each view. The new objective function becomes,

$$L_{\alpha,\beta} = -\sum_{i,j} n(i,j) \ln \frac{n(i,j)}{N} + N \left(\ln \frac{\sum_{i=1}^{N} \alpha^2 r_i}{N} + \ln \frac{\sum_{i=1}^{N} \beta^2 s_i}{N} \right) = L + N 2 \ln \alpha\beta \tag{3.11}$$

The added term is not a function of the clustering partition and thus will not affect the inference. **Q.E.D.**

3.3 Finding the Optimal Partitions

We use Annealed EM (AEM) to search for the optimal partitions that minimizes the description length function. The pseudo-code for the algorithm is as following:

$T \leftarrow T_0$

Do While $(T > \varepsilon)$ {

E Step: For Each $n \in \{1,...,N\}$ {

1. For Each $(i, j) \in \{1,...,K_1\} \times \{1,...,K_2\}$
   Compute The Description Length Function $L(i,j)$
   by Assigning Pattern n to Partition (i,j)
2. Compute Description Length Defined Probability
   $P(i, j)$ under Temperature T
3. Stochastically Choose Partition of Pattern n from P.

}

M Step: Update the Choice of Code to Minimize the Description Length with the Current Parition

A Step: $T \leftarrow \eta T$

}

E-Step. In step 1, the description lengths are computed with the current chosen code for every possible K_1K_2 partition assignment for pattern n while fixing other pattern assignments intact. In step 2, the probability distribution P under temperature T is computed as the following,

$$P(i, j) = \frac{\exp\left(-\frac{L(i, j)}{T}\right)}{\sum_{i,j} \exp\left(-\frac{L(i, j)}{T}\right)} \tag{3.12}$$

Step 3 commits the actual pattern assignment by sampling from the multinomial distribution $P(i, j)$.

As indicated in equation (3.12), when T is large, an assignment for pattern n with shorter description length is only marginally favored over an assignment with longer description length. The sampler has more freedom to traverse through the entire solution space in

order to escape local minimum. At later stage when T is near 0, the sampler "freezes" and becomes a greedy algorithm, always choosing the assignment with the shortest description length. Theoretically speaking, if T decreases slowly enough, the probability that the algorithm finds the global minimum converges to one [KGV83].

M-Step. M-step chooses the optimal code to encode the data given the assignments committed in E-step. Although the estimators coincide with maximum likelihood estimators, the philosophy is completely different from maximum likelihood estimation. The optimal codes for view X are,

$$P(i,j) = \frac{\sum_{n=1}^{N} \delta(P_1(n),i)\delta(P_2(n),j)}{N},$$
$$\mathbf{C_X}(k) = \frac{\sum_{n=1}^{N} \delta(P_1(n),k)\mathbf{x_n}}{\sum_{n=1}^{N} \delta(P_1(n),k)}, \sigma_X(k) = \frac{\sum_{n=1}^{N} \delta(P_1(n),k) r_n}{\sum_{n=1}^{N} \delta(P_1(n),k)} \tag{3.13}$$

The delta function takes 1 when the two function parameters are equal and takes 0 otherwise. The optimal codes for view Y can be computed analogously.

Theorem 3.2 (Monotonicity) The expected description length monotonically decreases in the AEM algorithm.

Proof: The M-step by definition monotonically decreases the description length. The A-step does not change the description length. We only need to prove that E-step monotonically decrease the expected description length. To see this, let $L(i,j)$ be the

description length associated with encoding a given pattern by assigning the pattern to the *i*th cluster in view *X* and the *j*th cluster in view *Y*.

$$\text{Let } C = \sum_{i,j} \exp\left(-\frac{L(i,j)}{T}\right)$$

$$Q(i,j) = \frac{1}{K_1 K_2}$$

$$P(i,j) = \exp\left(-\frac{L(i,j)}{T}\right) \Big/ C$$

$$L(i,j) = -T \ln C - T \ln P(i,j)$$

$$E_P[L] = \sum_{i,j} P(i,j) L(i,j) = -T \sum_{i,j} P(i,j)(\ln C + \ln P(i,j))$$

$$= -T\left(\sum_{i,j} P(i,j) \ln C + \sum_{i,j} P(i,j) \ln P(i,j)\right)$$

$$= -T \ln C - T \sum_{i,j} P(i,j) \ln P(i,j)$$

$$E_Q[L] = \sum_{i,j} Q(i,j) L(i,j) = -T \ln C - T \sum_{i,j} Q(i,j) \ln P(i,j)$$

Dropping the index (i,j) for simplicity,

$$E_P[L] - E_Q[L] = -T \sum_{i,j} (P - Q) \ln P$$

$$= -T \sum_{i,j} (P \ln P - Q \ln Q - Q \ln P + Q \ln Q)$$

$$= -T\left(-\sum_{i,j} Q \ln Q + \sum_{i,j} P \ln P + \sum_{i,j} Q \ln \frac{Q}{P}\right) \le 0$$

$$-\sum_{i,j} Q \ln Q - \left(-\sum_{i,j} P \ln P\right) \ge 0 \quad \text{(maximum entropy)}$$

$$\sum_{i,j} Q \ln \frac{Q}{P} \ge 0 \quad \text{(relative entropy)}$$

Q.E.D

The computational complexity of the algorithm is O(IK_1K_2N), where *I* is the number of iteration that is determined through T_0, ε and η. The computation complexity is of course also linear to the number of attributes from the larger view.

3.4 Empirical Results

We evaluate the MDL based multiple views clustering algorithm on a number of simulated and real world datasets. In addition to the description length as a universal metric, we also define two other metrics that have more immediate pragmatic implications.

3.4.1 Matching Rate (MR)

A matching rate measures the captured dependency between the two views. For N patterns, let $n(i, j)$ be the number of patterns assigned to ith cluster on view X and jth cluster on view Y simultaneously. Let

$I=(i_1,i_2,\ldots,i_{K1})$ be a permutation of $\{1,2,\ldots,K_1\}$

$J=(j_1,j_2,\ldots,j_{K2})$ be a permutation of $\{1,2,\ldots,K_2\}$

Then the matching rate is defined as

$$MR = \frac{1}{N} \max_{I,J} \sum_{m=1}^{\min(K_1,K_2)} n(i_m, j_m) \tag{3.14}$$

The definition of matching rate can be most easily understood by constructing a contingency table K_1 by K_2, with the (i, j) entry representing the number of patterns belong to cluster i from view X and cluster j from view Y. The matching rate is simply the largest possible sum of min (K_1, K_2) entries by using each row and column only once, divided by the total sum.

Matching rate establishes a correspondence of the clusters between the views. It is a measurement on the predictability of the partition from one view to the partition from another view, thus an evaluating on the associative dependency between the views.

3.4.2 Predictive Rate (PR)

If the patterns are labeled with external classes and one is interested in using the two views clustering partitions to predict the labels, one can associate each cluster combination (*i, j*) with a class. The predictive rate measures the accuracy of the predictions. For *N* patterns, let *n*(*i, j, k*) be the number of patterns assigned to *i*th cluster on view *X* and *j*th cluster on view *Y* labeled with class *k*, the predictive rate is defined as,

$$PR = \frac{1}{N} \sum_{i,j} \max_{k} [n(i, j, k)] \tag{3.15}$$

Predictive rate measures the association between the cluster partitions and the external class label. The prediction rate need not to be measured on a separate holdout set as typically in classical supervised learning, because the external labels are not used to supervise the clustering. Predicting rate is a post clustering evaluation to ensure the partitions carry some useful information in the problem context.

We use the description length together with the two metrics defined above to evaluate the performance of the multiple view clustering algorithms. In this section, we use a number of synthesized datasets as well as some real world ones. We abbreviate the description length for encode the partition information as Partition Description Length (PDL), the description length to encode the patterns given the partitions as Cluster Description

Length (CDL) and the sum of the two as Total Description Length (TDL). For each problem, we also report the matching rate and prediction rate where applicable.

We first demonstrate the property of MDL multiple views cluster with a synthesized dataset. In the dataset, 1000 patterns are randomly generated. Both view *X* and view *Y* containing two continuous attributes. For the first 500 patterns, all attributes from both views are independently sampled from normal distribution N(1,1) and for the last 500 patterns, all attributes are independently sampled from N(-1,1). The dependency between the two views is verified by the correlation matrix.

$$R = \begin{bmatrix} 1 & 0.5 & 0.5 & 0.5 \\ 0.5 & 1 & 0.5 & 0.5 \\ 0.5 & 0.5 & 1 & 0.5 \\ 0.5 & 0.5 & 0.5 & 1 \end{bmatrix} \tag{3.16}$$

The dependency between the two views is gradually reduced if we fix the positions of one view and randomly permutate a certain percentage of patterns in the other view. For each permutation, we compare the clustering solutions via dependent and independent encoding of the partitions. The number of clusters is set to 2 for each view.

Table 3.1 illustrates some important properties of MDL multiple views clustering. The dependent encoding captures the dependent information between the views. The number of bits saved with dependent encoding compared to independent encoding is most significant when the dependency between the views is strong. As the dependent information between the views start to diminish, the algorithm automatically manages the

tradeoff between Partition Description Length and Cluster Description Length. When the views are completely permutated and dependent encoding is no longer exploitable, the dependent encoding performs almost identically to the independent code. Table 3.1 also explains why minimizing the overall quantization error is not the optimal solution. Although the quantization error (represented by CDL) is always smaller for independent encoding, the additional description length on partition information makes greater total description length for independent encoding.

Table 3.1 MDL Multi-view Clustering on Synthesized Data

Permutation	Coding	PDL	CDL	TDL	MR	PR
0%	Dep	693.13	1353.19	2046.32	1	0.982
	Indep	1381.68	1174.17	2555.85	0.851	0.844
25%	Dep	919.6	1376.58	2296.18	0.94	N/A
	Indep	1381.68	1174.17	2555.85	0.765	N/A
50%	Dep	1235.54	1223.62	2459.16	0.766	N/A
	Indep	1381.68	1174.17	2555.85	0.673	N/A
100%	Dep	1370.02	1180.35	2550.37	0.568	N/A
	Indep	1381.68	1174.17	2555.85	0.539	N/A

With dependent encoding, the algorithm matches the two views very efficiently. Even when the views are 25% permutated, the method allows 94% of the matching to be recovered.

The second dataset we use is the pen-based handwritten digit dataset from the UCI data repository. Each pattern has 16 attributes, which are the horizontal and vertical positions of 8 sampled points when the digit is written. We naturally cleave the dataset into two views with 8 attributes each representing 4 sampled points on the written paths. The

externally labeled digit class is not used in the clustering but only used to evaluate the prediction rate. For clarity and simplicity, we reduce the problem of 10 different digits into a sub-problem with only 2 different digits. In particular, we are interested in two pairs, 0-1, 3-8 and 1-7. The 0-1 and 3-8 pairs represent simpler version of the multiple views clustering problem as both views are significantly different from each other. The 1-7 pair represents are more difficult problem given the second view (bottom half) of digit 1 and 7 are very similar. By fixing the number of clusters as 2 for both views, the results are reported in Table 3.2.

Table 3.2 Two View Clustering Results for Different Digit Pairs

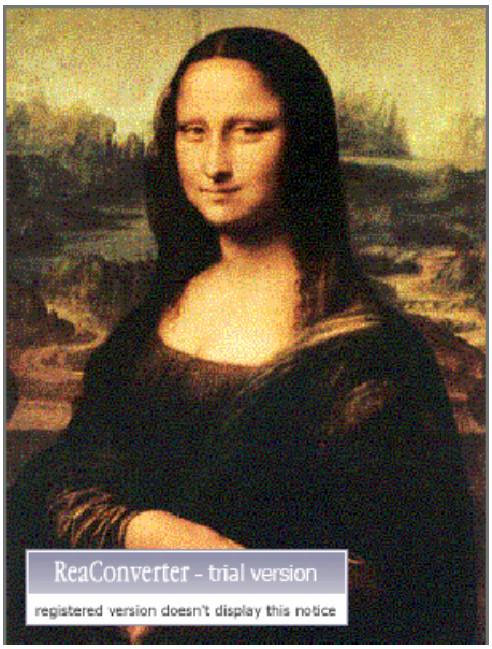
Digit 0-1					
Coding	**PDL**	**CDL**	**TDL**	**MR**	**PR**
Dep	1080.5	25329.8	26410.3	1	0.995
Indep	2139.4	25243.6	27383	0.906	0.985
Digit 1-7					
Coding	**PDL**	**CDL**	**TDL**	**MR**	**PR**
Dep	1079.2	24181.7	25260.9	1	0.795
Indep	1382.3	24443	25825.3	0.562	0.785
Digit 3-8					
Coding	**PDL**	**CDL**	**TDL**	**MR**	**PR**
Dep	996.6	22644.7	23641.3	1	0.988
Indep	1993.5	22513.2	24506.7	0.939	0.981

Table 3.2 illustrates that the MDL based multiple views clustering algorithm does not merely minimizes an abstract mathematical function, but have pragmatic implications. The shorter overall description length leads to better matching rate and prediction rate. The external class labels are not used in the clustering algorithm. The higher prediction rate with dependent encoding suggests that the algorithm achieves the cluster partition in

a more meaningful way by considering the potential dependent information between the views.

The MDL based multi-view clustering algorithm can also be readily applied to image segmentation problems. A color image consists thousands or millions of pixels, each represented by a RGB vector, whose three components correspond to the strength of red, green and blue. In addition to the color view on the pixels, each pixel also has X-Y coordination on the X-Y plane, which constitutes the location view of the image. Both color and position of the pixels are important in finding meaningful segmentation of the image, but different scales between the two views does not allow combination of two views into one. The problem is of classical multi-view clustering setting.

Multi-view clustering with pixel color and location view simultaneously can obtain better segmentation of the picture. Figure 3.1 shows an example of different levels of image recovery from segmenting image solely based on RGB color and by MDL based multi-view clustering on a BMP picture, each segments the picture with 10 clusters. For each pixel, the RGB color of the pixel is replaced by its assigned cluster center RGB color to show the segmentation. As the multi-view approach uses the spatial information as well as the color information, it achieves a better recovery of the images.



(a)

(b) (c)

Figure 3.1 MDL Based Multi-View Clustering on Image Segmentation.

(a) is the original image (b) is the MDL based multi-view segmentation (c) is the RGB segmentation

3.5 Model Selection

Until now, we have always assumed the number of clusters are predefined and fixed for each view in the problem. One trademark property of MDL principle is that it allows model selection. The description lengths computed from different models are directly comparable. With this property, we can find a good estimation of the number of clusters from each view by progressively attempting more complicated models.

The approach is very straightforward: starting with two clusters within each view, progressively increase the number of clusters. The best number of clusters combination is the one with the shortest description length. Table 3 demonstrates the method by find the optimal number of clusters in the digit pair 1-7 problem. The parametric complexity is approximated with their asymptotic expansion form for the multinomial distributions.

Table 3.3 Selecting Number of Clustering Within Each View

Negative Log Likelihood			
	K2=2	**K2=3**	**K2=4**
K1=2	25260.9	25124	25068.2
K1=3	25126.5	25062	24955.1
K1=4	25121.3	25052	24961.5
Approximated Parametric Complexity			
	K2=2	**K2=3**	**K2=4**
K1=2	8.3	13.8	19.3
K1=3	13.8	22.1	30.3
K1=4	19.3	30.3	41.3
Total Description Length			
	K2=2	**K2=3**	**K2=4**
K1=2	25269.2	25137.7	25087.5
K1=3	25140.2	25084.1	24985.4
K1=4	25140.6	25082.3	25002.8

It is easily identified from Table 3.3 that the number of clusters should be 3 and 4 respectively for the two views in the problem. Although there is possibility some higher number of clusters might yield even shorter description length, in practice we avoid too many clusters by imposing an upper bound of the number of clusters for each view.

3.6 Chapter Summary

In this chapter, we have introduced a MDL based multiple view clustering framework. It adopts a single metric to evaluate the clustering solutions, namely the number of bits to encode the patterns. This universal metric unifies the partition information with the cluster variance information, which allows not only automatic information tradeoff between dependency and quantization error, but also allows the model selection, allowing the data to inform the number of clusters within each view. Empirical evidence indicates the MDL multiple views clustering framework captures the dependent information among the views efficiently, leading to higher matching rate. Also, the cluster solutions are more informative, supported by higher prediction rate.

4 Semi-Supervised Clustering

4.1 Introduction

Semi-supervised clustering refers to clustering problems where a small percentage of the patterns are labeled. The situation arises usually because the process of obtaining abundant labeled data is expensive, if not impossible. As the limited amount of labeled data is not sufficient to build a model through standard supervised learning, the learner utilizes the information encompassed in the unlabeled data to improve performance. The data to be learnt come from set $\mathbf{X}^{\mathbf{D}} \times \mathbf{Y}$, where $\mathbf{x} \in \mathbf{X}^{\mathbf{D}}$ is a D-dimension vector and Y is a finite set that represents the partial labels, taking the values from a categorical set including missing values. Like plain clustering problems, the goal of semi-supervised clustering is to find the partition mapping from the patterns to a finite set of clusters. In addition to identifying partitioning structure among the patterns, semi-supervised clustering also concentrates on building classifier by exploiting the clustering structure and the restricted numbers of class labels.

There are two common approaches to encompassing the exterior label information in the clustering paradigm. The first approach is to derive instance-level clustering constraints from the labels, with patterns sharing the same class label forming must-link constraints and patterns with different labels forming cannot link constraints, which are enforced in the clustering process [BBM02][CCM03]. A second approach is to treat the labels as the consequence of different generating mechanisms from each cluster, building generative classifiers within each cluster with the available class labels. Homogeneity of exterior label within a cluster is preferred but not as strictly enforced as in the constrained clustering approach [GH04]. We concentrate on the second approach in this chapter and defer discussion on constrained clustering in chapter 5.

In the mixture Gaussian approach to semi-supervised clustering, each pattern is considered to have a latent variable that represents its cluster assignment. In addition, each cluster has a multinomial generating mechanism of the class labels. Thus semi-supervised clustering is also a classifier that each cluster corresponds to a discrete probability distribution on the class labels. To infer a class label for a pattern, one may find its most likely cluster assignment first and then find its most likely class label given the cluster assignment. However, due to the nature of semi-supervised clustering that it has few labels to offer to the learner, the associated model uncertainty is very significant. For this reason, Bayesian inference where the class label prediction is made upon all possible models, rather than the most likely model, is desirable in the semi-supervised clustering context. This chapter discusses how MDL principle can be applied in building an optimal Bayes classifier (OBC) for semi-supervised clustering.

4.2 Semi-Supervised Clustering with Mixture Gaussian Model

The mixture Gaussian model assumes the patterns to be clustered a generated from K different Gaussian distribution. In generating the patterns, each Gaussian component is assigned a marginal probability that it is chosen to generate a pattern. The likelihood of a pattern in the mixture Gaussian model is the weighted sum of the likelihood of all the components,

$$f(x \mid \Theta) = \sum_{j=1}^{K} f(j) f(x \mid \mu_j, \Sigma_j)$$
$$f(x \mid \mu_j, \Sigma_j) = \frac{1}{\sqrt{(2\pi)^D |\Sigma_j|}} \exp\left(-\frac{1}{2} (x - \mu_j)^T \Sigma_j (x - \mu_j) \right) \tag{4.1}$$

The likelihood for all the patterns is

$$f(x_1, x_2, ..., x_n \mid \Theta) = \prod_{i=1}^{n} \sum_{j=1}^{K} f(j) f(x_i \mid \mu_j, \Sigma_j) \tag{4.2}$$

The probability that a pattern belongs to a particular component is given by the posterior probability,

$$f(\theta_j \mid x_i) = \frac{f(j) f(x_i \mid \mu_j, \Sigma_j)}{\sum_{j=1}^{K} f(j) f(x_i \mid \mu_j, \Sigma_j)} \tag{4.3}$$

In semi-supervised clustering, the partial labels are considered in the overall likelihood. Let $D_l = \{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$ be the labeled data, $D_l = \{x_{n+1}, x_{n+2}, ..., x_{n+m}\}$ be the unlabeled data. Assuming that $\boldsymbol{X}$ and $\boldsymbol{Y}$ are conditionally independent given Θ, the likelihood function for semi-supervised clustering is,

$$f(x_1, x_2,..., x_{n+m}, y_1, y_2,..., y_n \mid \Theta) = \left(\prod_{i=1}^{n} P(y_i \mid \theta_j) \sum_{j=1}^{K} f(j) f(x_i \mid \mu_j, \Sigma_j) \right) \left(\prod_{i=n+1}^{n+m} \sum_{j=1}^{K} f(j) f(x_i \mid \mu_j, \Sigma_j) \right) \quad (4.4)$$

where patterns up to m are labeled and $P(. \mid \theta_j)$ is the probability measure on $\boldsymbol{Y}$ for component j.

4.3 Posterior Probability and Model Uncertainty

Bayes theorem connects marginal probability, conditional probability and posterior probability together. In machine learning, Bayes theorem typically takes the following form,

$$P(\theta \mid D) = \frac{P(\theta) P(D \mid \theta)}{P(D)} \quad (4.5)$$

Here, H is a random variable on the set of all considered hypotheses and D is a random variable on the set of all possible data. $P(\theta)$ is the prior probability which represents the learner's belief on a given hypothesis before observing the data. $P(D \mid \theta)$ is the likelihood of data given the hypothesis. $P(D)$ is the marginal probability of the data D, performing as a normalization factor. $P(\theta \mid D)$ is known as the posterior, the probability distribution on the set of all considered hypotheses after the learner updates its prior with the data.

In the learning philosophy of a Bayesian, the learning process corresponds to the update of the learner's belief on the hypotheses after seeing the data. The outcome of learning is a probability distribution on the hypotheses set rather than a single hypothesis. If a single

hypothesis has to be inferred, the maximum a posteriori (MAP) estimation [Deg70] is the hypothesis that maximizes the posterior probability,

$$\theta_{MAP} = \arg\max_{h \in H}\left(P(D \mid \theta)\right) \tag{4.6}$$

Model uncertainty arises when the posterior distribution is replaced by the MAP estimation, where the posterior distribution reduces to assigning all probability mass to a single hypothesis. The amount of model uncertainty depends on the probability density around the MAP estimator. For example, for three considered hypotheses $\theta = \{\theta_1, \theta_2, \theta_3\}$ and two possible posterior distributions *P* and *Q* on the hypotheses that are given by

$$P(\theta_1) = \frac{1}{10}, P(\theta_2) = \frac{4}{5}, P(\theta_3) = \frac{1}{10}$$
$$Q(\theta_1) = \frac{3}{10}, Q(\theta_2) = \frac{2}{5}, Q(\theta_3) = \frac{3}{10}$$

Posterior *P* would have less model uncertainty than *Q* if the posteriors are replaced by the MAP estimation because it has a more concentrated probability distribution.

4.4 Bayesian Model Averaging

When the availability of the exterior labels are limited, the uncertainty associated with the semi-supervised clustering classifier is more significant compared to a classifier built from fully labeled data. In semi-supervised clustering, the posterior distribution is more diffused compared to its supervised counter part. Figure 4.1 and Figure 4.2 illustrate a simple example of learning with half the patterns labeled and with all the patterns labeled in a mixture Gaussian model, with the posterior learnt from partially labeled data flatter than the fully labeled data.

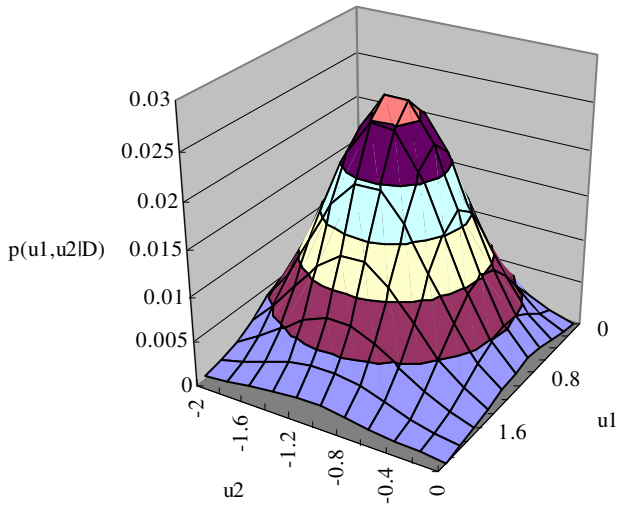


Figure 4.1 Posterior of a Mixture Gaussian with 8 Labeled Patterns

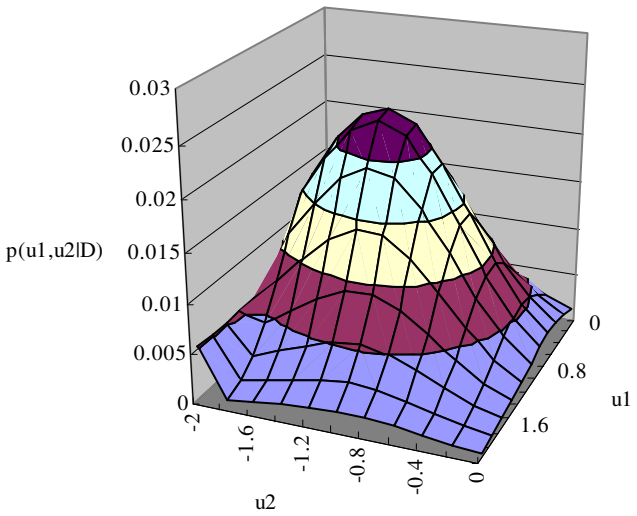


Figure 4.2 Posterior of a Mixture Gaussian with 4 Labeled and 4 Unlabeled Patterns

Point estimations such as maximum likelihood estimation (MLE) [Ald97] and maximum a posteriori estimation [Reg70] have reduced performance under considerable model

uncertainties in semi-supervised clustering. The model uncertainty is most well mitigated by Bayesian model averaging which averages inferences over all possible hypotheses, weighing each inference by the corresponding posterior probability of the hypothesis. For a given hypotheses set and prior distribution, Bayesian model averaging achieves the lowest risk [Mit97]. Mathematically, let Θ be the set of models, D_l be the set of labeled data and D_u be the unlabeled data, the Bayesian model averaging inference uses the entire posterior distribution for predictive inference. The most probable class label is predicted as

$$\arg\max_{y_i} : y_i = \int_{\Theta} P(y_i \mid x, \theta) P(\theta \mid D_l, D_u) d\theta \tag{4.7}$$

This contrasts to the MAP approach that makes predictions from the single model θ^* that has the largest posterior probability.

$$\arg\max_{y_i} P(y_i \mid x, \theta^*), \quad \theta^* = \arg\max_{\theta} P(\theta \mid D_l, D_u) \tag{4.8}$$

We can see that (4.8) approximates (4.7) if $p(\theta^* \mid D_l, D_u)$ dominates the posterior distribution. However, the two predictions can be different if the posterior distribution is not very peaked, which is typical in semi-supervised clustering. Under this situation, (4.7) integrates out the parameters to obtain the prediction not conditioned on any particular model in the model space, as shown in equation (4.9).

$$
\begin{aligned}
&\int_{\Theta} P(y \mid x,\theta) P(\theta \mid D_l, D_u) d\theta \\
&= \int_{\Theta} \frac{P(y,x,\theta)}{P(x,\theta)} \frac{P(\theta) P(D_l, D_u \mid \theta)}{P(D_l, D_u)} d\theta \\
&= \int_{\Theta} \frac{P(\theta) P(y,x \mid \theta)}{P(x)} \frac{P(D_l, D_u \mid \theta)}{P(D_l, D_u)} d\theta \\
&= \int_{\Theta} \frac{P(\theta) P(y,x,D_l, D_u \mid \theta)}{P(x) P(D_l, D_u)} d\theta \\
&= \frac{1}{P(x) P(D_l, D_u)} \int_{\Theta} p(y,x,D_l, D_u, \theta) d\theta \\
&= \frac{P(y,x \mid D_l, D_u)}{P(x)}
\end{aligned}
\tag{4.9}
$$

The main difficulty in performing Bayesian model averaging is to compute the integral over the posterior distribution $p(\theta \mid D_l, D_u)$ in (4.7). Uniform sampling on Θ typically is very inefficient way to estimate the integral as most of the samples would have small posterior probability and thus small weights. Importance sampling [Sri02] is desired to generate samples from Θ according to the posterior distribution. The integral is approximated by randomly generating models from the posterior distribution and averaging the inferences with unity weight. As more probable models are drawn more often, this approach asymptotically approaches the integral shown (4.7) [GRS96]. Typically it is achieved by constructing a Markov chain on Θ whose stationary distribution is equivalent to the posterior distribution.

4.5 Markov Chain Monte Carlo (MCMC)

4.5.1 Markov Chain

A Markov chain on set Θ is a collection of random variables θ^t that satisfies the Markov property,

$$P\left(\theta^{t+1} \mid \theta^0, \theta^1, ..., \theta^t\right) = P\left(\theta^{t+1} \mid \theta^t\right) \tag{4.10}$$

The Markov property states that the state of the chain at time t+1 only depends on its immediate previous state and conditionally independent of its historical path. With this property, a Markov chain is fully specified by the transition probability $P\left(\theta^{t+1} \mid \theta^t\right)$ and the probability on the initial state of the chain $P\left(\theta^0\right)$. A stationary distribution $\pi(\theta)$of a Markov chain exists if

$$\sum_{\theta^t \in \Theta} P\left(\theta^{t+1} \mid \theta^t\right)\pi\left(\theta^t\right) = \pi\left(\theta^{t+1}\right) \tag{4.11}$$

A path of Markov chain can be generated by sequentially sampling θ^t according to the transition probability distribution function.

In semi-supervised clustering, the set of model parameters that fully describes the model is $\Theta = \{k, \omega, z, \mu, \Sigma, \pi\}$, where k is the number of clusters, ω is the prior probability of each cluster, z is the vector of cluster assignment for the patterns, μ, Σ describes each of the Gaussian distributions in the mixture Gaussian model, and π is the parameter that describes the multinomial distributions on the class labels for each cluster. A state in the Markov chain is a member of Θ, which is a solution of the semi-supervised clustering problem.

4.5.2 Metropolis-Hastings and Gibbs Algorithm

The Metropolis-Hastings algorithm uses a propose-and-accept method to sample from the stationary distribution $\pi(.)$ by constructing a Markov chain. At each time *t*, a new state is proposed by an auxiliary proposal distribution $Q(.|.)$. Let $\theta^t = X$, a proposed new state $\theta^{t+1} = Y$ is accepted with probability of

$$P_{accept}(Y) = \min\left\{1, \frac{\pi(Y)Q(X \mid Y)}{\pi(X)Q(Y \mid X)}\right\} \tag{4.12}$$

For symmetrical proposal distribution functions, the probability to accept reduces to,

$$P_{accept}(Y) = \min\left\{1, \frac{\pi(Y)}{\pi(X)}\right\} \tag{4.13}$$

If the state is multivariate $\theta = \{\theta_1, \theta_2, ..., \theta_M\}$, a single component Metropolis-Hastings proposes new states that is only different from the current state by one component. To update component *i*, the probability for acceptance of a new state is,

$$P_{accept}(\theta_1, ..., \theta_i', ..., \theta_M) = \min\left\{1, \frac{\pi(\theta_1, ..., \theta_i', ..., \theta_M)Q(\theta_1, ..., \theta_i, ..., \theta_M \mid \theta_1, ..., \theta_i', ..., \theta_M)}{\pi(\theta_1, ..., \theta_i, ..., \theta_M)Q(\theta_1, ..., \theta_i', ..., \theta_M \mid \theta_1, ..., \theta_i, ..., \theta_M)}\right\} \tag{4.14}$$

If the proposal distribution is the full conditional distribution,

$$Q(\theta_1, ..., \theta_i', ..., \theta_M \mid \theta_1, ..., \theta_i, ..., \theta_M) = \frac{\pi(\theta_1, ..., \theta_i', ..., \theta_M)}{\int \pi(\theta_1, ..., \theta_i', ..., \theta_M) d\theta_i'} \tag{4.15}$$

The acceptance probability becomes,

$$P_{accept}(\theta_1, ..., \theta_i', ..., \theta_M) = \min\{1,1\} = 1 \tag{4.16}$$

In other words, if the new component is proposed from the full conditional distribution, the Metropolis-Hastings algorithm always accepts the newly proposed state. This sampling algorithm is known as the Gibbs sampling. A sweep in Gibbs sampler refers to

an iteration of sampling each individual component with the corresponding full conditional distributions.

4.6 MDL Coupled MCMC

As discussed in chapter 2, an efficient prefix code is equivalent to a probability distribution. If a description length function can be fully specified as a function of the set of parameters in semi-supervised clustering model, each full conditional distribution required in Gibbs sampling can be derived from the description length function. Let L be such a description length function mapping from the model set Θ to positive real numbers, the marginal probability of a state is given by the following transformation,

$$P(\theta_1,\theta_2,...,\theta_i,...,\theta_M) = \exp(-L_D(\theta_1,\theta_2,...,\theta_i,...,\theta_M)) \tag{4.17}$$

The full conditional distribution for the ith parameter is,

$$P(\theta_1,\theta_2,...,\theta_i',...,\theta_M \mid \theta_1,\theta_2,...,\theta_i,...,\theta_M) = \frac{\exp[-L_D(\theta_1,\theta_2,...,\theta_i',...,\theta_M)]}{\sum_{\theta_i}\exp[-L_D(\theta_1,\theta_2,...,\theta_i,...,\theta_M)]} \tag{4.18}$$

The MDL coupled MCMC sampler is superior to the traditional MCMC sampler in the following ways

- The MDL coupled sampler allows easier accommodation of exterior class labels. The label information is readily encompassed in the sampler by creating codes of the labels within each cluster.

- The MDL coupled MCMC allows jumping across models with different numbers of components without the need to explicitly specify the prior probability on the components. Rather, the prior is automatically derived from the parametric complexity and is consistent with Occam's razor philosophy.

- When normalized likelihood distribution is used in the encoding, only parameters which are potentially maximum likelihood estimators need to be considered, essentially discretizing and reducing the size of the state space.

4.7 Encoding Semi-supervised Clustering with MDL

We now propose the encoding scheme for probabilistic models in semi-supervised clustering. The description length formulation for a probabilistic model in semi-supervised clustering problem includes the following steps.

1. Draw the graphical representation of the probabilistic model that implies our prior assumption.

2. Encode the model following the links in the graphical representation from root nodes to leaf nodes, until the observed data are encoded. For labeled data, we encode both independent attributes $\boldsymbol{x}$ and class label $\boldsymbol{y}$. For unlabeled data, we only encode independent attributes $\boldsymbol{x}$.

3. Drop the constant terms in the description length distribution that does not vary with the considered model parameters.

We assume that there are total K Gaussian components in the mixture Gaussian model. Let latent variable $\boldsymbol{z}$ be the component index. For each component, it generates $\boldsymbol{x}$ according to independent Gaussian distributions with parameters characteristic to this component. Similarly, each component generates class label $\boldsymbol{y}$ using multinomial distribution with parameters characteristic to this component. For labeled data, we can observe both $\boldsymbol{x}$ and $\boldsymbol{y}$ while for unlabeled data we only observe $\boldsymbol{x}$**.** To predict the class label for a new pattern x_{new}, we first find its component index using the link between $\boldsymbol{x}$ and $\boldsymbol{z}$ and then predict its class label using the link between $\boldsymbol{z}$ and $\boldsymbol{y}$**.** A graphical representation of a mixture Gaussian model following the convention of [Bun94] is given in Figure 4.3, where solid arrows indicate conditional probability of the observed pattern given the model parameters and dashed arrow represents the choice of parameters. The solid lines contribute to the likelihood part of the MDL encoding and the dashed lines correspond to the parametric complexity in MDL encoding. A transparent rectangle indicates an array of objects, here in particular indicates the array of components.

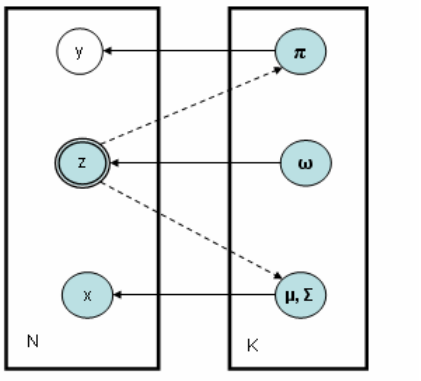


Figure 4.3 Graphical Representation of Mixture Gaussian Model

The likelihood part to code an unlabeled pattern x is,

$$L_{unlabel}(x_i) = -\sum_{j=1}^{K} z_i(j)\left(\left(\ln \omega_j\right) - \ln f\left(x_i \mid \mu_j, \Sigma_j\right)\right) \tag{4.19}$$

The likelihood part to code a labeled pattern (x, y) is,

$$L_{unlabel}(x_i) = -\sum_{j=1}^{K} z_i(j)\left(\left(\ln \omega_j\right) - \ln f\left(x_i \mid \mu_j, \Sigma_j\right) - \ln f\left(y_i \mid \pi_j\right)\right) \tag{4.20}$$

Three parametric complexities need to be included in the total description length function: multinomial model to encode the component index, Gaussian model to encode the unlabeled part of the pattern, multinomial distribution to encode labeled part of the pattern.

$$PC\left(\boldsymbol{\Theta}_K, N\right) = PC\left(\Omega_K, N\right) + PC\left(\boldsymbol{\Sigma}, N\right) + PC\left(\boldsymbol{\Pi}, N\right) \tag{4.21}$$

The total description length function becomes

$$\begin{aligned} &L\left(x_1, x_2, ..., x_{n+m}, y_1, y_2, ..., y_n\right) = PC\left(\Omega_K, N\right) + PC\left(\boldsymbol{\Sigma}, N\right) + PC\left(\boldsymbol{\Pi}, N\right) \\ &- \sum_{i=1}^{n}\sum_{j=1}^{K} z_i(j)\left(\left(\ln \omega_j\right) - \ln f\left(x_i \mid \mu_j, \Sigma_j\right) - \ln f\left(y_i \mid \pi_j\right)\right) \\ &- \sum_{i=n+1}^{n+m}\sum_{j=1}^{K} z_i(j)\left(\left(\ln \omega_j\right) - \ln f\left(x_i \mid \mu_j, \Sigma_j\right)\right) \end{aligned} \tag{4.22}$$

4.8 MDL Coupled MCMC in Semi-Supervised Clustering

The standard approach to sampling from the posterior distribution is to construct a Markov chain on the model space that has the posterior distribution as its stationary distribution. The state of the chain at time $t, \Theta^t = \{k^t, \omega^t, z^t, \mu^t, \Sigma^t, \pi^t\}$, will only depend on the state of the chain at time $t-1$, $\Theta^{t-1} = \{k^{t-1}, \omega^{t-1}, z^{t-1}, \mu^{t-1}, \Sigma^{t-1}, \pi^{t-1}\}$. The iteration from time *t-1* to *t*, is a sweep that consists of sampling each parameter conditionally on all other remaining parameters. In the MDL-MCMC sampler for mixture component model, there are six moves in each sweep.

1. Sample ω from $f(\omega \mid k, z, \mu, \Sigma, \pi)$
2. Sample z from $f(z \mid k, \omega, \mu, \Sigma, \pi)$
3. Death and Re-Birth of a component
4. Split and Combine of a component
5. Sample μ, Σ from $f(\mu, \Sigma \mid k, \omega, z, \pi)$
6. Sample π from $f(\pi \mid k, \omega, z, \mu, \Sigma)$

Step 1, 2, 5 and 6 use Gibbs sampling to sample from the full conditional probability distribution. Step 3 and 4 use Metropolis-Hasting algorithm to handle empty components and jump across subspaces.

4.8.1 Sample ω

Parameter ω represents the marginal probability of each cluster and must satisfy the following constraint,

$$\sum_{j=1}^{K} \omega_j = 1 \tag{4.23}$$

According to equation (4.22), the description length part that changes with ω is,

$$L(\omega) = -\sum_{i=1}^{n+m} \sum_{j=1}^{K} z_i(j) (\ln \omega_j) \tag{4.24}$$

The challenge in the sampling is to have a proposal function that always satisfies the unity constraint in (4.23). To fulfil the constraint, we devise the following mapping to construct the proposal function as illustrated in Figure 4.4,

1. Divide a circle with unity circumference into $n+m$ equally separated segments by $n+m$ points on the circle.

2. Any combination of K points of the $n+m$ possible on the circle corresponds to a state of ω. For example, in Figure 4.4, the state is represented as,

$$\omega_1 = AB, \omega_2 = BC, \omega_3 = CD, \omega_4 = DA$$

3. Starting from the previous state, a new state is proposed by moving each of the K points one step towards a random direction.

Because the proposal function is symmetrical, the acceptance probability in Metropolis-Hastings algorithm is simply

$$P_{accept}(\omega_{new}) = \min\left\{1, \frac{\exp(-L(\omega_{new}))}{\exp(-L(\omega))}\right\}$$

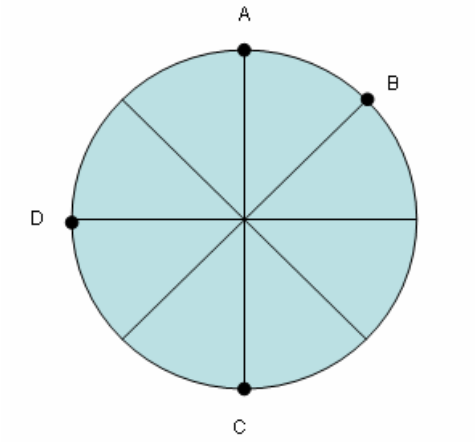


Figure 4.4 Sampling clustering frequency with constraints, K=4, N=8

4.8.2 Sampling z

To sample the latent variable z that represents the cluster assignment of the pattern, we first write the description length function as a function of z,

$$\begin{aligned} L(z) = &-\sum_{i=1}^{n}\sum_{j=1}^{K} z_i(j)\left((\ln \omega_j) - \ln f(x_i \mid \mu_j, \Sigma_j) - \ln f(y_i \mid \pi_j)\right) \\ &- \sum_{i=n+1}^{n+m}\sum_{j=1}^{K} z_i(j)\left((\ln \omega_j) - \ln f(x_i \mid \mu_j, \Sigma_j)\right) \end{aligned} \tag{4.25}$$

Assume the patterns are identically independently distributed (i.i.d.), the sampling is done with each individual pattern independently. For a labelled pattern,

$$L(z_i = j) = -(\ln \omega_j) - \ln f(x_i \mid \mu_j, \Sigma_j) - \ln f(y_i \mid \pi_j) \tag{4.26}$$

For an unlabled pattern,

$$L(z_i = j) = -(\ln \omega_j) - \ln f(x_i \mid \mu_j, \Sigma_j) \tag{4.27}$$

For each z_i, there are totally K considered alternative encodings, each corresponds to a different cluster assignment. The probability distribution from which to sample z_i is defined by equation (4.18).

4.8.3 Death and Rebirth

Completely empty components and components that contain only a single pattern require special attention, as they usually indicate a redundant part of the model that increases the description length to specify the model yet will not help compress the data. To increase the mixing rate and shorten the total description length, better parameters can be proposed to help encode the data. The death and rebirth moves involve destroying an empty component or a nearly empty component and reinitialize it with new parameters, which hopefully encode the data more efficiently.

Because an empty component only encodes parametric complexity, the description length is always the same no matter what the parameters values are. Reinitializing the parameter values for the empty component does not change the total description length. Also, we maintain a symmetrical parameter proposal function by reinitialize the parameters randomly so that the detail balance will be satisfied [Nea93]. If a component contains one pattern, we cannot always reinitialize the component without a penalty since changes on the parameters of the component will affect the description length to encode the single pattern in that component. The increase of the description length is $-\ln f(x \mid \theta_{new})$ since

it takes no description to encode the pattern previously (the pattern will overlap with the cluster center and the distance from cluster center is zero). Thus the probability of accepting the move is $f(x \mid \theta_{new})$. If the dimensionality of the data is high, then the acceptance rate becomes very low. One way of overcoming this difficulty is by only reinitializing the parameter only in one random dimension.

4.8.4 Split and Combine

This is the move that enables sampling across subspaces with different *k* values. At each split and combine move, we will stochastically determine whether to attempt to split or to combine. When *k=1*, we always attempt the split move and when *k* equals the maximum number of components *K*, we always attempt the combination move. At all other *k* values, both the probability to split and the probability to combine are 0.5.

Split. First a random component is chosen as the split candidate. Then we choose the dimension with the largest standard deviation to generate the split pivot. The split pivot *sp* is randomly generated from $[\mu - \sigma, \mu + \sigma]$ in the chosen dimension and all patterns inside the component are divided into two groups: those larger than the pivot and those smaller in the chosen dimension. All the parameters of the two groups are estimated using the maximum likelihood estimator. Let *j* be the candidate component proposed to split into j_1 and j_2, the change of the description length after the proposed split can be calculated from

$$L_{split}(j) = \sum_{i=1}^{n} \sum_{s=1,2} z_i(j,s) \left(\left(\ln \frac{\omega_j}{\omega_{j,s}} \right) + \ln \frac{f\left(x_i \mid \mu_j, \Sigma_j\right)}{f\left(x_i \mid \mu_{j,s}, \Sigma_{j,s}\right)} + \ln \frac{f\left(y_i \mid \pi_j\right)}{f\left(y_i \mid \pi_{j,s}\right)} \right)$$
$$+ \sum_{i=n+1}^{n+m} \sum_{s=1,2} z_i(j,s) \left(\left(\ln \frac{\omega_j}{\omega_{j,s}} \right) + \ln \frac{f\left(x_i \mid \mu_j, \Sigma_j\right)}{f\left(x_i \mid \mu_{j,s}, \Sigma_{j,s}\right)} \right) \tag{4.28}$$

The move is subject to a Metropolis-Hasting test and will pass the test with a probability of $\min\{1, \exp(-L_{split}(j))\}$.

It is also important that the split proposal function and the combination proposal function be symmetrical. That is, if component j splits into j_1 and j_2, then the probability of choosing s for the split attempt should equals the probability of choosing j_1 and j_2 for the combination attempt. To achieve this, we enforce that after the split, **at least** one of the two newly produced components must be the most adjacent component of the other. Here, when we say component *j1* is the most adjacent component to *j2*, we mean *j1* has the shortest Euclidean distance to *j2*. Note that this property is not mutual, that is, *j1* is most adjacent to *j2* does not imply that *j2* is most adjacent to *j1*. If none of the two components is most adjacent to the other, the split attempt is unconditionally rejected. In later section, we discuss in greater detail in section 4.9 to illustrate that the proposal function enforces symmetry.

Combine. We pick the two candidate components to combine by choosing the first candidate component randomly and enforce its most adjacent component as the second candidate component. The proposed combined component parameters can be easily

estimated from the candidate component's sufficient statistics. The message length change for a combination step is the reverse of the split step.

$$L_{combine}(j1, j2) = -\sum_{i=1}^{n}\sum_{s=1,2} z_i(j,s)\left(\left(\ln\frac{\omega_j}{\omega_{j,s}}\right) + \ln\frac{f(x_i \mid \mu_j, \Sigma_j)}{f(x_i \mid \mu_{j,s}, \Sigma_{j,s})} + \ln\frac{f(y_i \mid \pi_j)}{f(y_i \mid \pi_{j,s})}\right)$$
$$-\sum_{i=n+1}^{n+m}\sum_{s=1,2} z_i(j,s)\left(\left(\ln\frac{\omega_j}{\omega_{j,s}}\right) + \ln\frac{f(x_i \mid \mu_j, \Sigma_j)}{f(x_i \mid \mu_{j,s}, \Sigma_{j,s})}\right) \quad (4.29)$$

The combination move is evaluated by the Metropolis-Hasting test with an acceptance probability $\min\{1, \exp(-L_{combine}(j1, j2))\}$. The combination move is the symmetrical move to the split move. The two moves are reversible and satisfy the detail balancing equilibrium as we will show in section 4.9.

4.8.5 Sampling μ, Σ

For easy sampling, we assume the covariance matrix Σ is of diagonal form that,

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \ldots & 0 \\ 0 & \sigma_2^2 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \sigma_d^2 \end{bmatrix} \quad (4.30)$$

It states the attributes of the patterns are independent from one another. The assumption can be satisfied via rotating the original patterns through principle component analysis (PCA) to make a new set of attributes that are orthogonal to one another. Once the covariance matrix is diagonalized, the means and variances of each attribute can be sampled independently. The description length function for the *k*th Gaussian component and *j*th attribute is

$$L(\mu_{i,j},\sigma_{i,j}) = (n+m)\ln\sigma_{k,j} + \sum_{i=1}^{n+m}\frac{(x_{i,j}-\mu_{k,j})^2}{2\sigma_{k,j}^2} \tag{4.31}$$

From the description length function (4.31), $\mu_{k,j}$ can be sampled from a Gaussian distribution while $\frac{1}{\sigma_{k,j}^2}$ can be sampled from a Chi square distribution.

4.8.6 Sampling π

The description length part that depends on π_j is,

$$L(\pi_j) = \sum_{i:z(i)=j} -\ln f(y_i \mid \pi_j) \tag{4.32}$$

The sampling of the multinomial distribution is the same as sampling ω in 4.8.1.

4.9 Convergence

If the stationary distribution of a Markov chain is to converge towards the posterior distribution, the chain must satisfy the following three conditions [GRS96].

- The chain must be aperiodic, which means there should **not** be any positive integer, *T*, that satisfies $\{k^t,\omega^t,z^t,\mu^t,\Sigma^t,\pi^t\} = \{k^{t+T},\omega^{t+T},z^{t+T},\mu^{t+T},\Sigma^{t+T},\pi^{t+T}\}$ for **all** $t \geq t_0$. If there is such a *T* then the chain is periodic and the period of the chain would be *T*.
- The chain must be irreducible, that is, the transition time takes from any two states $\{k,\omega,z,\mu,\Sigma,\pi\}$ and $\{k',\omega',z',\mu',\Sigma',\pi'\}$ must not be infinity.

- The chain must satisfy the detail balance condition for every move, which is given by

$$p(k,\omega,z,\mu,\Sigma,)p(k,\omega,z,\mu,\Sigma,\rightarrow k',\omega',z',\mu',\Sigma',\pi') = p(k',\omega',z',\mu',\Sigma',\pi')p(k',\omega',z',\mu',\Sigma',\pi'\rightarrow k,\omega,z,\mu,\Sigma,) \quad (4.33)$$

Given any state at time *t*, the probability the next state is the same state is greater than zero. Thus it is possible that the chain will stay at one state for arbitrary number of iterations and move to other states. The chain can only repeat the history with a probability less than 1. Therefore, the chain can never get into the deterministic cycle that satisfies the periodicity condition. The chain is also irreducible as the transition probability between any two states is greater than zero thus it will not take infinite time for the transition to take place. We now prove that detail balance holds for the six moves.

In the six sampling moves the parameters are sampled from the full conditional distributions transformed from the message length distribution. In move 1, 2, 5 and 6 where Gibbs sampling is used, it is easy to see the detail balance holds since

$$p(\theta_1)p(\theta_1\rightarrow\theta_2) = \frac{\exp(-L(\theta_1))}{Z}\cdot\frac{\exp(-L(\theta_2))}{Z} = p(\theta_2)p(\theta_2\rightarrow\theta_1) \quad (4.34)$$

Here θ stands for whichever parameter being sampled in the move and Z is the normalization factor $\sum_{\theta}\exp(-L(\theta))$.

In move 3 and 4 where Metropolis algorithm is used,

$$p(\theta_1)p(\theta_1\rightarrow\theta_2) = \frac{e^{-m_1}}{Z}\min\{e^{-(m_2-m_1)},1\} = \frac{e^{-m_2}}{Z}\min\{e^{-(m_1-m_2)},1\} = p(\theta_2)p(\theta_2\rightarrow\theta_1) \quad (4.35)$$

It remains to prove that in the Metropolis test, the proposal function is symmetrical. In the death and rebirth move, since these parameters are randomly reinitialized, the

probability of a proposal is independent of the current state and is obviously symmetrical. In the split/combine move, the probability of proposing a component as the split candidate equals *1/k*. The proposed component *j* is split into *j1* and *j2*. We also enforce that **at least one** component resulted from the split must the most adjacent of the other. Without losing generality, let *j2* be the most adjacent component of *j1*. In the combination step, the probability of choosing *j1* and *j2* equals to the sum probability of choosing *j1*(which will automatically choose *j2* subsequently) and the probability of choosing *j2* and then *j1* as its most adjacent component. Let $p(j1, j2)$ be the probability of proposing components *j1* and *j2* as the combination candidates and $p(j)$ be the probability of proposing component *j* as the split candidate, then

$$p(j1, j2) = \frac{1}{k+1} + \frac{1}{k+1}\frac{1}{k} = \frac{1}{k} = p(j) \tag{4.36}$$

The proposing function is symmetrical and the detail balance holds.

In summary, the proposed MDL coupled MCMC sampler consists of six moves. The Markov chain grown by the sampler is aperiodic, irreducible and detail balanced therefore its stationary distribution converges to the MML defined posterior distribution of the models.

4.10 MCMC Diagnosis

In this section, we empirically diagnose the MDL coupled MCMC sampler to verify the convergence and analyze the mixing rate. A four component two dimension Gaussian mixture (Figure 4.5) dataset is used for the purpose. We run the chain for 200,000

iterations with the first 50,000 as the burn-in period. We diagnose the convergence by comparing the posterior probabilities of k among different segments of the chain, each with a size of 50,000 iterations. If the chain has converged then the posterior probabilities should be constant across the segments. The probability of a particular value of k is the number of iterations the sampler stays in the given model sub-space. The comparison results are presented in Figure 4.6. Trace plots for k (Figure 4.7) indicates efficient mixing across the subspaces of different k, with split move and the combine move have an acceptance rate of 11.2% and 11.3% respectively.

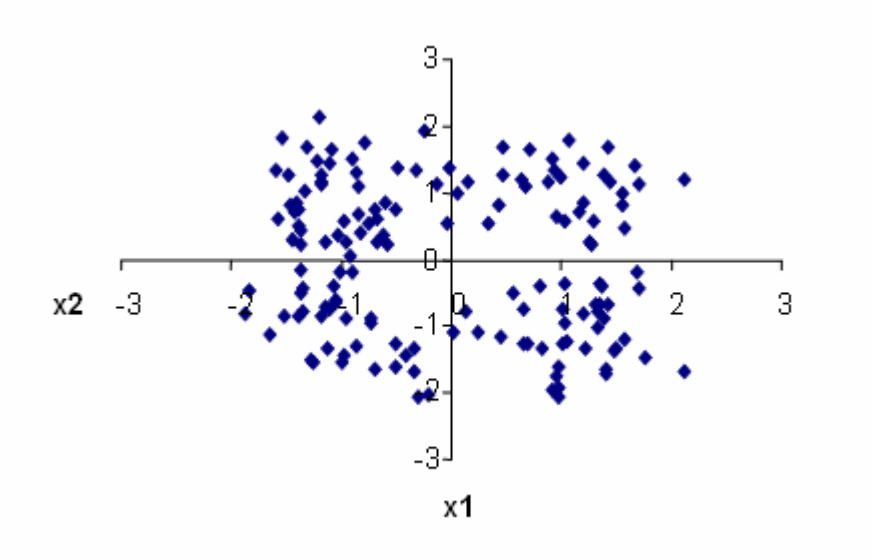


Figure 4.5 Mixture Gaussian Model with Four Components and Two Dimensions

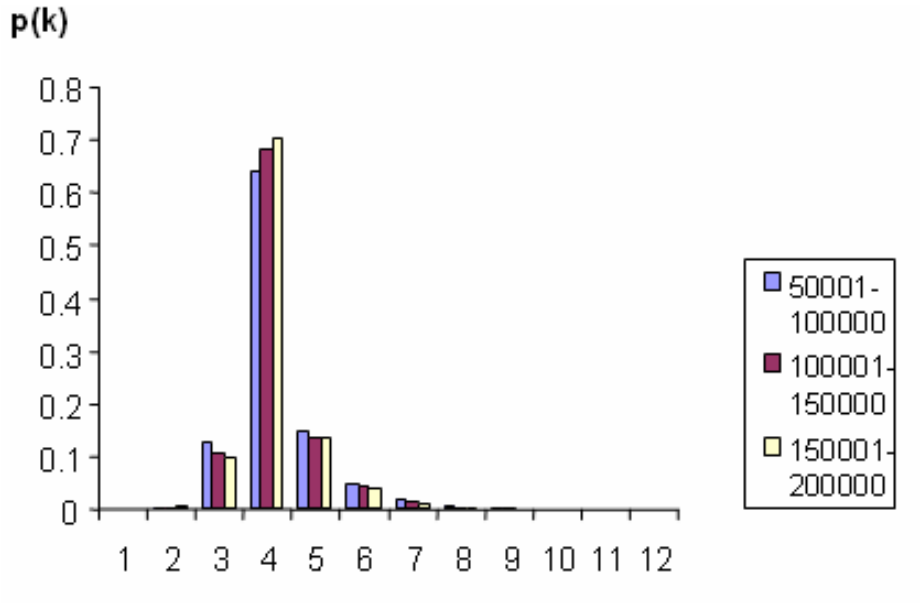


Figure 4.6 Posterior Distribution of k among different time segments in MCMC chain

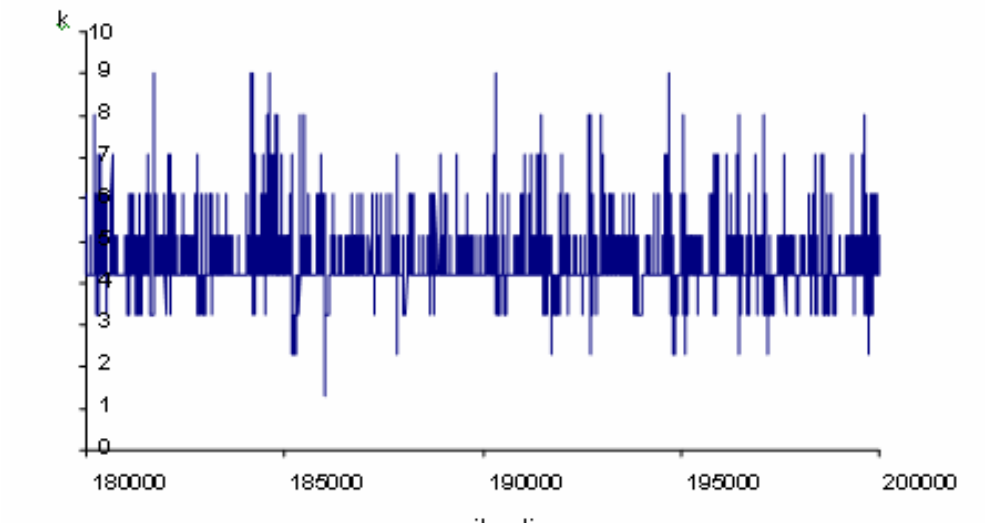


Figure 4.7 Trace Plot of k (Iteration 180000 to 200000)

4.11 Empirical Results

In this section, we compare the predictive performance between an optimal Bayes classifier as constructed above and the maximum likelihood classifier usually found by the EM algorithm. We abbreviate the semi-supervised optimal Bayes classifier as SS-OBC, and abbreviate the semi-supervised maximum likelihood classifier as SS-EM.

We use standard data sets from the UCI machine learning repository. For each dataset, we use 10% of the data as labeled data, 10% as the unlabeled data and 80% as the testing data. We choose small training set size mainly to test the classifiers' performance when data is scarce. We report the prediction error and standard deviation over 100 trials. We also include the p-value of a paired T-test of errors to indicate whether the error reduction is statistically significant. We summarize our results in Figure 4.1.

Table 4.1 Predictive Performance Comparison between SS-OBC and SS-EM.

Data	SS-EM	SS-OBC	P value
Iris	17.5 (9.9)	10.9(6.9)	6.00E-08
Diabetes	21.2 (7.8)	20.6(6.8)	0.15
Wine	18.1(13.0)	12.4(7.9)	5.20E-05
Glass	56.3 (5.1)	53.7(7.8)	0.0006
Shuttle	21.6 (4.5)	18.6(5.0)	6.50E-08

***10% labelled data and 10% unlabeled data**

We see that for all but one data set that SS-OBC performs significantly better than its SS-EM rival. Furthermore this improvement in accuracy is often accompanied by a reduction of the standard deviation of the performance. The reason that SS-OBC showed a non-statistical significant improvement on the Diabetes dataset is probably that the posterior

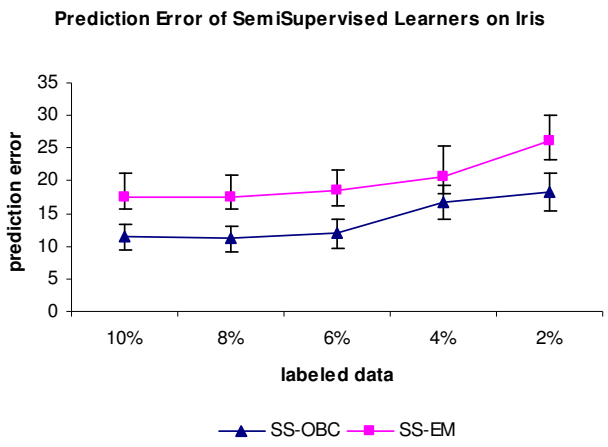
distribution is already well peaked for the problem even with limited amount of data, thus an SS-EM can approximate SS-OBC fairly well as the Bayesian integral in equation (4.7) is dominated by the shortest model.

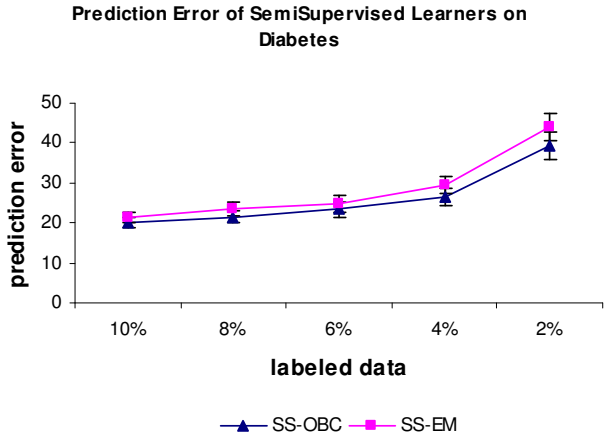
Next, we gradually decrease the amount of labeled data given to the learner and replace with unlabeled data. We show the general trend fond for all data sets using Iris, Diabetes and Wine dataset, as illustrated in Figure 4.8.

We see that in Iris data, an SS-OBC with only 2% labeled data can perform almost as well as a SS-EM using 10% labeled data. Similarly, in the Wine data, with 4% labeled data, the SS-OBC classifier achieves comparable prediction accuracy as SS-EM using 10% labeled patterns. This indicates that SS-OBC performs well even when labeled patterns are very limited, which is an important property in semi-supervised clustering.

In some semi-supervised clustering problems, not only the amount of labeled but also the amount of unlabeled data is also restricted. In the last experiment, we empirically investigate the impact of the unlabeled data size on the classifiers. We gradually decrease the unlabeled data and measure the prediction errors.

Through Figure 4.9, we see that the performance of SS-OBC is superior to that of SS-EM in semi-supervised learning situations when the unlabeled data as well as the labeled data is limited. The learner, under this situation, must utilize both labeled and unlabeled data as efficiently as possible.





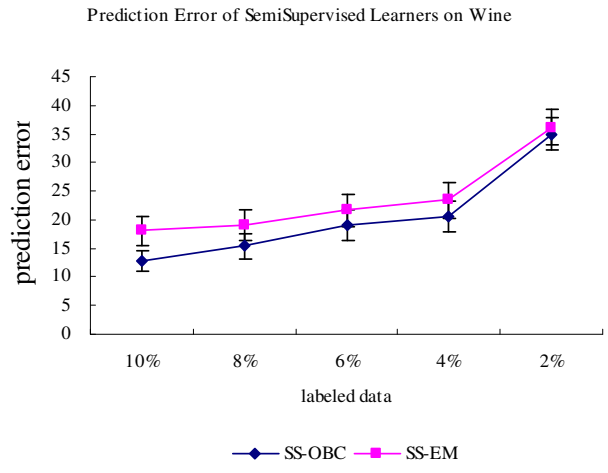
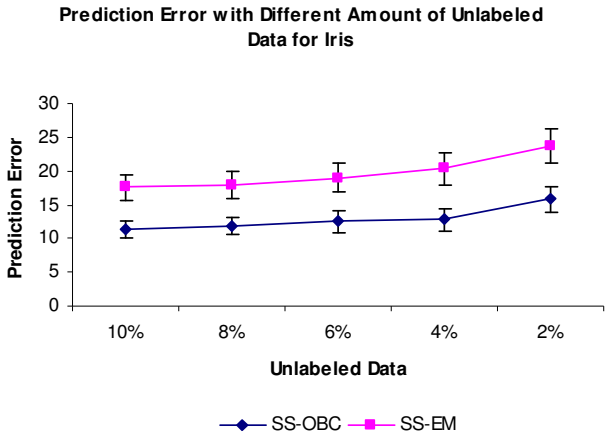
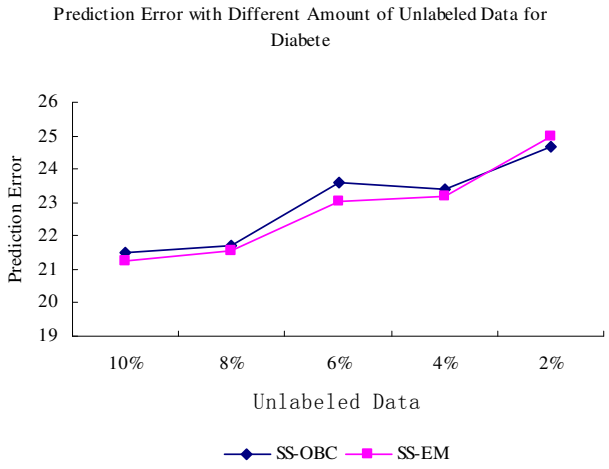


Figure 4.8 SS-OBC and SS-EM on Size of Labele Patterns





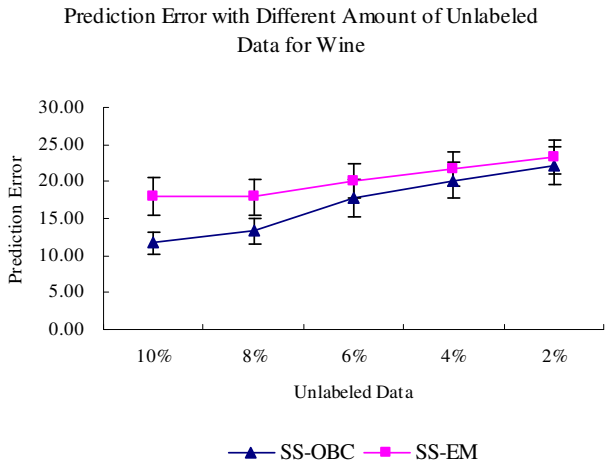


Figure 4.9 SS-OBC and SS-EM on Size of Unlabeled Patterns

4.12 Chapter Summary

MDL principle provides description length as the measurement of model complexity from which we can calculate the posterior probability of the model. In this chapter, we present procedures to construct optimal Bayes classifiers for probabilistic models in semi-supervised clustering. The form of the description length calculation can be derived from the graphical representation of the probabilistic model by encoding the model parameters and the data in a top-down manner from root to leaf. The description function implies the full conditional probabilities and can be used to construct a Markov Chain whose stationary distribution represents the posterior distribution of the model, which serves as the "weights" used in the optimal Bayes classifier. We verify empirically that MDL-coupled Optimal Bayes Classifier makes better predictions in semi-supervised clustering problems compared to the maximum likelihood classifier found by EM in learning situations where the amount of data is scarce. The semi-supervised optimal Bayes classifier shows great robustness when very limited amounts of labeled and unlabeled data are available. This property makes optimal Bayes classifier a very useful predictor in semi-supervised problems.

5 Constrained Clustering

5.1 Introduction

Clustering algorithm finds partitions for a set of patterns by minimizing dissimilarity function within clusters. For example, K-means clustering uses squared Euclidean distance among the patterns for such measure. The found cluster corresponds to implicit labels. However, in real world problem, it is not immediately clear that these implicit labels meet the learning purposes. Feedback from expert opinion on the clustering results, under this scenario, can be beneficial in directing the clustering towards desired learning goals. Cohn et al. give a Yahoo! Document clustering example [CCM03] where user can provide feedbacks on clustered patterns advising two patterns belong to the same cluster or two patterns be exclusive in cluster assignment. The clustering algorithm adopts the feedback and reconstructs clusters following the constraint added by the user. Constraints act as background knowledge in learning that help build more meaningful clusters if handled correctly. The constraints commonly introduced in the clustering context come

into three levels, namely instance-level constraint, cluster-level constraint and model-level constraint.

Instance-Level Constraint

There are two types of instance-level constraints, known as must-link (ML) and cannot-link (CL) constraints.

Definition 5.1 (Must-Link Constraint) Let $P : x \to \{1,2,...,K\}$ be the cluster assignment mapping from the pattern space to the cluster indices, pattern x_i and x_j are subjective to must-link constraints if $\forall k \in \{1,2,...,K\} \quad (P(x_i) = k) \Leftrightarrow (P(x_j) = k)$.

Definition 5.2 (Cannot-Link Constraint) Let $P : x \to \{1,2,...,K\}$ be the cluster assignment mapping from the pattern space to the cluster indices, pattern x_i and x_j are subjective to cannot-link constraints if $\forall k \in \{1,2,...,K\} \quad (P(x_i) = k) \cap (P(x_j) = k) \Rightarrow F$.

The source of the instance-level constraints can be from user feedback as in the Yahoo! example or be derived from the semi-supervised clustering setting where patterns with same class labels are imposed must-link constraints and patterns with different class labels are enforced to be assigned to different clusters. High quality constraints from expertise opinion can potentially boost the performance of the clustering learner. Wagstaff et al proposed COP-K-means algorithm [WCR+01] which yields better performance than plain K-means algorithm by respecting the instance-level constraints randomly generated from the pattern clusters. Some other algorithm allows violation of the constraints with an associated penalty [BBM04b].

Cluster-Level Constraint

Davidson and Ravi [DR05] propose two types of cluster-level constraints, named as the ε-constraint and δ-Constraint.

Definition 5.3 (δ-Constraint) Let $P: x \to \{1,2,...,K\}$ be the cluster assignment mapping from the pattern space to the cluster indices and $D(x_i, x_j)$ the distance function, cluster C_i and C_j are subject to δ-constraint if $(\min\{D(x,y); P(x)=i, P(y)=j\} \geq \delta) \Rightarrow T$.

Definition 5.4 (ε-Constraint) Let $P: x \to \{1,2,...,K\}$ be the cluster assignment mapping from the pattern space to the cluster indices and $D(x_i, x_j)$ the distance function, cluster C_i is subject to δ-constraint if $(P(x)=i) \Rightarrow (\min\{D(x,y); P(y)=i, y \neq x\} \leq \varepsilon)$.

Cluster-level constraints control the quality of the clusters. δ-Constraint prohibits two clusters be too similar to each other by specifying the minimal distance allowed between patterns from two distinctive clusters. ε-Constraint, on the other hand, ensures the similarity within the same cluster, preventing the distribution of patterns within the same cluster becoming too loose. The cluster level constraints can be converted into either conjunctions or disjunctions of the instances-level constraints [DR05].

5.1.1 Model-Level Constraints

In some problems, constraints are put on the maximum size of a cluster to prevent too small or dominating clusters.

Definition 5.5 (Cluster Size Constraint) Let $P : x \to \{1,2,...,K\}$ be the cluster assignment mapping from the pattern space to the cluster indices and $\delta(i, j)$ be the disparity function

$$\delta(i, j) = \begin{cases} 1 & if\ i = j \\ 0 & if\ i \neq j \end{cases}$$

The clustering model is subject to the cluster size constraint $CSC(a,b)$ if

$$\forall k \in \{1,2,...,K\} \quad a \leq \sum_{x} \delta(P(x), k) \leq b$$

must hold.

In this chapter, we focus on clustering under the instance-level constraints, as they serve as building blocks of higher level constraints. We investigate encoding the patterns with instance-level constraints as background knowledge. The constraints imposed on the clustering solution essentially induce simpler model by excluding a subset of the solution space. We show that the simpler model induced by constraints can lead to either shorter or longer encoding, depending on the expected encoding length on the subset of solution space. With this philosophy, the encoding length can serve as a yardstick in evaluating the constraints, thus respect only constraints that facilitate the encoding and ignore the constraints that result in lengthened codes. We illustrate how good constraints improve the model performance and bad ones deteriorate the model performance, as well as how to actively choose good constraints and ignore bad ones within the MDL framework.

5.2 Clustering under Constraints

5.2.1 Feasibility

A fundamental question to ask in constrained clustering is the feasibility of finding clusters that satisfies the constraints. The question should be answered before any clustering is attempted in constrained clustering problems where constrains must be complied. Davidson and Ravi [DR05] investigate the feasibility on various instance-level and cluster-level constraints. The results indicate that while some constraints such as must-link constraints are tractable, which means there is a polynomial algorithm in deciding whether a feasible clustering partition exists, there are intractable constraints where the feasibility cannot be efficiently decided.

5.2.2 Flexibility

Constraints algorithms fall into two categories. The first type of algorithm faithfully complies with every constraint specified in the problem, an example of which is the COP-K-means algorithm. The constraints are said to be hard in this case. Other algorithms treat the constraints as soft, which can be violated with an associated penalty. An algorithm enforcing the constraints must subjective to the feasibility problem mentioned in the previous section. The first level of flexibilities on constraint is whether a constraint is hard or soft.

Constraints are background knowledge that supposedly augments the performance of the learner. Indeed, it has been widely reported that learning with constraints, be it hard or

soft, can enhance the learning accuracies [WCR+01] [BBM04a] [GH04] [GVG05]. However, recently research indicates that constraints can potentially have adverse effects. For example, enforcing a must-link constraint between two patterns with large distance is likely to weaken the clustering quality. There are two approaches to addressing the issue. The first solution is to trust the constraints and learn the distance function to accommodate the constraints [DWB06] [BBM04c]. Alternatively, one can trust the distance function and evaluate on the constraints. Davidson et al. proposed informativeness and coherence measures on constraints, enabling the learning to identify constraints with adverse effects and ignore them [DWB06]. The second level of flexibility in constraints is whether a constraint is beneficial or harmful.

In the scope of this work, we adopt the second approach: the learner is being faithful to using description length as universal metric measuring model quality, with which the constraints are evaluated.

5.3 Constraints and Codes

Previous chapters have already introduced the MDL code to encode patterns with clustering models without loss of information in unconstrained clustering. In constrained clustering, the constraints are considered as background knowledge or prior knowledge shared by the sender and receiver of the code. Depending on the relevance of the prior knowledge, the code in constrained clustering may or may not be shorter compared to its unconstrained counterpart. This essentially provide a yardstick in evaluating constraint qualities and allows flexible usage of the constraints: a constraint is considered to be

beneficial if the total code length is reduced and should be respected; on the other hand, a constraint can be decided as detrimental to the model if the code length is augmented by incorporating the prior knowledge and such constraints should be ignored.

As discussed in chapter 2, the description length costs breaks into two parts in encoding the patterns with clustering models. First the cluster assignment has to be encoded for each pattern. Then the distance between the pattern and assigned cluster center is encoded. In constrained clustering, there are less partition solutions than the corresponding unconstrained problem. From the perspective of coding, the constrained clustering model is a simpler model that the unconstrained counterpart. The constraints define a subset of the models from the unconstrained model space and reduce the parametric complexity of the model. However, the total encoding length may increase if such model simplification leads to poor data fitting.

Definition 5.6 (Description Length Density) For probability measure f on set P, the description length density of f on $Q \subseteq P$ is defined as,

$$DLD_f(Q) = \frac{-\int_Q f(x) \ln f(x) dx}{\int_Q f(x) dx} \tag{5.1}$$

The description length density measures the average encoding length within a subset. A large description length density on a subset indicates encoding the events within the subset is not efficient and vice versa. In constrained clustering, the subset of events excluded by the constraints need to be of high description length density in order to results in shorter encoding if constraints are used.

Theorem 5.1 Let P be the set of possible partition events for unconstrained clustering and Q be the set of partition events of constrained clustering. Let ω be the probability measure on P that corresponds to the efficient prefix MDL encoding. If

$$DLD_{\omega}(Q) \le DLD_{\omega}(P-Q)$$

Then encoding with constraints results in shorter expected description length.

Proof: The expected description length for the non-constraint clustering is given by,

$$L_{NC} = E_P[-\ln \omega(p)] = -\int_P \omega(p) \ln \omega(p) dp \tag{5.2}$$

After the events set is reduced from P to Q, the prefix code is renormalized, the new probability density on Q becomes,

$$\psi(q) = \frac{\omega(q)}{\int_Q \omega(q)} \tag{5.3}$$

The expected description length for the constrained clustering is

$$L_{CC} = E_Q[-\ln \psi(q)] = -\int_Q \psi(q) \ln \psi(q) dq = -\int_Q \frac{\omega(q)}{\int_Q \omega(p) dp} \ln \frac{\omega(q)}{\int_Q \omega(p) dp} dq$$

$$= -\frac{\int_Q \omega(q) \ln \omega(q) dq}{\int_Q \omega(p) dp} + \ln \int_Q \omega(p) dp$$

The change of the expected description length is given by,

$$\Lambda L = L_{CC} - L_{NC} = -\frac{\int_{Q} \omega(q) \ln \omega(q) dq}{\int_{Q} \omega(p) dp} + \ln \int_{Q} \omega(p) dp + \int_{P} \omega(p) \ln \omega(p) dp$$

Let $$\frac{1}{\int_{Q} \omega(p) dp} = 1 + \alpha$$

$$\begin{aligned}
&\Delta L = L_{CC} - L_{NC} \\
&= -(1+\alpha) \int_{Q} \omega(q) \ln \omega(q) dq + \ln \int_{Q} \omega(p) dp + \int_{P-Q} \omega(p) \ln \omega(p) dp + \int_{Q} \omega(p) \ln \omega(p) dp \\
&= \int_{P-Q} \omega(p) \ln \omega(p) dp - \alpha \int_{Q} \omega(q) \ln \omega(q) dq + \ln \int_{Q} \omega(p) dp \\
&= \int_{P-Q} \omega(p) dp \left(\frac{\int_{P-Q} \omega(p) \ln \omega(p) dp}{\int_{P-Q} \omega(p) dp} - \left(\frac{1}{\int_{Q} \omega(p) dp} - 1 \right) \frac{\int_{Q} \omega(q) \ln \omega(q) dq}{\int_{P-Q} \omega(p) dp} \right) + \ln \int_{Q} \omega(p) dp \\
&= \int_{P-Q} \omega(p) dp \left(\frac{\int_{P-Q} \omega(p) \ln \omega(p) dp}{\int_{P-Q} \omega(p) dp} - \frac{\int_{Q} \omega(q) \ln \omega(q) dq}{\int_{Q} \omega(p) dp} \right) + \ln \int_{Q} \omega(p) dp \\
&= \left(DSD_{\omega}(Q) - DSD_{\omega}(P-Q) \right) \int_{P-Q} \omega(p) dp + \ln \int_{Q} \omega(p) dp \\
&\leq 0
\end{aligned}$$

Q.E.D.

Theorem 5.1 states that the learner expects to encode with shortened description length if the subset of events which has been removed by the constraints have a higher description length density than the subset of events that are compatible with the constraints. A constraint is "sound" if it decreased the expected description length by removing the lengthy encoding subsets from the entire set of events.

Theorem 5.2 $DLD_{\omega}(P-Q) \geq DLD_{\omega}(Q) \Leftrightarrow DLD_{\omega}(P) \geq DLD_{\omega}(Q)$

Proof: The proof is straightforward,

$$W(Q) = \int_{Q} \omega(q) dq$$

By the definition of description length density,

$$W(Q)DSD_{\omega}(Q) + W(P-Q)DSD_{\omega}(P-Q) = DSD_{\omega}(P)$$

$$\frac{DLD_{\omega}(P-Q)}{DLD_{\omega}(Q)} = \frac{DLD_{\omega}(P) - W(Q)DSD_{\omega}(Q)}{W(P-Q)DLD_{\omega}(Q)} = \frac{\frac{DLD_{\omega}(P)}{DSD_{\omega}(Q)} - W(Q)}{W(P-Q)}$$

Since $W(Q) + W(P-Q) = 1$

$$\frac{DLD_{\omega}(P-Q)}{DLD_{\omega}(Q)} \geq 1 \Leftrightarrow \frac{DLD_{\omega}(P)}{DSD_{\omega}(Q)} \geq 1$$

Q.E.D.

Theorem 5.2 together with 5.1 states that it is sufficient to compare the description length density of the unconstrained event set with that of the constrained event set to decide the soundness of a constraint.

5.4 MDL Clustering with Instance-Level Constraints

5.4.1 Encoding Must-Link Constraints

We view constraints are prior knowledge or agreements on codes shared by the sender and receiver. For example, if pattern x_i and x_j form a must-link constraint, the sender

can encode the clustering assignment information of the two patterns together. The receiver, on the other hand, should expect such encoding and knows that the cluster assignment would not be encoded redundantly once the cluster assignment information of x_i is assigned.

The must-link constraints have following entailment property,

$$ML(x_i, x_j) \cap ML(x_j, x_k) \Rightarrow ML(x_i, x_k) \tag{5.4}$$

Such property allows identifying must-link pattern sets within which patterns must make the same clustering assignments. Must-link constraints allow economical coding on clustering assignments, but the same inflexibility may lead to larger encoding costs on the disparities between the pattern and cluster center.

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The must-link subsets are identified by searching for the connected components in an auxiliary graph *G(V,E)* in the following steps.

1. The set of vertices *V* form a one-to-one mapping to the set of patterns
2. Connect undirected edge $E(v_i, v_j)$ if $ML(x_i, x_j)$
3. Find the set of connected components of *G* by breadth first search algorithm

We use a flag f_{CC_i} to indicate if a connected component is already encoded. The flag does not have to be part of the description that the sender sends to the receiver. It is only used in constructing the code. The receiver can construct the flags unambiguously from the constraints when decoding the message. The steps to construct the code for the cluster assignment information with the auxiliary graph are,

1. Initialize the encoding flag for each connected component as 0

2. For each pattern x_i, identify its connected component.

3. If the flag of the connected component is 0, then encode the cluster assignment of the pattern and set the encoding flag of the connected component to 1. If the flag of the connected component is 1, then no encoding is needed for cluster assignment of x_i.

4. Encode the distances of each pattern from its assigned cluster center.

Example 5.1 (Must-Link Encoding) Let $x_1 = 0.1, x_2 = 0.2, x_3 = 0.5, x_4 = 0.8, x_5 = 0.9$ be five patterns to be clustered into three clusters. The must-link constraints are $ML(x_1, x_2), ML(x_4, x_5)$. A feasible partition is $\{x_1, x_2, x_3\}\{x_4, x_5\}$. Further, the prefix code to encode the cluster assignment corresponds to probability measure *P* such that

$$P(1) = \frac{3}{5}, P(2) = \frac{2}{5}$$

The encoding of the patterns can be accomplished with the following steps,

1. A Breadth-First search identifies the connected components are $\{x_1, x_2\}\{x_3\}\{x_4, x_5\}$.

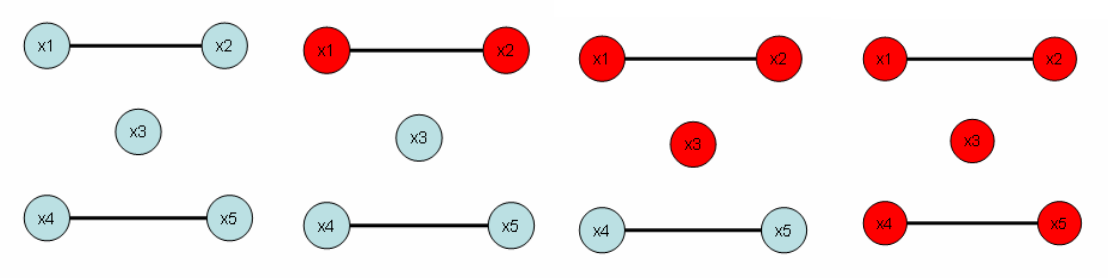
2. Encode x_1 with description length $-\ln P(1)$ and set flag $f_{CC_1} = 1$, which is indicated by Figure 5.1 (b).

3. When encode x_2, the sender check that $x_2 \in CC_1$ and $f_{CC_1} = 1$. Thus no encoding is needed for x_2. The receiver of the code can determine the cluster assignment of x_2 from the constraints and earlier part of the code.

4. x_3 is encoded with description length of $-\ln P(1)$ and set flag $f_{CC_2} = 1$.

5. x_4 and x_5 are encoded similarly as x_1 and x_2 using the must-link constraint.

6. The distances of the patterns from the assigned clusters are encoded with equation (2.29).



(a) (b) (c) (d)

Figure 5.1 Encoding with Must-Link Constraints in Example 5.1

5.4.2 Encoding Cannot-Link Constraints

Because cannot-link constraints do not have the entailment property as must-link constraints, the encoding is more complicated. As mentioned previously, the feasibility problem for cannot-link constraints is NP-complete. Thus there is no known polynomial algorithm to decide if a code exists to encode the patterns while fulfilling the constraints. However, assuming that a feasible clustering solution has already been found, the patterns can be encoded with the following steps,

1. Construct an auxiliary graph for the cannot-link constraints similarly as in the must-link constraints.

2. For each pattern x_i, initialize coding flag as 0.

3. For each pattern x_i, if all adjacent vertices in the auxiliary graph have coding flag 0, encode the cluster assignment with the same prefix code as unconstrained clustering and change coding flag to 1. If some adjacent vertices in the auxiliary graphs have

coding flag 1, code cluster assignment by renormalizing the unconstrained code and change coding flag to 1.

4. Encode the distances of each pattern from its assigned cluster center.

Example 5.2 (Cannot-Link Encoding) Let $x_1 = 0.1, x_2 = 0.2, x_3 = 0.5, x_4 = 0.8, x_5 = 0.9$ be five patterns to be clustered into three clusters. The cannot-link constraints are $CL(x_1, x_3), CL(x_3, x_5)$. A feasible partition is $\{x_1, x_2\}\{x_3\}\{x_4, x_5\}$. Further, the prefix code to encode the cluster assignment corresponds to probability measure P such that

$$P(1) = \frac{2}{5}, P(2) = \frac{1}{5}, P(3) = \frac{2}{5}$$

To encode the cluster assignments of the patterns, we first construct the auxiliary graph,

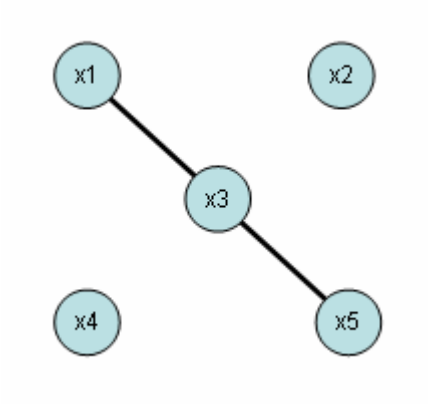


Figure 5.2 Cannot-Link Encoding Auxiliary Graph for Example 5.2

The encoding of the patterns are done sequentially with inference to the auxiliary graph G in Figure 5.2,

1. x_1 is encoded with description length $-\ln P(1)$.

2. x_2 is encoded with description length $-\ln P(1)$.

3. In encoding x_3, the sender checks the neighboring vertices in the auxiliary graph G and found x_1 is already encoded to be assigned to cluster 1. x_3 can only be assigned to either cluster 2 or 3. Thus prefix code *P* becomes redundant by reserving code to encode the event of assigning x_3 to cluster 1. The probability measure *P* is renormalized into *Q* by excluding events that conflicts the cannot-link constraint.

$$Q(2) = \frac{1}{3}, Q(3) = \frac{2}{3}$$

The description length to encode the cluster assignment of x_3 to cluster 2 is $-\ln Q(2)$. The description length saved is $\ln Q(2) - \ln P(2) = \ln \frac{5}{3}$.

4. x_4 is encoded with description length $-\ln P(3)$.

5. x_5 is encoded in the similar way as x_3, by excluding the event of assigning x_5 to cluster 2, the probability measure is renormalized into

$$Q(2) = \frac{1}{2}, Q(3) = \frac{1}{2}$$

The description length saved is $\ln Q(3) - \ln P(3) = \ln \frac{5}{4}$

6. The distances of the patterns from the assigned cluster centers are encoded with code in equation (2.29).

5.4.3 Optimization

The optimization is done in a similar fashion to K-means clustering, while replacing the quantization error with description length cost. Within each iteration, a pattern is assigned to the cluster that offers shortest encoding of the pattern while maintaining the integrity

of the constraints. The encoding cost of the patterns can be represented by an encoding cost matrix C, where each row represents a pattern and each column a potential cluster assignment of the pattern. $C[i, j]$ entry represents the encoding cost associated with assigning pattern i to cluster j. To minimize the total encoding cost, the cluster assignment for each pattern is simply,

$$P(x_i) = \arg\min_j C[i, j] \tag{5.5}$$

The minimization is less straightforward when it subjects to a number of must-link and cannot-link constraints. Again, the problem is NP-complete in nature and we cannot hope to find an exact solution. Instead, we assume the constraints form an easy set [DR06] where iterative algorithms will converge to a feasible solution.

The cannot-link constraints may potentially enforce the learner to make a cluster assignment that is not the shortest description length in the row of the coding matrix representing a pattern. The worst case scenario is the clustering assignment associated with the longest description length has to be chosen due to constraints. We define maximum coding risk (MCR) as the largest possible extra encoding cost of a constrained assignment versus when the assignment is unconstrained for a given pattern,

$$MCR(C[i,.]) = \max(C[i,.]) - \min(C[i,.]) \tag{5.6}$$

Within the scope of respecting the constraints, the learner should prefer to make assignment for patterns with larger MCR first.

In [DR06], Davidson and Ravi proposed an algorithm that generates the inductive ordering of the patterns to achieve convergence for a clustering problem with easy

constraints set. Here, we modify the algorithm slightly to accommodate our need to minimize the description length within the scope of satisfying the constraints.

1. Generate connected components with breadth-first search.
2. Generate auxiliary graph G (*V, E*) with each node corresponding to a connected component and each edge corresponding to a cannot-link constraint.
3. E-Step
    a. Generate encoding cost matrix *C*.

$$C[i, j] = -\ln \omega_j + \sum_{x \in CC_i} \frac{\left\| x - \mu_j \right\|^2}{\sigma_j^2}$$

    b. Generate *Q*-inductive Order cc_i

    While $V \neq \Phi$

        i. Find a node $v \in V$ with minimum degree. For nodes with the same number of degrees, find the node with smallest MCR defined in (5.6)

        ii. Insert *v* at the head of the list *L*

        iii. $V = V - v$

    End While

    c. For each cc_i, set constraint list $CList(cc_i) = \Phi$

    d. For each $cc_i \in L$ from head to tail

i. $z(cc_i) = \arg\min_{j \notin CList(i)} C[i, j]$

ii. For each cc_k that $E(cc_k, cc_i) = 1$

$$CList(cc_k) = CList(cc_k) \cup z(cc_i)$$

4. M-Step

a. $$\omega_j = \frac{\sum_{i=1}^{N} \delta(z(x_i), j)}{N}$$

b. $$\mu_j = \frac{\sum_{i=1}^{N} \delta(z(x_i), j) x_i}{\sum_{i=1}^{N} \delta(z(x_i), j)}$$

c. $$\sigma_j^2 = \frac{\sum_{i=1}^{N} \delta(z(x_i), j) \| x_i - \mu_j \|^2}{\sum_{i=1}^{N} \delta(z(x_i), j)}$$

5. Repeat step 3 and 4 until the solution converges.

5.5 Constraints Violation

Not all constraints are beneficial to the clustering process. Poorly specified constraints such as must-link constraints among very disparate patterns give rises to clusters with large within-cluster dissimilarities. For example, the feedback in the Yahoo! example is not guaranteed to be of high quality as anyone can potentially provide any constraints. It

is essentially important to evaluate constraint quality and ignore poorly specified constraints.

Theorem 5.1 and 5.2 provides a method in determining the quality of the constraints. Constraints, as background knowledge in the clustering problem, should supposedly shorten the overall description length. Any imposed constraints that necessarily increase the encoding cost should be ignored if the constraints are not enforced to be hard, as the choice between encoding with constraints and without is essentially a model selection problem and the description length of the pattern is the ubiquitous metric that decides the outcome of the model selection.

The algorithm in the previous section can be readily modified to accommodate the constraint evaluation mechanism implied by theorem 5.1 and 5.2 in the E-Step, when the patterns are assigned to clusters by evaluating the encoding costs associated with each of the clusters. The expected encoding cost with the constraints can be compared to that without, and the learner only enforces a constraint if it allows shortening of the description. To address the decoding issue, the code reserves a single bit as a flag to indicate if a constraint is enforced so that the receiver can decipher the code accordingly.

5.6 Empirical Results

In this section, we use UCI dataset to empirically validate the MDL based instance-level constrained clustering approach proposed in the chapter. All datasets have continuous attributes, which are standardized. Each dataset is randomly divided into training set

(80%) and test set (20%). Within the training set, must-link constraints and cannot-link constraints are generated with different constraint percentages (CP) from the class labels. A derivation of the algorithm outline in 5.5 by incorporating the encoding cost of the class labels is used to find the cluster solutions. Each cluster is associated with a class label by majority counting. This allows classification of the patterns in the test set with two steps: first assign a pattern to a cluster (there is no constraint in the test set) and then the predicted label is the one that corresponds to the assigned cluster. The reported accuracy is an average over 10 runs.

In the first experiment, all constraints are faithfully generated from the class labels. For patterns with the same class label, we assign must-link constraints and for patterns with different class labels, we assign must-link constraints. The empirical results are indicated in Figure 5.1. With increased percentage of constraints, both the accuracy of the training set and testing set improves steadily, indicating that the constraints derived from the class labels have influenced the cluster solutions towards befitting the purpose of predicting the class labels. It also suggests that class labels can provide more information than passively serving as associating clusters with classes by simple majority counting, they can actively participate in the clustering solution search process and thus boost the overall performance.

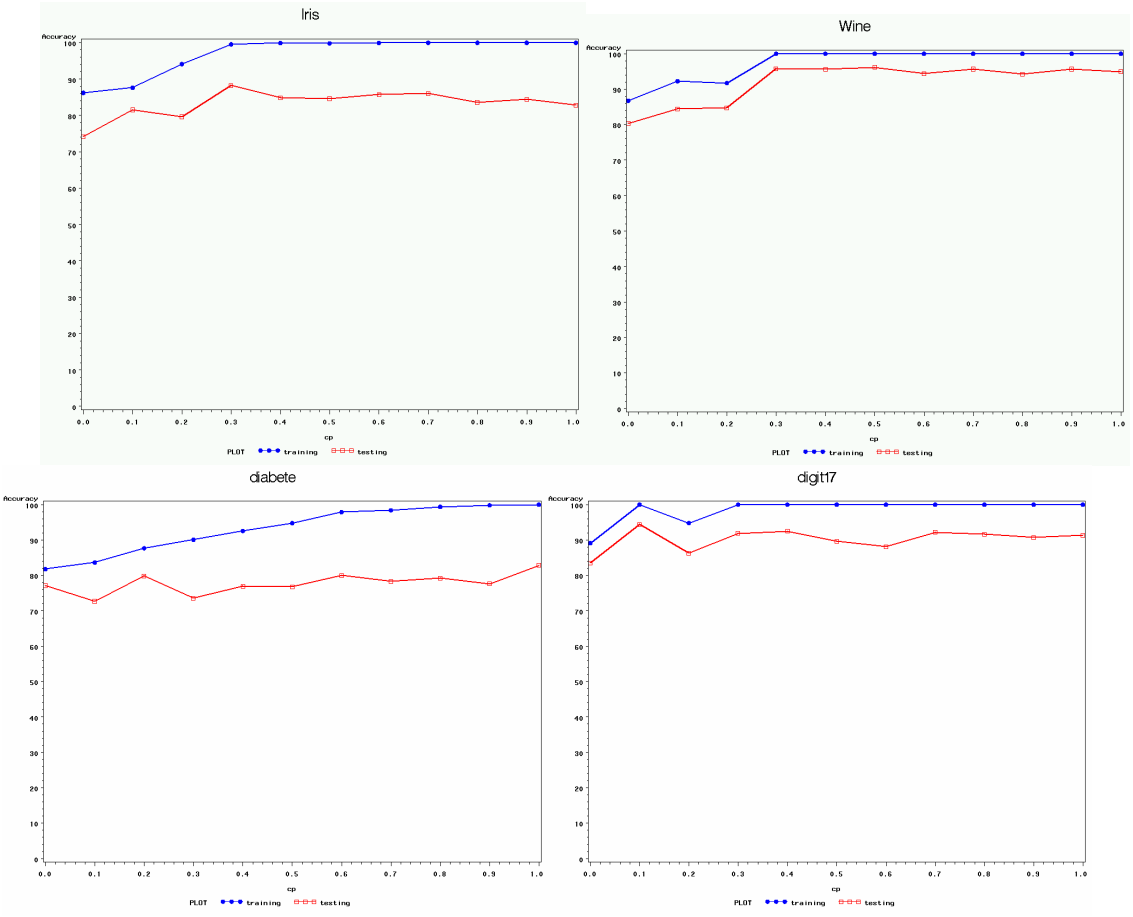


Figure 5.3 Performance of UCI Datasets from Different Percentage of Constraints Generated from Class Labels

The second experiment is similar to the first one, except that the constraints are generated purely randomly, independent of the class labels. Such constraints with no insights should be detrimental to the learner and lengthens the encoding cost if the constraints are to be enforced. The results are shown in Figure 5.4, where both the training and testing sets have impaired performance when more randomly generated constraints are introduced. It shows poorly specified constraints can deteriorates the clustering solution significantly.

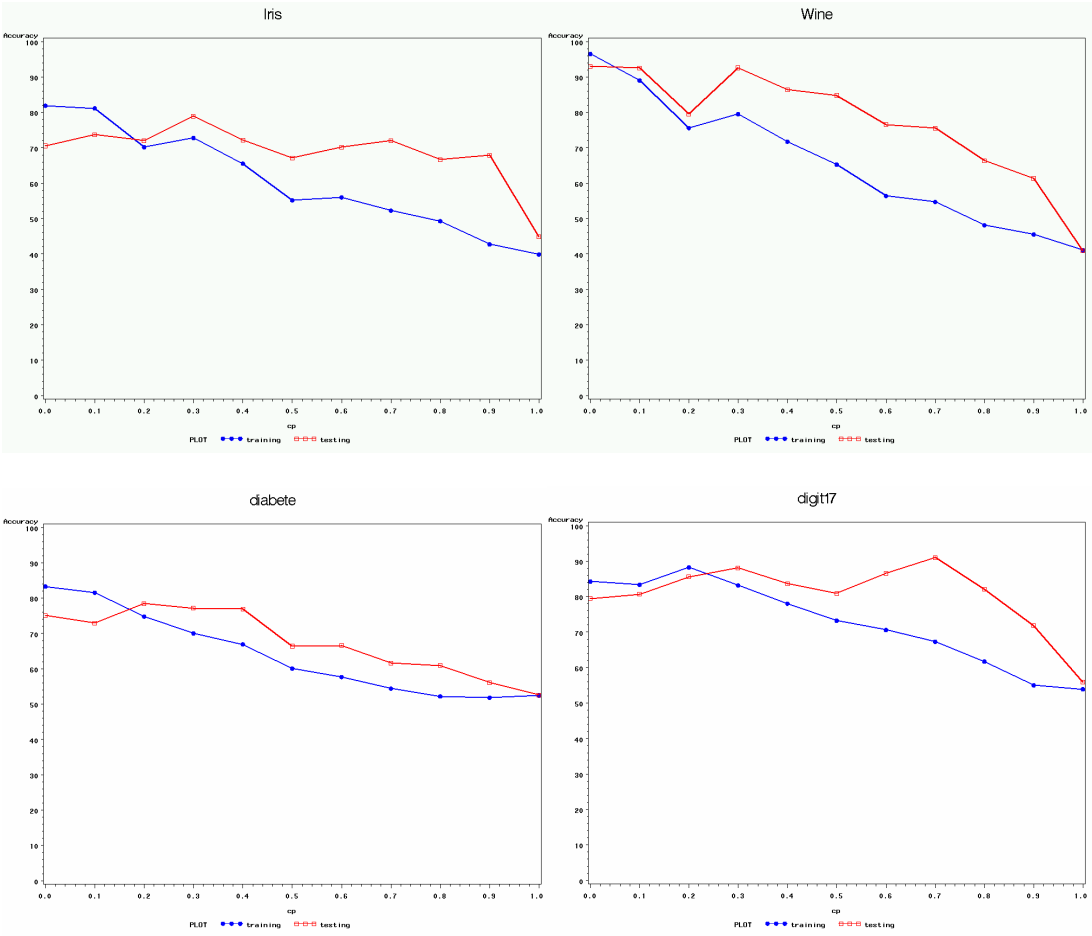


Figure 5.4 Performance of UCI Datasets from Different Percentage of Constraints Generated Randomly

In the third experiment, 60% of the generated constraints are from class labels and 40% are generated randomly. We compare the results between “soft constraints”, which allow MDL actively choosing “sound” constraints that lead to shortened description length, and “hard constraints”, where the clustering results are partially dictated by the constraints. Empirical results show that MDL can evaluate the quality of the constraints correctly and improves the performance of the training set. However, empirical results indicate that even without actively choosing the “good” constraints, the performance of the testing set is resistant to the certain percentage of bad constraints. A possible reason is that the “bad”

constraints are generated randomly introduces more variance in the system, but will not affect the estimations of the cluster centers much. The clusters found are relatively good to predict on the testing set even with some randomly noisy constraints.

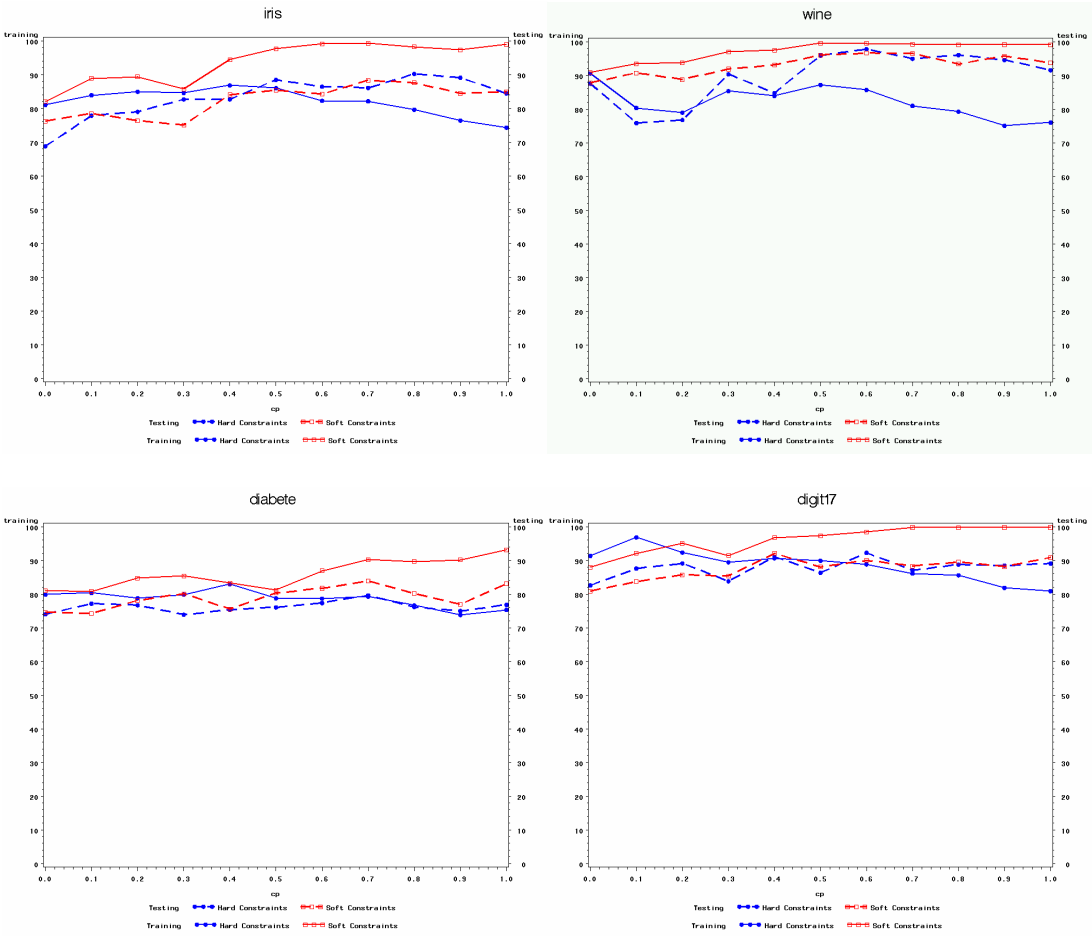


Figure 5.5 Comparison between Hard Constraints MDL Selected Soft Constraints on UCI Datasets from Different Percentage of Constraints Generated from Class Labels with 40% Noise

In the fourth experiment, we use the same setting as experiment 3, but generate the 40% "bad" constraints systematically. This reflects a bias in the constraints, to which the hard constrained clustering is no longer resistant. Empirical results show that MDL evaluation

of the constraints actively choosing the good constraints and yield significantly better accuracies than if all the constraints are faithfully respected.

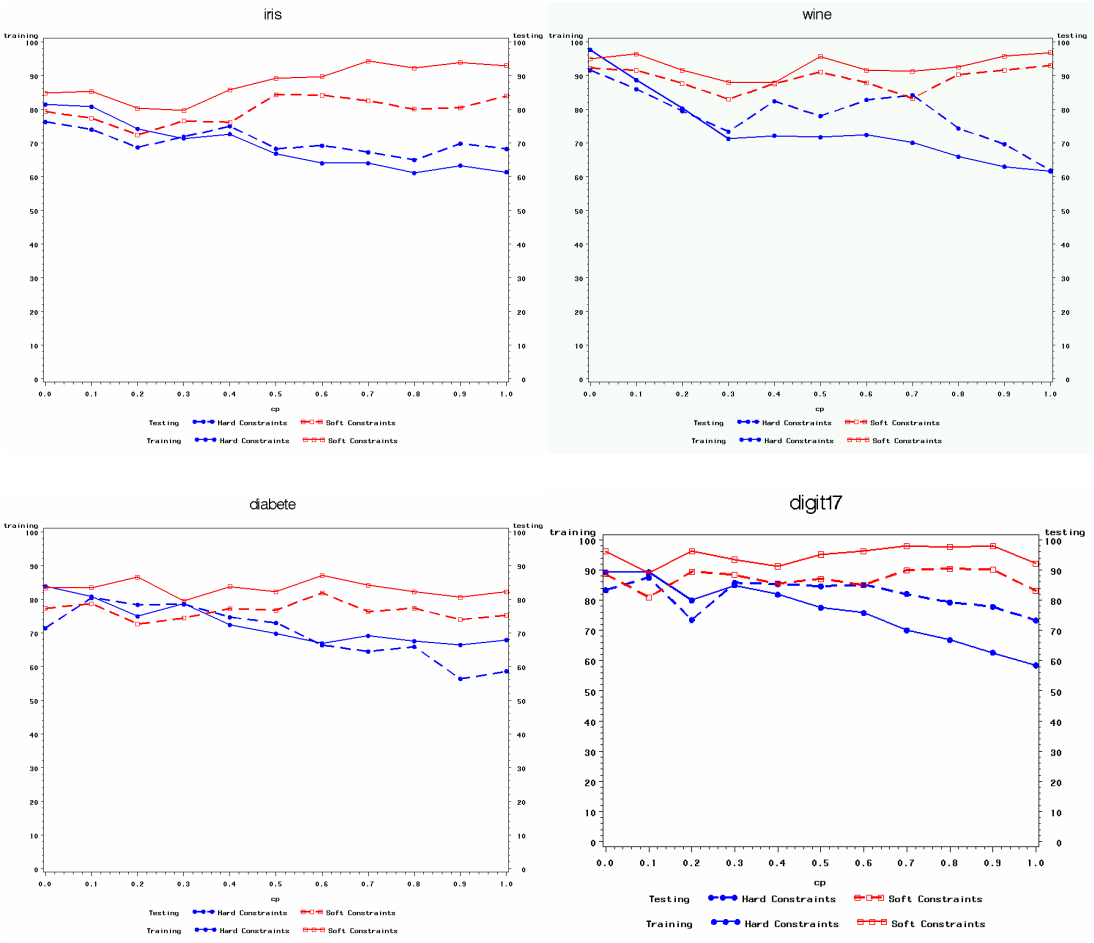


Figure 5.6 Comparison between Hard Constraints MDL Selected Soft Constraints on UCI Datasets from Different Percentage of Constraints Generated from Class Labels with 40% Bias

5.7 Chapter Summary

In constrained clustering, the cluster partition solution is subject to a set of must-link and cannot-link constraints which are generated either from expert opinion or class labels. While well specified constraints increase the performance of the learner, poorly defined constraints can mitigate the learning quality. In this chapter, we propose the MDL

approach to solving the constrained clustering problem, which allows active identification of randomly bad constraints due to variance and systematically bad constraints due to bias. The empirical results indicate that the method performs well in both cases by ignoring the bad constraints. In particular, it is most useful in identifying bad constraints due to bias to which the performance of a learner is most vulnerable.

6 Conclusion and Future Work

This thesis explores three informed clustering problems by utilizing minimum description length principle. Within the established MDL informed clustering framework, various information are all encoded into binary strings and information amount is measured ubiquitously by the string lengths. This allows straightforwardly managing the trade-off among information of various types. In particular, for each type of informed clustering problem, the thesis describes the following aspects:

- How to encode patterns within the clustering context. This includes encoding pattern assignments to clusters and the disparities between patterns and cluster centers. In addition, in multi-view clustering, the thesis proposes the joint encoding of the views; in semi-supervised clustering, the thesis describes the encoding of the partial labels; in constrained clustering, the thesis discusses encoding with constraints as background knowledge.

- How to search for the shortest code. The thesis uses EM optimization algorithm when model uncertainty is less significant such as in multi-view clustering and constrained clustering. While in semi-supervised clustering where the limited partial label induces significant model uncertainty, the thesis proposes a MDL based Markov Chain Monte Carlo sampler, which allows efficient sampling of the posterior distribution and constructing the Optimal Bayes Classifier (OBC).

- How to decide the model selection problem. A major advantage of the MDL based informed clustering framework proposed in the thesis is that model selection problem can be conveniently addressed within the framework. As MDL considers both model complexity and goodness of data fitting, models of different complexity can be directly compared using the encoding length as the yardstick. In multi-view clustering, the framework allows model selection between modelling the views as independent and as dependent; in semi-supervised clustering, it allows automatic jumping across mixture Gaussian model space with different number of components; in constrained clustering, it allows the learner to judge the soundness of the constraints, thus exploiting the beneficial constraints and ignores the detrimental ones.

Empirical results indicated that the MDL based inference yields improved performances in various informed clustering problems. The framework proposed in the thesis avail itself as a learning flexible tool to handle various types of background information in informed clustering problems and make inferences that are immune to model over-fitting or under-fitting.

Future Research Directions

The thesis is the first attempt in establishing a unified framework among various types of informed clustering problems. The thesis explores to certain level of details of the encoding of various types of background information, but it requires further supplementation and refinement at least in the following aspects:

- In multi-view clustering, when the number of views increases from two, the algorithm proposed in chapter 3 has an exponential computational complexity to the number of views. Automatic selecting the most informative views from large number views of the data is a challenging problem.

- In semi-supervised clustering, a very simple multinomial model is built within each cluster in predicting class labels. In principle, any classifier can be combined with clustering to give rise to local classifier for each cluster, known as the divide and conquer approach. Incorporating other classifiers into the semi-supervised clustering can potentially further improve the model performance.

- In constrained clustering, the thesis explored encoding with instance-level constraints. To have a complete framework, further research is needed for encoding under cluster-level constraints and model-level constraints.

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