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Semi-supervised clustering aims to improve clustering performance by considering user supervision in the form of pairwise constraints. In this paper, we study the active learning problem of selecting pairwise must-link and cannot-link constraints for semi-supervised clustering. We consider active learning in an iterative manner where in each iteration queries are selected based on the current clustering solution and the existing constraint set. We apply a general framework that builds on the concept of neighborhood, where neighborhoods contain "labeled examples" of different clusters according to the pairwise constraints. Our active learning method expands the neighborhoods by selecting informative points and querying their relationship with the neighborhoods. Under this framework, we build on the classic uncertainty-based principle and present a novel approach for computing the uncertainty associated with each data point. We further introduce a selection criterion that trades-off the amount of uncertainty of each data point with the expected number of queries (the cost) required to resolve this uncertainty.

This allows us to select queries that have the highest information rate. We evaluate the proposed method on the benchmark datasets and the results demonstrate consistent and substantial improvements over the current state-of-the-art.

Active Learning of Constraints for Semi-Supervised Clustering

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I understand that my thesis will become part of the permanent collection of Oregon State University libraries. My signature below authorizes release of my thesis to any reader upon request.

Sicheng Xiong, Author

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To my family and friends.

Chapter 1: INTRODUCTION

Semi-supervised clustering aims to improve clustering performance with the help of user-provided side information. One of the most studied types of side information is pairwise constraints, which include must-link and cannot-link constraints specifying that two points must or must not belong to the same cluster. A number of previous studies have demonstrated that, in general, such constraints can lead to improved clustering performance [2,3,4]. However, if the constraints are selected improperly, they may also degrade the clustering performance [9, 11]. Moreover, obtaining pairwise constraints typically requires a user to manually inspect the data points in question, which can be time consuming and costly. For example, for document clustering, obtaining a must-link or cannot-link constraint requires a user to potentially scan through the documents in question and determine their relationship, which is feasible but costly in time. For those reasons, we would like to optimize the selection of the constraints for semi-supervised clustering, which is the topic of active learning.

While active learning has been extensively studied in supervised learning [7, 12, 13, 14, 16, 21], the research on active learning of constraints for semi-supervised clustering is relatively limited [2,11,15,19,26]. Most of the existing work on this topic has focused on selecting an initial set of constraints prior to performing semi-supervised clustering [2, 11, 19, 26]. This is not suitable if we wish to iteratively improve the clustering model by actively querying the user.

In this thesis we consider active learning of constraints in an iterative framework. Specifically, in each iteration we determine what is the most important information toward improving the current clustering model and form queries accordingly. The responses to the queries (i.e., constraints) are then used to update (and improve) the clustering. This process repeats until we reach a satisfactory solution or we reach the maximum number of queries allowed. Such an iterative framework is widely used in active learning for supervised classification [12, 13, 14, 16], and has been generally observed to outperform non-iterative methods where the whole set of queries is selected in a single batch.

We focus on a general approach based on the concept of neighborhoods, which has been successfully used in a number of previous studies on active acquisition of constraints [2, 15, 19]. A neighborhood contains a set of data points that are known to belong to the same cluster according to the constraints and different neighborhoods are known to belong to different clusters. Simply put, neighborhoods can be viewed as containing the "labeled examples" of different clusters. Well-formed neighborhoods can provide valuable information regarding what the underlying clusters look like. Analogous to supervised active learning, an active learner of constraints will then seek to select the most informative data point to include in the neighborhoods. Once a point is selected, we query the selected point against the existing neighborhoods to determine to which neighborhood it belongs.

Specifically, our approach builds on the classic uncertainty-based principle. Here we define the uncertainty in terms of the probability of the point belonging to different known neighborhoods and propose a novel non-parametric approach using random

forest [5] for estimating the probabilities. Different from supervised learning where each point only requires one query to obtain its label, in semi-supervised clustering, we can only pose pairwise queries and it typically takes multiple queries to determine the neighborhood of a selected point. In general, points with higher uncertainty will require larger number of queries. This suggests that there is a trade-off between the amount of information we acquire by querying about a point, and the expected number of queries (cost) for acquiring this information. We propose to balance this trade-off by normalizing the amount of uncertainty of each data point by the expected number of queries required to resolve this uncertainty, and as such, select queries that have the highest rate of information.

Note that an obvious alternative approach would be to evaluate all potential pairs and select the one that has the highest uncertainty regarding wether they are must-linked or cannot-linked. This idea has previously been explored by Huang et al. [15] in the context of document clustering. In this thesis, we note a critical issue with this approach that it only considers the pairwise uncertainty of the first query, and fails to measure the benefit of the ensuing queries that are required to determine the neighborhood for a point. Our method, instead, focuses on the point-based uncertainty, allowing us to select the queries according to the total amount of information gained by the full sequence of queries as a whole.

We empirically evaluate the proposed method on eight datasets of different complexity. The evaluation results demonstrate that our method achieves consistent and substantial improvements over three competing methods.

The remainder of the thesis is organized as follows. Chapter 2 presents a brief review

of the related work on active learning of constraints. Chapter 3 introduces our general active learning framework and the proposed method within the framework. Experimental evaluations are presented in Chapter 4. Finally, we conclude the thesis and discuss future directions in Chapter 5.

Chapter 2: LITERATURE REVIEW

Active learning has been studied extensively for supervised classification problems [7, 12, 13, 14, 16, 21]. In contrast, the research on active learning for constraint-based clustering has been limited. As mentioned previously, most of the existing research studied the selection of a set of initial constraints prior to performing semi-supervised clustering. Specifically, the first study on this topic was conducted by Basu et al. [2]. They proposed a two-phase approach, which we refer to as the Explore and Consolidate (E & C) approach. The first phase (Explore) incrementally selects points using the farthest-first traversal scheme and queries their relationship to identify c disjoint neighborhoods, where c is the total number of clusters. The second phase (Consolidate) iteratively expands the neighborhoods, where in each iteration it selects a random point outside any neighborhood and queries it against the existing neighborhoods until a must-link is found. More recently, Mallapragada et al. [19] proposed an improvement to Explore and Consolidate named Min-Max, which modifies the Consolidate phase by choosing the most uncertain point to query (as opposed to randomly).

Xu et al. [26] proposed to select constraints by examining the spectral eigenvectors of the similarity matrix, which is unfortunately limited to two-cluster problems. In [1, 11], constraints are selected by analyzing the co-association matrix (obtained by applying cluster ensembles to the data). A key distinction of our method from the above mentioned work is that we iteratively select the next set of queries based on the current

clustering assignment in order to improve the solution. This is analogous to supervised active learning where data points are selected iteratively based on the current classification model such that the model can be improved most efficiently [12, 13, 14, 16].

More relevant to our work is an active learning framework presented by Huang et al. [15] for the task of document clustering. Specifically, this framework takes an iterative approach that is similar to ours. In each iteration, their method performs semi-supervised clustering with the current set of constraints to produce a probabilistic clustering assignment. It then computes, for each pair of documents, the probability of them belonging to the same cluster and measures the associated uncertainty. To make a selection, it focuses on all unconstrained pairs that has exactly one document already "assigned to" one of the existing neighborhoods by the current constraint set, and among them identifies the most uncertain pair to query. If a "must-link" answer is returned, it stops and moves onto the next iteration. Otherwise, it will query the unassigned point against the existing neighborhoods until a "must-link" is returned.

While Huang's method is developed specifically for document clustering, one could potentially apply the underlying active learning approach to handle other types of data by assuming appropriate probabilistic models. We would like to highlight a key distinction between Huang's method and our work, that is Huang's method makes the selection choice based on *pairwise uncertainty* whereas we focus on the uncertainty of a point in terms of which neighborhood it belongs to. This difference is subtle, but important. Pairwise uncertainty captures only the relationship between the two points in the pair. Depending on the outcome of the query, we may need to go through a sequence of additional queries. Huang's method only considers the pairwise uncertainty of the first

query, fails to measure the benefit of the ensuing queries. This is why our method instead focuses on point-based uncertainty, which measures the total amount of information gained by the full sequence of queries as a whole. Furthermore, our method also takes into account the expect number of queries to resolve the uncertainty of a point, which has not been considered previously.

Finally, we want to mention another line of work that uses active learning to facilitate clustering [22, 25] where the goal is to cluster a set of objects by actively querying the distances between one or more pairs of points. This is different from the focus of this thesis, where we only request pairwise must-link and cannot-link constraints, and do not require the user to provide specific distance values.

Chapter 3: METHODOLOGY

The problem addressed in this thesis is how to effectively choose pairwise queries in order to produce an accurate clustering assignment. Through active learning, we aim to achieve query efficiency, i.e., we would like to reduce the number of queries/questions asked in order to achieve a good clustering performance. We view this as an iterative process such that the decision for selecting queries should depend on what has been learned from all the previously formulated queries. In this section, we will introduce our proposed method. Below we will begin by providing a precise formulation of our active learning problem.

3.1 Problem Formulation

Formally, we define the problem as follows: given a set of data instances $\mathcal{D} = \{\mathbf{x}_1, \cdots, \mathbf{x}_n\}$, we assume that there exists an underlying class structure that assigns each data instance to one of the c classes. We denote the unknown labels by $\mathbf{y} = \{y_1, \cdots, y_n\}$, each label $y_i \in \mathcal{Y} \triangleq \{1, \cdots, c\}$, $\forall i \in \{1, \cdots, n\}$. In this setting, we cannot (directly) observe these labels. Instead, information can be obtained through query of the form: *Do instances $\mathbf{x}_i$ and $\mathbf{x}_j$ belong to the same class?* We denote a query by a pair of instances $(\mathbf{x}_i, \mathbf{x}_j)$, and the answer to the query by $l_{ij} \in \mathcal{A} \triangleq \{\mathrm{ML}, \mathrm{CL}\}$. In particular, the label "ML" ("CL") is returned if $y_i = y_j$ ($y_i \neq y_j$). In each iteration, we need to select one or

more queries based on $\mathcal{D}$ and the current set of constraints $\mathcal{C}$.

Note that must-link and cannot-link constraints satisfy the following properties:

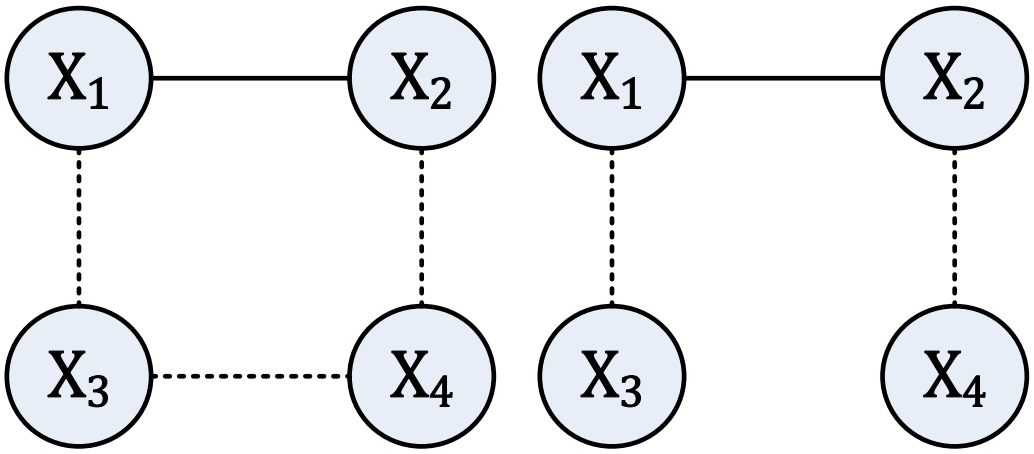
- $(\mathbf{x}_i, \mathbf{x}_j, ML) \wedge (\mathbf{x}_i, \mathbf{x}_k, ML) \Rightarrow (\mathbf{x}_j, \mathbf{x}_k, ML)$
- $(\mathbf{x}_i, \mathbf{x}_j, ML) \wedge (\mathbf{x}_i, \mathbf{x}_k, CL) \Rightarrow (\mathbf{x}_j, \mathbf{x}_k, CL)$

Based on these properties, we introduce the concept of neighborhood, which is instrumental in the design of many existing methods for active learning of pairwise constraints [2, 15, 19].

3.2 A Neighborhood-based Framework

Definition 1. *A neighborhood contains a set of data instances that are known to belong to the same class (i.e., connected by must-link constraints). Further more, different neighborhoods are connected by cannot-link constraints and thus are known to belong to different classes.*

Given a set of constraints denoted by $\mathcal{C}$, we can identify a set of l neighborhoods $\mathcal{N} = \{N_1, \cdots, N_l\}$, such that $l \leq c$ and c is the total number of classes. Consider a graph representation of the data where vertices represent data instances and edges represent must-link constraints. The neighborhoods, which are denoted by $N_i \subset \mathcal{D}, i \in \{1, \cdots, l\}$, are simply the connected components of the graph that have cannot-link constraints between one another. Note that if there exists no cannot-link constraints, we can only identify a single known neighborhood even though we may have multiple connected components because some connected components may belong to the same



(a) (b)

Figure 3.1: Two examples to show how to identify neighborhoods from a set of pairwise constraints.

class. In such cases, we will treat the largest connected component as the known neighborhood.

Figure 3.1 illustrates two examples that explain how we can form the neighborhoods from a set of pairwise constraints. The nodes denote data instances, and the solid lines denote must-link constraints while the dashed lines denote cannot-link constraints. Note that in our definition, each neighborhood is required to have a cannot-link constraint with all other neighborhoods. Therefore, Figure 3.1(a) contains three neighborhoods: $\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}$, and $\{\mathbf{x}_4\}$, whereas Figure 3.1(b) contains only two known neighborhoods, which can be either $\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}$ or $\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_4\}$.

One way to interpret the neighborhoods is to view them as the "labeled examples" of the underlying classes because instances belonging to different neighborhoods are guaranteed to have different class labels, and instances of the same neighborhood must belong to the same class. A key advantage of using the neighborhood concepts is that

by leveraging the knowledge of the neighborhoods, we can acquire a large number of constraints via a small number of queries. In particular, if we can identify the neighborhood of an instance $\mathbf{x}$, we can immediately infer its pairwise relationship with all other points that are currently confirmed to belong to any of the existing neighborhoods. This naturally motivates us to consider an active learning strategy that incrementally expands the neighborhoods by selecting the most informative data point and querying it against the known neighborhoods. We summarize this strategy in Algorithm 1.

Briefly, the algorithms begins by initializing the neighborhoods by selecting a random point to be the initial neighborhood (line 1). In each iteration, given the current set of constraints $\mathcal{C}$, it performs semi-supervised clustering on $\mathcal{D}$ to produce a clustering solution π (line 3). A selection criterion is then applied to select the "most informative" data point $\mathbf{x}^*$ based on the current set of neighborhoods and the clustering solution π (line 4). The selected point $\mathbf{x}^*$ is then queried against each existing neighborhood N_i to identify where $\mathbf{x}^*$ belongs, during which the constraint set $\mathcal{C}$ is updated (lines 5-12). In Line 5, we go through the neighborhoods in decreasing order based on $p(\mathbf{x}^* \in N_i)$, $i \in \{1, \cdots, l\}$, i.e. the probability of $\mathbf{x}^*$ belonging to each neighborhood, which is assumed to be known. This query order will allow us to determine the neighborhood of $\mathbf{x}^*$ with the smallest number of queries. This process is repeated until we reach the maximum number of queries allowed (line 13).

In this work, we consider the semi-supervised clustering algorithm as a black-box and any existing algorithm can be used here. The key question we aim to answer is how to select the "most informative" instance to query against, i.e., the design of the function MostInformative in line 4. In the remaining part of this section, we will focus on this

question and describe our proposed solution.

Algorithm 1 The Neighborhood-based Framework

Input: A set of data points $\mathcal{D}$; the total number of classes c; the maximum number of pairwise queries T.
Output: a clustering of $\mathcal{D}$ into c clusters.

Initializations: $\mathcal{C} = \emptyset$; $N_1 = \{\mathbf{x}\}$, where $\mathbf{x}$ is a random point in $\mathcal{D}$; $\mathcal{N} = N_1$; $l = 1$; $t = 0$;
repeat
  π = Semi-Supervised-Clustering($\mathcal{D}$, $\mathcal{C}$);
  $\mathbf{x}^*$ = MostInformative ($\mathcal{D}$, π, $\mathcal{N}$);
  for each $N_i \in \mathcal{N}$ in decreasing order of $p(\mathbf{x}^* \in N_i)$ **do**
    Query $\mathbf{x}^*$ against any data point $\mathbf{x}_i \in N_i$;
    $t++$;
    Update $\mathcal{C}$ based on returned answer;
    if $(\mathbf{x}^*, \mathbf{x}_i, \mathrm{ML})$ **then** $N_i = N_i \cup \{\mathbf{x}^*\}$; break;
  end for
  if no must-link is achieved
  then $l++$; $N_l = \{\mathbf{x}^*\}$; $\mathcal{N} = \mathcal{N} \bigcup N_l$;
until $t > T$
return Semi-supervised-clustering($\mathcal{D}$, $\mathcal{C}$)

3.3 Selecting the Most Informative Instance

Given a set of existing neighborhoods, we would like to select an instance such that knowing its neighborhood will allow us to gain maximal information about the underlying clustering structure of the data. Our method is based on the following key observation. If we can predict with high certainty to which neighborhood an instance belongs based on our current understanding of the clustering structure, querying about that instance will not lead to any gain of information. Similar observations have been used

to motivate the widely used uncertainty-based sampling principle for active learning of classifiers [21].

To apply uncertainty-based sampling for selecting the most informative instance, we need to address a number of important issues. First, how can we reliably measure the uncertainty of a data point? Second, we can only ask pairwise queries, and it may take multiple queries to resolve the uncertainty about a data point. How can we take this into consideration in our decision. Below we present our approach for dealing with these two issues.

Measuring uncertainty

In uncertainty-based sampling for supervised learning, an active learner queries the instance about which the label uncertainty is maximized. Numerous studies have investigated different approaches for measuring uncertainty given probabilistic predictions of the class labels [21]. In our context, one can take a similar approach and measure the uncertainty of each data instance belonging to different clusters.

For example, one could also take a model-based clustering approach such as Mixture of Gaussians, which will allow us to produce a probabilistic assignment of each instance to different Gaussian clusters and then compute the associated uncertainty in cluster assignment using measures such as entropy. While this may appear to be a natural approach, there are some potential issues. First, this approach can be overly sensitive to the current clustering solution. An ill-formed clustering solution will lead to meaningless models and poor choices of queries. Furthermore, it is also sensitive to the modeling

assumption. If the clusters can not be properly represented using the assumed model, this approach will not provide reliable uncertainty estimation.

To address the first issue, we will not estimate the probability of an instance belonging to each of the learned clusters. Instead, we estimate the probability of it belonging to each of the existing "labeled" neighborhoods. In particular, we will estimate the neighborhood assignment probability of a particular instance by focusing on its relationship with only the labeled instances (those with known neighborhood assignments). All other instances are ignored for this purpose because their cluster assignment may be inaccurate and misleading. As such, we reduce the sensitivity of our method to poor clustering results. Since different neighborhoods contain "labeled" examples of different underlying clusters, this will allow us to more accurately estimate the probability of an instance belonging to the true underlying clusters. Given the neighborhood assignment probability, we then compute the uncertainty of an instance using a measure such as entropy[1].

To address the second issue, i.e., the sensitivity to the probabilistic assumptions, we will avoid making such assumptions at all. Instead, our approach estimates the probability of each instance belonging to each neighborhood using a similarity-based approach where the similarity measure is discriminatively learned under the supervision of the current clustering solution. That is, for instances belonging to different clusters (according to the current solution) their learned similarity will likely to be low and vice

[1]Note that the choice to use entropy here is not critical. Other uncertainty or certainty (to be minimized) measures could potentially be used as well. For example, one could measure the certainty of a point by the maximum probability, or by the difference between the largest and the second largest probabilities.

versa. This learning based approach allows us to transfer the knowledge that we have learned from the constraints to the similarity measures.

Below we explain in detail how we learned the similarities and estimate the probabilities.

We are given a current clustering assignment π, and a set of neighborhoods $\mathcal{N} = \{N_1, ..., N_l\}$. Our goal is to estimate $p(\mathbf{x} \in N_i)$, i.e. for each data instance $\mathbf{x} \in \mathcal{D}$, the probability of it belonging to N_i for $i \in \{1, ..., l\}$.

Supervised learning of similarities. We first learn a similarity measure using a random forest based approach. In particular, we leverage the current clustering assignment π by creating a labeled training set using $\pi(\mathbf{x})$ as the label of $\mathbf{x}$ for all $\mathbf{x} \in \mathcal{D}$. Using this training set, we build a random forest classifier (containing 50 decision trees) that predicts the cluster label $\pi(\mathbf{x})$ from $\mathbf{x}$. Random forest [5] is an ensemble learning algorithm that learns a collection of decision trees. Each decision tree is trained using a randomly bootstrapped sample of the training set and the test for each node of the tree is selected from a random subset of the features. While one could also use other supervised classifiers, we choose random forest because it is not prone to overfitting [6], and as described below it provides a natural definition of similarities (proximities) among instances once a random forest is built.

Given the learned random forest classifier, we compute the similarity between a pair of instances by sending them down the decision trees in the random forest and count the number of times they reach the same leaf, normalized by the total number of trees. This will result in a value between zero and one, with zero for no similarity and one for maximum similarity. Note that random forest has previously been successfully applied

to estimating similarities between unsupervised objects [23]. In that work, a random forest classifier is built to distinguish the observed data from synthetically generated data, whereas our work builds the random forest classifier to distinguish the different clusters. Because the clusters are identified by applying constraint-based clustering to data using the constraint set $\mathcal{C}$, thus the resulting proximities can be also viewed as a supervised similarity measure learned indirectly using the constraint set $\mathcal{C}$.

Estimating neighborhood probability. Given the similarity matrix M generated by previous steps, let $M(\mathbf{x}_i, \mathbf{x}_j)$ denote the similarity between instance $\mathbf{x}_i$ and instance $\mathbf{x}_j$. For any unconstrained data point $\mathbf{x}$, we assume that its probability of belonging to a neighborhood N_i to be proportional to the average [2] similarity between $\mathbf{x}$ and the instances in N_i. More formally, we estimate the probability of an instance $\mathbf{x}$ belonging to neighborhood N_i as:

$$p(\mathbf{x} \in N_i) = \frac{\frac{1}{|N_i|} \sum_{\mathbf{x}_j \in N_i} M(\mathbf{x}, \mathbf{x}_j)}{\sum_{p=1}^{l} \frac{1}{|N_p|} \sum_{\mathbf{x}_j \in N_p} M(\mathbf{x}, \mathbf{x}_j)} \tag{3.1}$$

where $|N_i|$ indicates the number of instances in neighborhood N_i, and l is the total number of existing neighborhoods. Note that in early stages of our algorithm, when all neighborhoods are small, it is possible for an unconstrained data point $\mathbf{x}$ to have zero average similarity with every neighborhood. In such cases, we assign equal probabilities to all neighborhoods for $\mathbf{x}$. This will essentially treat instance $\mathbf{x}$ as highly uncertain, making it a good candidate to be selected by our algorithm. This behavior is reasonable

[2] Note that instead of average, one can also consider minimum or maximum here. We have observed empirically that minimum and maximum tend to be more sensitive to outliers and lead to less robust solutions.

because it will encourage the discovery of more neighborhoods in early stages.

Finally, we measure the uncertainty of an instance by the entropy of its neighborhood membership, which we denote $H(\mathcal{N}|\mathbf{x})$:

$$H(\mathcal{N}|\mathbf{x}) = -\sum_{i=1}^{l} p(\mathbf{x} \in N_i) \log_2 p(\mathbf{x} \in N_i). \tag{3.2}$$

where l is the total number of existing neighborhoods.

Normalizing uncertainty with expected cost

Note that we query a selected instance against the existing neighborhoods to determine to which neighborhood it belongs. Given a selected data instance, it may take multiple pairwise queries to decide its neighborhood. In our selection criterion, we should take this into consideration. In particular, we can consider the number of queries required to reach a must-link as the cost associated with each data instance. To define and quantify this cost more precisely, let's take a closer look at the querying process.

Given a selected instance $\mathbf{x}$, and the probabilities of it belonging to different neighborhoods, which neighborhood should we query against first? Assume the estimated probabilities $p(\mathbf{x} \in N_i)$ is accurate for all $\mathbf{x} \in \mathcal{D}$ and $N_i \in \mathcal{N}$, we should always start by querying $\mathbf{x}$ against the neighborhood that has the highest probability of containing $\mathbf{x}$ to minimize the total number of required queries. If a must-link is returned, we can stop with only one query. Otherwise, one should ask the next query against the neighborhood that has the next highest probability of containing $\mathbf{x}$. This procedure is repeated

until a must-link constraint is returned or we have a cannot-link constraint against all neighborhoods, at which point a new neighborhood will be created using $\mathbf{x}$.

Let $q(\mathbf{x})$ denote the random variable of the total number of queries that we need to determine the neighborhood membership of $\mathbf{x}$. Assuming that the neighborhoods are ranked based on their probability of containing $\mathbf{x}$ in descending order, i.e., $p(\mathbf{x} \in N_1) \geq p(\mathbf{x} \in N_2) \geq \cdots \geq p(\mathbf{x} \in N_l)$, where l is the total number of existing neighborhoods, it is straightforward to show that $p(q(\mathbf{x}) = i) = p(\mathbf{x} \in N_i)$. The expectation $\mathbb{E}[q(\mathbf{x})]$ is thus computed by the following equation:

$$\mathbb{E}[q(\mathbf{x})] = \sum_{i=1}^{l} i * p(\mathbf{x} \in N_i) \tag{3.3}$$

where l is the total number of existing neighborhoods.

Algorithm 2 MostInformative($\mathcal{D}$,π, $\mathcal{N}$)

Input: A set of data instances $\mathcal{D}$; the cluster assignments π; A set of neighborhoods $\mathcal{N} = \bigcup_{i=1}^{l} N_i$;
Output: The most informative data point $\mathbf{x}^*$;

1: Learn a random forest classifier on $\mathcal{D}' = \{\mathbf{x}_i, \pi(\mathbf{x}_i)\}_{i=1}^{n}$, and compute the similarity matrix M;
2: **for** each $\mathbf{x} \in \mathcal{D}$, and $\notin \bigcup_{i=1}^{l} N_i$ **do**
3: **for** $i = 1$ to l **do**
4: Compute $p(\mathbf{x} \in N_i)$ using Eq. 3.1;
5: **end for**
6: Compute $H(\mathcal{N}|\mathbf{x})$ using Eq. 3.2;
7: Compute $\mathbb{E}[q(\mathbf{x})]$ using Eq. 3.3;
8: **end for**
9: **Return**
$\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathcal{U}} \frac{H(\mathcal{N}|\mathbf{x})}{\mathbb{E}[q(\mathbf{x})]}$ where $\mathcal{U} = \mathcal{D} \setminus \bigcup_{i=1}^{l} N_i$

If we consider $H(\mathcal{N}|\mathbf{x})$, the entropy of the neighborhood membership of $\mathbf{x}$ (defined by Equation 3.2), as the amount of information we gain by querying about data instance $\mathbf{x}$, $\mathbb{E}\left[q(\mathbf{x})\right]$ is simply the cost for obtaining this information as measured by the number of queries consumed. Ideally we would like to maximize the gain of information, i.e. $H(\mathcal{N}|\mathbf{x})$, and at the same time minimize the cost, i.e. $\mathbb{E}\left[q(\mathbf{x})\right]$. However, these two objectives are at odds and we trade-off them by selecting the instance that maximizes the ratio between them:

$$\mathbf{x}^* = \underset{\mathbf{x}\in\mathcal{U}}{\operatorname{argmax}} \frac{H(\mathcal{N}|\mathbf{x})}{\mathbb{E}\left[q(\mathbf{x})\right]} \tag{3.4}$$

where $\mathcal{U}$ denotes the set of unconstrained instances (i.e., the set of points that do not belong to any neighborhood). This criterion can be interpreted as selecting the instance that has the highest rate of information per query.

So far we have described our proposed method for selecting the most informative instance to query. We summarize this selection algorithm in Algorithm 2. This completes the description of our overall algorithm which is summarized in Algorithm 1.

3.4 Run Time Analysis

In this section, we analyze the runtime of our proposed algorithm. In particular, we will focus on Algorithm 2 since it is the core part of our active learning algorithm.

In line 1, we build a random forest classifier, whose running time is $O(N_T n \log n)$[3],

[3]Strictly speaking it should be $O(N_T d n \log n)$, where d corresponds to the size of the random feature subset that is considered for selecting each test. Here we drop d because it is generally much smaller than n and can be viewed as a constant factor in this case.

where N_T is the number of decision trees in RF and n is the number of instances in the data [6]. Once the RF classifier is built, constructing a full similarity matrix will take $O(n^2)$. However, we do not need to estimate the full similarity matrix, instead we only need to estimate a subset of the matrix of size $m \times n$, where m is the total number of points in the neighborhoods. As a result, the total runtime of line 1 is $O(N_T n \log n + nm)$.

The for-loop in line 2 is executed at most $O(n)$ times, and the runtime of each execution is $O(m + c)$, where m is the total number of "labeled" instances, i.e., the instances that are assigned to a known neighborhood. We can generally bound both m and c by T, the total number of queries allowed to ask, because it takes at least one query to assign an instance to a neighborhood and T is generally greater than c. Therefore we can bound the total runtime between line 2-8 by $O(nT)$.

Putting it together, the total runtime of Algorithm 2 is $O(N_T n \log n + nT)$. Empirically, with a non-optimized matlab implementation on an Intel 8-Core i7-2600 CPU at 3.40GHz, the average time to select an instance to query for the largest dataset we experimented with (i.e., Digits-389 with 3165 instances) is approximately 0.02 second (using random forest of 50 decision trees). For significantly larger datasets with millions of instances and thousands of features, additional strategies could be applied to scale up our method. For example, the random forest learning step can be easily parallelized to increase the efficiency. Another possibility would be to develop and apply an incremental semi-supervised clustering method that updates the clustering solution incrementally when new constraints are incorporated.

Chapter 4: EXPERIMENTS

In this section, we empirically evaluate the performance of our proposed method in comparison with current state of the art methods. Below we will first explain our experimental setup.

4.1 Experimental Setup

Datasets

In our experiments, we use eight benchmark UCI datasets [10] that have been used in previous studies on constraint-based clustering [2,3,4]. Out datasets include breast [20], pen-based recognition of handwritten digits (3,8,9), ecoli, glass identification, statlog-heart, parkinsons [18], statlog-image segmentation and wine. For the ecoli dataset, we removed the smallest three classes, which only contain 2, 2, and 5 instances respectively. The characteristics of the eight datasets are shown in Table 4.1.

Experimental setting

Our active learning framework assumes the availability of a constraint-based clustering algorithm. For this purpose, we use the well-known MPCKMeans [4] algorithm, as implemented in the WekaUT package [24]. We set the maximum number of iterations

Table 4.1: Characteristics of the Datasets

Datasets	# of Classes	# of Features	# of Examples
Breast	2	9	683
Digits-389	3	16	3165
Ecoli	5	7	327
Glass	6	9	214
Heart	2	13	270
Parkinsons	2	22	195
Segment	7	19	2310
Wine	3	13	178

of MPCKmeans to 200, and used default values for other parameters. Note that the choice of this algorithm is not critical and our method can be used with any constraint-based clustering algorithm.

When evaluating the performance of a particular method on a given dataset $\mathcal{D}$, we apply it to select up to 150 pairwise queries, starting from no constraint at all. The queries are answered based on the ground-truth class label for the dataset. MPCKmeans is then applied to the data with the resulting constraints (and their transitive closures). To account for the randomness in both active learning and MPCKmeans, we repeat this process for 50 independent runs and report the average performance using evaluation criteria described below.

Evaluation criteria

Two evaluation criteria are used in our experiments. First, we use Normalized Mutual Information (NMI) to evaluate the clustering assignments against the ground truth class

labels [17]. NMI considers both the class label and clustering assignment as random variables, and measures the mutual information between the two random variables, and normalizes it to a zero-to-one range. In general, let C be the random variable representing the cluster assignments of instances, and K be the random variable representing the class labels of the instances, the NMI is computed by the following equation:

$$NMI = \frac{2I(C;K)}{H(C) + H(K)}$$

where $I(X;Y) = H(X) - H(X|Y)$ is the mutual information between random variables X and Y. $H(X)$ is the entropy of X, and $H(X|Y)$ is the conditional entropy X given Y.

Second, we consider F-measure as another criterion to evaluate how well we can predict the pairwise relationship between each pair of instances in comparison to the relationship defined by the ground truth class labels [2]. F-measure is defined as the harmonic mean of precision and recall, which are computed by the following equations:

$$\begin{aligned} Precision &= \frac{\#PairsCorrectlyPredictedInSameCluster}{\#TotalPairsPredictedInSameCluster} \\ Recall &= \frac{\#PairsCorrectlyPredictedInSameCluster}{\#TotalPairsActuallyInSameCluster} \\ F-measure &= \frac{2 \times Precision \times Recall}{Precision + Recall} \end{aligned}$$

Baseline methods

To demonstrate the effectiveness of the proposed method, we first compare its performance to a set of competing methods, including a random policy, the Min-Max approach introduced by [19] and a variant of Huang's method [15] to make it applicable to non-document data types. Below we briefly explain these baseline methods.

Random. This policy selects random pairwise queries that are not included in or implied by the current set of constraints $\mathcal{C}$. It is not a neighborhood based approach, and is a commonly used baseline for active learning studies.

Min-Max. As reviewed in Chapter 2, Min-Max is a neighborhood-based approach that works in two phases. The first phase, Explore, builds c disjoint neighborhoods using farthest-first traversal, where c is the total number of clusters. The second phase, Min-Max incrementally expands the neighborhoods by selecting a point to query using a distance-based Min-Max criterion [19].

Huang's method. As noted in Chapter 2, the language-model based method by Huang et al. is only applicable to document clustering because it assumes a specific language model for each cluster. This model is used to estimate the probability of each document belonging to different clusters. In our experiments, to apply the underlying active learning method to general-type data, we replace the language with a discriminative approach for estimating the probabilities. In particular, we train a random forest classifier using the cluster labels as classes. We then estimate for each data point $\mathbf{x}$ its probability of belonging to different clusters using the out-of-bag probabilistic prediction for $\mathbf{x}$. That is, we consider all decision trees in the random forest that were trained

without using the data point $\mathbf{x}$, and use them to estimate the probability of $\mathbf{x}$ belonging to different clusters.

4.2 Experimental Results

This section presents the experiment results, which compare our proposed method to the baseline methods. In the remaining discussion, we will refer to our method as the Normalized Point-based Uncertainty (NPU) method.

Evaluation based on clustering performance

The NMI values of NPU and the baseline methods are shown in Figure 4.1. The x-axis indicates the total number of pairwise queries and the y-axis shows the resulting clustering performance (as measured by NMI) by running MPCKmeans with the constraints returned from the queries (and their transitive closures). As mentioned previously, each curve shows the average performance of a method across 50 independent random runs. The error bar on each data point indicates the confidence interval (t-test at 95% significance level). Note that we use up to 150 queries for all but two datasets, namely Breast and Wine. For these two datasets, NPU converges before using up 150 queries, therefore we show the results up to 100 queries.

From Figure 4.1 we can see that the constraints selected by NPU generally leads to clustering results that are more consistent with the underlying class labels, as can be seen by the dominating curve of NPU compared to other baseline curves. It is inter-

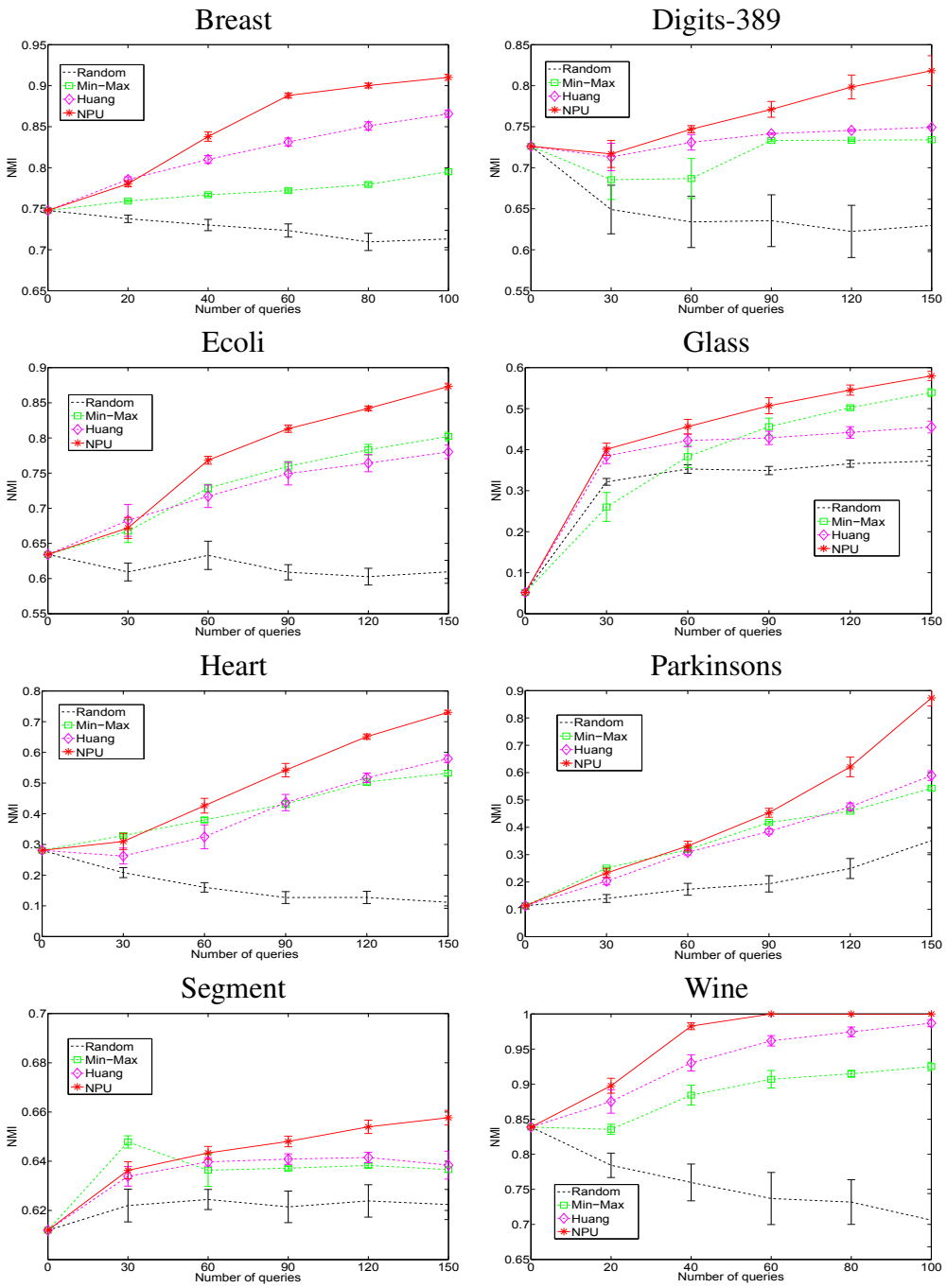


Figure 4.1: The NMI values of different methods on eight datasets as a function of the number of pairwise queries (mean and the confidence interval of t-test at 95% significance level).

esting to note that Random actually degrades the performance in some datasets as we include more constraints, namely the breast, heart and wine datasets. Previous studies on semi-supervised clustering [8,9,11] have reported similar results where randomly selected constraints actually degrades the clustering performance for some datasets. This further demonstrates the importance of selecting the right set of constraints. In comparison, Min-Max and Huang's methods are generally able to improve the performance consistently as we increase the number of queries, but their performance are dominated by NPU in most cases.

We also note that in the early stages, the performance of the three non-random methods are fairly close. As we increase the number of queries, the performance advantage of our method becomes more and more pronounced. This is expected because our method make more explicit usage of the current clustering solution when selecting the queries. As we increase the number of queries, the clustering solution will become better and better, leading to more pronounced performance advantage of our method.

Evaluation based on pairwise relationship

F-measure focuses on how accurately we can predict the pairwise relationship between any pair of instances. In Table 4.2, we shows the F-measure values achieved by different methods with query sizes of 20, 40, 60, 80 and 100. For each query size, we compare different methods against each other using paired *t*-test at 95%-significance level and the best performing method(s) are then highlighted in boldface. Finally Table 4.3 provides a summary of the win/tie/loss counts of the proposed method versus the other methods.

This set of results are very similar to what we observe when evaluating using NMI. When using only 20 queries, the performance of the non-random methods often do not demonstrate statistically significant difference. However, as we increase the number of queries, our method begins to dominate all other methods.

Table 4.2: Comparison on F-measure (mean $\pm$ std). The best performance and its comparable performances based on paired *t*-tests at 95% significance level are highlighted in boldface.

Data	Algorithm	Number of queries				
		20	40	60	80	100
Breast	Random	0.927 ± 0.005	0.924 ± 0.008	0.921 ± 0.010	0.916 ± 0.013	0.918 ± 0.012
	Min-Max	0.934 ± 0.001	0.937 ± 0.002	0.939 ± 0.002	0.941 ± 0.002	0.946 ± 0.002
	Huang	0.941 ± 0.004	0.951 ± 0.005	0.957 ± 0.004	0.963 ± 0.004	0.967 ± 0.004
	NPU	$\mathbf{0.943 \pm 0.003}$	$\mathbf{0.959 \pm 0.005}$	$\mathbf{0.972 \pm 0.003}$	$\mathbf{0.976 \pm 0.003}$	$\mathbf{0.978 \pm 0.003}$
Digits-389	Random	0.762 ± 0.104	0.774 ± 0.100	0.749 ± 0.108	0.752 ± 0.107	0.752 ± 0.107
	Min-Max	$\mathbf{0.805 \pm 0.080}$	0.788 ± 0.093	0.797 ± 0.087	0.842 ± 0.001	0.842 ± 0.002
	Huang	$\mathbf{0.814 \pm 0.072}$	0.826 ± 0.061	0.842 ± 0.034	0.851 ± 0.002	0.853 ± 0.003
	NPU	$\mathbf{0.808 \pm 0.077}$	$\mathbf{0.848 \pm 0.011}$	$\mathbf{0.857 \pm 0.013}$	$\mathbf{0.870 \pm 0.023}$	$\mathbf{0.883 \pm 0.032}$
Ecoli	Random	0.642 ± 0.076	0.628 ± 0.050	0.700 ± 0.092	0.653 ± 0.064	0.659 ± 0.076
	Min-Max	0.648 ± 0.043	0.779 ± 0.060	0.836 ± 0.009	0.851 ± 0.008	0.858 ± 0.010
	Huang	$\mathbf{0.687 \pm 0.058}$	0.762 ± 0.069	0.801 ± 0.047	0.833 ± 0.036	0.829 ± 0.046
	NPU	0.673 ± 0.032	$\mathbf{0.798 \pm 0.048}$	$\mathbf{0.858 \pm 0.007}$	$\mathbf{0.879 \pm 0.008}$	$\mathbf{0.900 \pm 0.007}$
Glass	Random	0.440 ± 0.051	0.403 ± 0.033	0.410 ± 0.037	0.410 ± 0.032	0.413 ± 0.034
	Min-Max	0.432 ± 0.034	0.418 ± 0.067	0.463 ± 0.059	0.484 ± 0.060	0.493 ± 0.040
	Huang	$\mathbf{0.480 \pm 0.039}$	$\mathbf{0.481 \pm 0.042}$	$\mathbf{0.476 \pm 0.043}$	0.474 ± 0.038	0.473 ± 0.039
	NPU	$\mathbf{0.493 \pm 0.036}$	$\mathbf{0.492 \pm 0.045}$	$\mathbf{0.481 \pm 0.056}$	$\mathbf{0.496 \pm 0.056}$	$\mathbf{0.495 \pm 0.043}$
Heart	Random	0.659 ± 0.033	0.636 ± 0.035	0.612 ± 0.036	0.598 ± 0.043	0.587 ± 0.041
	Min-Max	$\mathbf{0.700 \pm 0.012}$	$\mathbf{0.726 \pm 0.013}$	0.743 ± 0.015	0.760 ± 0.017	0.790 ± 0.018
	Huang	0.680 ± 0.042	0.682 ± 0.064	0.709 ± 0.080	0.744 ± 0.076	0.789 ± 0.045
	NPU	0.682 ± 0.046	$\mathbf{0.725 \pm 0.049}$	$\mathbf{0.766 \pm 0.047}$	$\mathbf{0.812 \pm 0.016}$	$\mathbf{0.845 \pm 0.014}$
Parkinsons	Random	$\mathbf{0.594 \pm 0.023}$	0.607 ± 0.023	0.635 ± 0.032	0.657 ± 0.040	0.682 ± 0.059
	Min-Max	0.593 ± 0.005	0.615 ± 0.015	0.666 ± 0.007	0.705 ± 0.010	0.747 ± 0.008
	Huang	0.593 ± 0.015	0.605 ± 0.012	0.652 ± 0.024	0.694 ± 0.023	0.736 ± 0.033
	NPU	$\mathbf{0.597 \pm 0.012}$	$\mathbf{0.637 \pm 0.031}$	$\mathbf{0.695 \pm 0.036}$	$\mathbf{0.759 \pm 0.039}$	$\mathbf{0.814 \pm 0.068}$
Segment	Random	0.546 ± 0.028	0.553 ± 0.030	0.552 ± 0.030	0.548 ± 0.035	0.549 ± 0.036
	Min-Max	$\mathbf{0.571 \pm 0.009}$	$\mathbf{0.582 \pm 0.022}$	0.569 ± 0.022	0.566 ± 0.015	0.569 ± 0.004
	Huang	$\mathbf{0.567 \pm 0.017}$	$\mathbf{0.576 \pm 0.015}$	$\mathbf{0.577 \pm 0.013}$	0.573 ± 0.024	0.575 ± 0.012
	NPU	$\mathbf{0.565 \pm 0.027}$	$\mathbf{0.579 \pm 0.017}$	$\mathbf{0.581 \pm 0.014}$	$\mathbf{0.585 \pm 0.013}$	$\mathbf{0.587 \pm 0.014}$
Wine	Random	0.871 ± 0.044	0.853 ± 0.073	0.836 ± 0.102	0.843 ± 0.082	0.827 ± 0.095
	Min-Max	0.909 ± 0.018	0.935 ± 0.037	0.945 ± 0.035	0.953 ± 0.010	0.959 ± 0.012
	Huang	$\mathbf{0.931 \pm 0.042}$	0.964 ± 0.031	0.982 ± 0.012	0.988 ± 0.011	0.994 ± 0.007
	NPU	$\mathbf{0.945 \pm 0.025}$	$\mathbf{0.992 \pm 0.008}$	$\mathbf{1.000 \pm 0.000}$	$\mathbf{1.000 \pm 0.000}$	$\mathbf{1.000 \pm 0.000}$

Table 4.3: Win/tie/loss counts of NPU versus the other methods with varied numbers of queries based on F-measure.

Algorithms	Number of queries					In All
	20	40	60	80	100	
Random	5/3/0	8/0/0	8/0/0	8/0/0	8/0/0	37/3/0
Min-Max	4/3/1	6/2/0	8/0/0	8/0/0	8/0/0	34/5/1
Huang	2/5/1	6/2/0	6/2/0	8/0/0	8/0/0	30/9/1
In All	11/11/2	20/4/0	22/2/0	24/0/0	24/0/0	101/17/2

Table 4.4: Number of queries to discover all c neighborhoods

Data (# of Classes)	Methods	
	Explore	NPU
Breast (2)	1.42	2.68
Digits-389 (3)	14.22	5.50
Ecoli (5)	76.12	50.34
Glass (6)	98.90	73.94
Heart (2)	2.76	2.08
Parkinsons (2)	1.82	4.22
Segment (7)	102.98	36.92
Wine (3)	9.40	6.14

Further analysis of results

Below we provide some more in-depth analysis of the performance to understand what are the key factors contributing to the performance advantage of our method.

With or without Explore. In the Min-Max method, the first phase is Explore, which uses furthest first traversal to find at least one example from each neighborhood to obtain a good "skeleton" of the clusters. Basu et al. [2] showed that given a set of c disjoint balls (clusters) of uneven sizes, Explore is guaranteed to get at least one example from

each cluster with a small number of queries. Our method does not use a separate Explore stage to deliberately build c neighborhoods. Does this help or hurt our performance?

To answer this question, we consider a two-phase variant of NPU, which performs Explore first (as used by Min-Max), followed by the NPU selection criterion. We examine this method (referred to as E & NPU) and compare it with NPU. The results are shown in Figure 4.2, where each point in the figure represents a comparison between the two methods using NMI on one of the eight datasets, and with one of five different query sizes including 20, 40, 60, 80 and 100. The x-axis shows the performance of E & NPU, and the y-axis shows the performance of NPU. We observe that most points lie above the diagonal line, suggesting that NPU is superior to E & NPU. This indicates that eliminating the Explore stage actually allows more efficient use of the queries. Note that the difference is most pronounced in the areas of low NMI values, indicating they happen in the early stages (small query sizes). This is understandable because the two variants differ only by the initial stages.

Note that NPU can discover c neighborhoods by itself, where c is the number of classes. Could our method be more efficient in discovering all of the neighborhoods than Explore? We record the number of queries used before finding all c neighborhoods for each dataset using Explore and NPU. Table 4.4 shows the average number of queries required by each method to find c neighborhoods for each dataset. The results show that despite the theoretical guarantees of Explore, NPU is empirically more efficient in finding all neighborhoods for multi-class datasets (3 or more classes). This is possibly due to the fact that real datasets may not have ball-shaped clusters, violating the condition that is assumed by Explore for its theoretical guarantees.

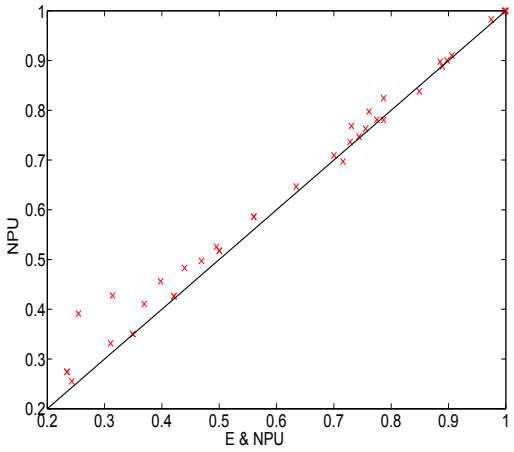


Figure 4.2: Comparing the performance(NMI) of NPU with and without Explore

Can our method still outperform its competitors if we put them on equal footing in terms of the use of Explore? Figures 4.3 and 4.4 represent the comparison between our method and Min-Max and Huang's method when each method is applied with Explore as the common initial stage.

From this comparison we observe that majority of the points lie either on or above the diagonal lines. It is worth noting that many of the points that are on or close to the diagonal line have low NMI values, suggesting that they correspond to comparisons at the early stages of the active learning process. This is precisely what we expect because in this comparison we use the same Explore phase to initialize all three methods, thus they should behave exactly the same for the early stages. For higher performance areas (presumably when using more queries), we observe that more points lie above the diagonal line. This suggests that after eliminating the compounding factor of the Explore phase, our NPU method remains superior to Min-Max and Huang's method.

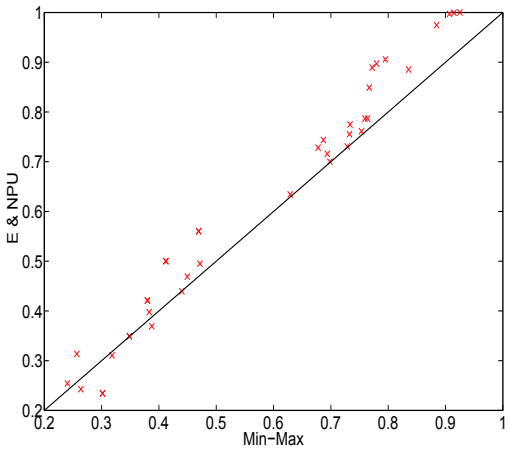


Figure 4.3: Comparing performance(NMI) of Min-Max with E & NPU.

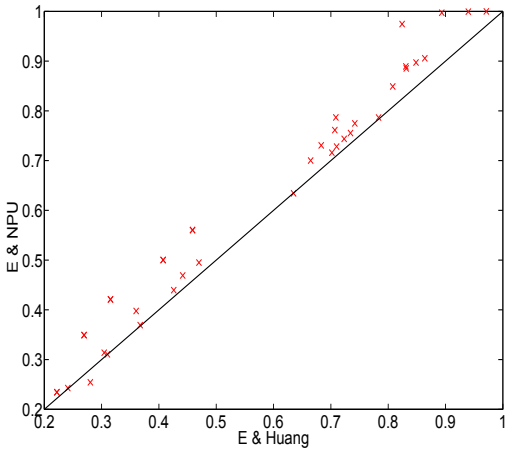


Figure 4.4: Comparing performance(NMI) of E & Huang with E & NPU.

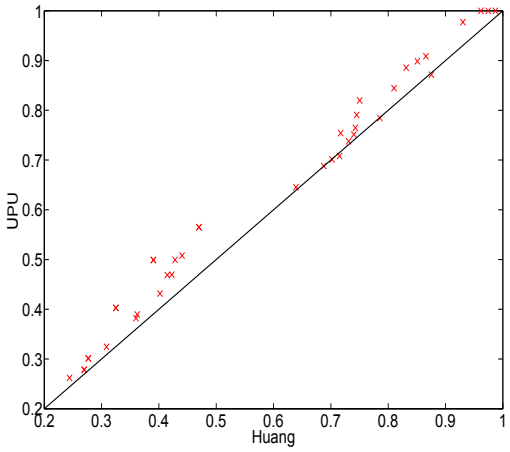


Figure 4.5: Comparing performance(NMI) of Huang with Unnormalized Point-based Uncertainty (UPU).

Point-based v.s. pairwise uncertainty. Huang's method is our closest competitor. A key difference between the approach we propose and Huang's method is that our method considers point-based uncertainty whereas Huang's method is based on pairwise uncertainty. In Chapter 3, we identify a potential issue with Huang's method. That is, it only considers the information content of the first query, even though multiple queries may be needed to identify the neighborhood of a selected instance. Here we would like to make a direct comparison between these two approaches. As such, we consider our method without the normalization step and compare it with Huang's method in Figure 4.5. The x-axis shows the performance of Huang's method, and the y-axis shows the performance of our method without normalization, i.e. directly using Eq. 3.2 as the selection criterion (referred to as Unnormalized Point-based Uncertainty, or UPU for short), both measured in NMI. Each point in the figure corresponds to a particular dataset with a particular query size. As we can see from the figure, UPU generally out-

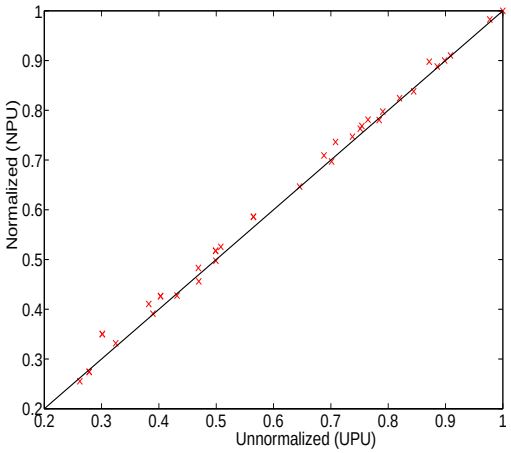


Figure 4.6: Comparing performance(NMI) of the point-based uncertainty method with and without normalization. The y-axis shows the performance of the normalized version (NPU) whereas the x-axis shows the performance of the unnormalized version (UPU).

performs Huang's method, providing strong evidence that point-based uncertainty leads to better and more informative queries.

Effect of normalization. Finally, we would like to examine the effect of normalization. In Figure 4.6, we show the performance comparison between the two variants of our method with or without the normalization step, namely NPU and UPU. The x-axis shows the performance of the unnormalized version (UPU) whereas the y-axis shows the performance of the normalized version (NPU). From the figure we can see that most of the points lie either above or close to the diagonal line, suggesting that the normalization step leads to some mild improvement in performance. To understand the significance of the differences, we performed paired student t-tests at 95% significance level. The results show that for four of the eight datasets (Digits, Ecoli, Parkinsons, and Segment), the normalization step was able to improve the performance in a statistically significant

way. On the other hand, it never hurts the performance significantly. This suggests that it is advisable to include the normalization step since it may provide additional benefit for some datasets and generally does not hurt the performance.

Chapter 5: CONCLUSION

5.1 Conclusion

In this thesis, we study an iterative active learning framework to select pairwise constraints for semi-supervised clustering and propose a novel method for selecting the most informative queries.

Our method takes a neighborhood based approach, and incrementally expands the neighborhoods by posing pairwise queries. We devise an instance-based selection criterion that identifies in each iteration the best instance to include into the existing neighborhoods. The selection criterion trades-off two factors, the information content of the instance, which is measured by the uncertainty about which neighborhood the instance belongs to; and the cost of acquiring this information, which is measured by the expected number of queries required to determine its neighborhood.

We empirically evaluate the proposed method on the eight benchmark datasets against a number of competing methods. The evaluation results indicate that our method achieves consistent and substantial improvements over its competitors.

5.2 Future Work

There are a number of interesting directions to extend our work. The iterative framework requires repeated re-clustering of the data with an incrementally growing constraint set.

This can be computationally demanding for large datasets. To address this problem, it would be interesting to consider an incremental semi-supervised clustering method that updates the existing clustering solution based on the neighborhood assignment for the new point. An alternative way to lower the computational cost is to reduce the number of iterations by applying a batch approach that selects a set of points to query in each iteration. A naive batch active learning approach would be to select the top k points that have the highest normalized uncertainty to query their neighborhoods. However, such a strategy will typically select highly redundant points. Designing a successful batch method requires carefully trading-off the value (normalized uncertainty) of the selected points and the diversity among them — a direction that we plan to pursue for future work.

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