Paper #782:Identifying and Generating Easy Sets of Constraints For Clustering

Ian Davidson * and **S.S. Ravi** †

Abstract

Clustering under constraints is a recent innovation in the artificial intelligence community that has yielded significant practical benefit. However, recent work has shown that for some negative forms of constraints the associated sub-problem of just finding a feasible clustering is **NP**-complete. These *worst case* results for the entire problem class say nothing of where and how prevalent easy problem instances are. In this work, we show that there are large pockets within these problem classes where clustering under constraints is easy and that using easy sets of constraints yields better empirical results. We then illustrate several sufficient conditions from graph theory to identify apriori where these easy problem instances are and present algorithms to create large and easy to satisfy constraint sets.

Introduction and Motivation

Clustering is a ubiquitous unsupervised learning activity used within artificial intelligence for object identification in images, information retrieval and natural language understanding (Wagstaff et al. 2001). A recent innovation has been the introduction of clustering under instance level constraints which effectively provide hints to the composition of a desirable clustering of the instances. The most prevalent form of constraints are must-link (ML) where two instance must be in the same cluster and cannot-link (CL) where they are in different clusters. These two types of constraints offer the ability to incorporate strong background knowledge into the clustering process. For example when clustering automobile GPS trace information to form clusters that are traffic lanes (Wagstaff et al. 2001) the physical distance between lanes (4 meters) can be used to generate cannot-link constraints between instances. However, in practice constraints are typically randomly generated from labeled data. If two randomly chosen instances have the same (different) label a ML (CL) constraint is generated between them.

The main uses of ML and CL constraints have been in the context of three classes of algorithms listed below. a) Algorithms that satisfy every constraint, such as COP-k-means (Wagstaff et al. 2001), b) algorithms that satisfy as many constraints as possible, such as PKM (Bilenko et al. 2004), and c) algorithms that learn a distance function (Xing et al. 2003) so that points which are part of a ML (CL) constraint are close (far) according to the distance function. Some algorithms have multiple objectives, such as MPKM (Bilenko et al. 2004) which attempts both b) and c).

*Department of Computer Science, University at Albany - State University of New York, Albany, NY 12222. Email: davidson@cs.albany.edu.

†Department of Computer Science, University at Albany - State University of New York, Albany, NY 12222. Email: ravi@cs.albany.edu.

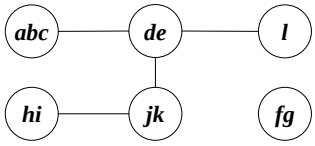
However, when clustering under constraints the feasibility sub-problem arises: Does there exist *any* solution that satisfies all constraints? For example, there is no possible clustering under the constraints $ML(a, b)$, $CL(a, b)$, but even for self-consistent constraints set such as $CL(a, b)$, $CL(b, c)$ and $CL(a, c)$, there is no clustering for $k \leq 2$. Formally:

Definition 1. ***The Feasibility Problem***. *Given a set D of data points, a collection C of ML and CL constraints on some points in D, upper (K_u) and lower bounds (K_l) on the number of clusters, does there exist at least one partition of D into k clusters such that $K_l \leq k \leq K_u$ and all constraints in C are satisfied?*

If this question can be answered efficiently, then one can generate feasible clustering at each iteration of a clustering under constraints algorithm. Previous work (Davidson & Ravi, 2005a) has produced *worst case* results for the feasibility problem for clustering under ML and CL constraints amongst others. The feasibility problem for clustering under ML constraints is in **P** while clustering under CL only and ML and CL is **NP**-complete, as can be shown by a reduction from graph coloring. It is tempting then to abandon the use of CL constraints, however, the transitivity and entailment property of ML and CL constraints respectively (Wagstaff et al. 2001) can result in many entailed CL constraints and hence are quite useful. For example, the constraints $ML(a, b)$, $ML(a, c)$, $ML(d, e)$, $CL(a, e)$ entail the additional constraints $ML(a, c)$, $CL(a, d)$, $CL(b, d)$, $CL(b, e)$, $CL(c, d)$ and $CL(c, e)$.

The worst case complexity results just make a general statement about the feasibility problem, namely that it contains a core of difficult problem instances. Of more practical importance to users and A.I. researchers are more pragmatic questions such as how does one apriori identify an easy problem instance and how does one generate them? How we define an *easy* problem instance is important. An idealized definition would of course be a set of constraints where there is at least one feasible solution. However, since the feasibility problem is **NP**-complete for CL constraints, testing any necessary and sufficient condition to apriori identify feasible constraint sets cannot be carried out efficiently so long as **P** $\neq$ **NP**. Furthermore, knowing that a constraint set has a feasible solution does not make it easy to find the solution. As we shall see later, the ordering of the instances in D plays an important role for most iterative style clustering algorithms such as k-means and EM which assign instances to clusters in a fixed pre-determined order. Therefore, we will adopt the definition that a problem instance is easy for a clustering algorithm if a feasible solution can be found given an *ordering* of the instances in the data set which in turn determine the order of how the instances will be assigned clusters. Formally:

Figure 1: A graphical representation of the feasibility problem for *ML(a,b), ML(a,c), ML(d,e), ML(f,g), ML(h,i), ML(j,k), CL(a,e), CL(i,j), CL(d,k), CL(e,l)*



Definition 2. *A feasibility problem instance is β-**easy** if a feasible solution can be found by an algorithm β given the ordering of instances in the training set which determines the order they will be assigned to clusters.*

It may help the reader to loosely interpret an easy problem as being under-constrained and a hard problem as being over-constrained such that a feasible solution is difficult to find. In this paper we shall focus on using definition 2 with respect to the simplest constrained clustering algorithm, COP-k-means (Wagstaff et al. 2001). As we shall see constraint sets which are easy for COP-k-means are also easy for other algorithms that assign instances to clusters in a fixed order.

This paper attempts to make a contribution to answering the question of what properties identify easy problems apriori and how we can generate them in a manner that is useful for practitioners and algorithm designers. We begin by summarizing the previous worst case results for the feasibility problem (Davidson & Ravi, 2005a). We then empirically investigate properties in the feasibility landscape showing there are large parts which are easy. We also empirically illustrate that using easy sets of constraints affects the performance of a wide variety of algorithms that use constraints. We then discuss two sufficient conditions to identify easy feasibility problems and then develop an algorithm to generate large constraint sets and an ordering of the instances that makes the feasibility problem easy (see definition 2).

A Graph Coloring Interpretation of Clustering Under Constraints and Worst Case Results

Consider the problem of clustering under an expanded version of the set of constraints described earlier: $ML(a,b), ML(a,c), ML(d,e), ML(f,g), ML(h,i),$ $ML(j,k), CL(a,e), CL(i,j), CL(d,k), CL(e,l)$.

Regardless of the number of instances in the data set the feasibility problem is limited to instances $a, b, \ldots, l$. We can represent this problem as a graph by following the construction:

1. Compute the transitive closure of the must-linked constraints, producing connected components $C_1, ..., C_r$.
2. Create one node for each connected component and for each instance that is part of only a CL constraints.
3. Place an edge between those nodes that represent instances that are part of CL constraints.

Figure 1 shows the result for our simple example. Finding a feasible solution to satisfy all of the must-link constraints, simply involves computing the transitive closure in step 1) above and determining if the number of connected components is not too much smaller than k_u. Since the transitive closure computation takes time $O(n + m)$ where n is the number of nodes and m the number of edges, the feasibility problem for ML constraints is in the class **P**. Clustering to satisfy the CL constraints is then a case of assigning each node a value from 1 to k so that no nodes connected by an edge have the same value. This is at least as hard as the graph coloring problem (West, 2001), which is known to be intractable and hence clustering under CL constraints is **NP**-complete. To find a feasible clustering in our example we can assign instances f and g to any cluster so long as they are together. However, care must be taken to assign the instances de so that the assigned value does not clash with the assignments for l and jk and abc. We shall see later on that the node in the graph (namely, de) with the maximum degree (namely, 3) has special significance in determining easy problem instances as does the ordering of how the graph nodes are assigned values. Reference (Davidson & Ravi, 2005a) presents complete complexity proofs.

Investigating the Difficulty Landscape

The previous section's worst case complexity results stated the clustering under CL or ML and CL constraints is, in general, difficult. In this section, we shall empirically explore the difficulty landscape to identify the prevalence of easy problem as per definition 2 using a popular clustering under constraints algorithm, COP-k-Means (Wagstaff et al. 2001). This algorithm is a common method of extending k-Means to ensure that all ML and CL constraints are satisfied at each iteration. It is important to note that the COP-k-Means algorithm is sensitive to the ordering of the points to be clustered; therefore, if it does converge for a set of constraints, then the constraint set can be deemed easy with respect to given the ordering of the points. The COP-k-Means algorithm handles ML constraints by first computing the transitive closure and then replacing all the points in each transitive closure set (connected component) with a single point which is the centroid of all the points in that set, weighted by the size of the connected component. Since k is typically small, infeasibility due to ML constraints does not occur. The algorithm incorporates CL constraints by changing nearest-centroid assignment to *nearest-feasible-centroid* assignment. This is easily programmed by creating for each point a sorted list of centroids (in increasing order of distances) and progressing down the list until a feasible centroid is found to assign the point (Wagstaff et al. 2001) without violating a CL constraint. For any point, if the algorithm reaches the bottom of this list and still cannot find a feasible assignment, the algorithm halts with an indication that it cannot find a feasible solution.

In all our experiments, we use the following common method for generating ML and CL constraints. If the labels of the two points agree, then an ML constraint is generated; otherwise, a CL constraint is generated. We generate a variety of constraint set sizes 500 times and then determine what proportion of them are easy according to the above definition. The instance labels are of course not given to the clustering algorithm and we cluster with k equaling the number

Figure 2: Graph of the proportion of the 500 randomly created constraint sets that are easy (Solid Line) according to Definition 2 and (Crossed Line) our sufficient condition: $k > 1 +$ MaxDegree(CLGraph).

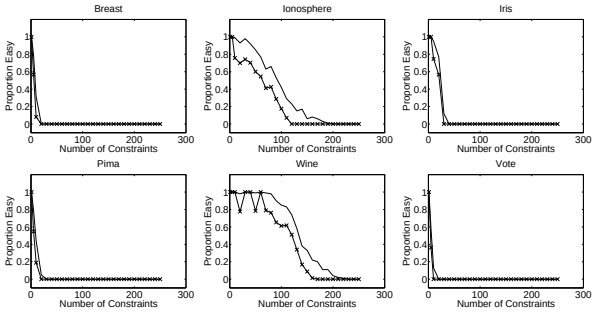
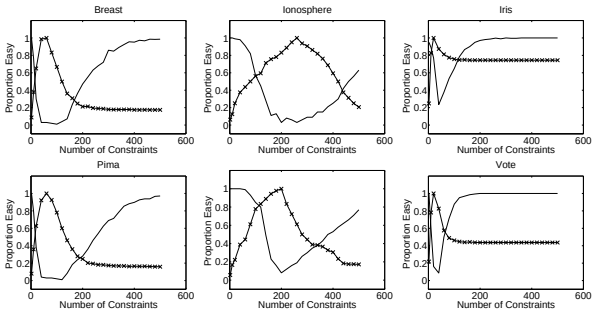


Figure 3: Graph of the proportion of the 500 randomly created constraint sets that are easy (Solid Line) according to the definition 2 and (Crossed Line) the average number of connected components (rescaled to fit on the same axes).



of extrinsic classes in the UCI data sets.

With only CL-constraints (Figure 2) we see that for the solid line as the number of constraints increases the proportion of easy constraint sets decreases and we also note that the transition point from being easy to not-easy is abrupt and is at different position for each data set. The crossed line is the proportion of times our yet to be identified sufficient condition occurs.

With ML and CL constraints, we note a quite unusual phenomenon. Figure 3 (solid line). This result is quite counterintuitive. Initially for a small number of constraints the feasibility problem is easy for the vast majority of the 500 trials. However, the number of easy constraint sets diminishes as the number of constraints increases only to become more prevalent again!

Why Problems are Difficult

It is of course interesting to investigate the question, why some problem instances are easy for COP-k-means and others are difficult. There are two potential reasons. Firstly, the problem may have no feasible solution such as clustering a dataset containing the constraints $CL(a,b), CL(b,c), CL(a,c)$ with $k = 2$. Secondly, the ordering of instances in the training set can make finding the solution difficult. Once again consider Figure 1. The graph is 2 colorable; however, suppose the nodes are considered in the order $\langle abc, hi, de, jk, l, fg \rangle$. The algorithm may assign color 1 to both nodes abc and hi and color 2 to node de. Now, when node jk is considered, it cannot be assigned either color 1 or color 2 without violating a CL constraint. Thus, the algorithm may terminate with an indication that no feasible solution exists. Since all the non-hierarchical clustering algorithms we shall empirically investigate process instances in a fixed ordering, they may not converge or converge to a poor solution depending on the instance ordering.

Effects of Using Easy Sets of Constraints

Our previous sections have defined feasibility and shown that easy sets of constraints occur frequently for some constraint set sizes despite worst case complexity results. But is there any benefit to identifying and using easy sets of constraints? This section attempts to answer this question empirically.

The effect of using an easy set of constraints on algorithms that attempt to satisfy all constraints is clear: they will converge to a feasible solution. However, as mentioned in the introductory section, there are other algorithms that make use of constraints. In this section we shall explore the effect of *Cop-k-means*-easy sets of constraints on a) the PKM (partial constraint satisfaction k-means) algorithm that attempts to satisfy as many constraints as possible (Bilenko et al. 2004), b) the MPKM (metric learning partial constraint satisfaction k-means) algorithm that learns a distance function and attempts to satisfy as many constraints as possible (Bilenko et al. 2004) and c) a simple closest-cluster-join agglomerative hierarchical clustering (CHC) algorithm that attempts to satisfy all constraints and terminates building the dendrogram once it cannot (Davidson & Ravi, 2005b).

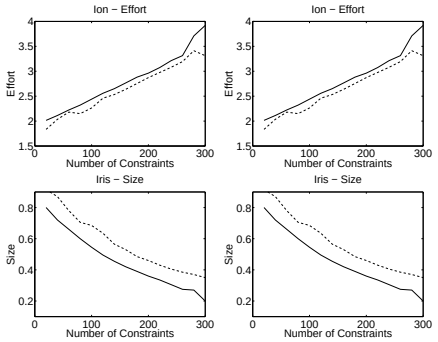
Firstly, we explore algorithms that learn distance functions and perform clustering when constraints can be ignored. We present the results for all six data sets for when the number of constraints sets that are easy or not-easy are approximately the same (i.e. number of constraints in Figure 2 when y-axis equals approximately 0.5). For each data set and non-hierarchical clustering technique we present the number of iterations until convergence and error of the algorithm as measured on the extrinsic class label for *all* of the instances, not just those used to generate constraints. We see (Table 1) that for both algorithms, for easy constraint sets, the reduction in number of iterations and error is significant at the 99% confidence level and in particular, the error rate improvement is practically significant.

Due to space reasons Figure 4 shows the results for the agglomerative hierarchical clustering algorithm CHC for only two of the data sets; similar results hold for the remaining four data sets. The first row of graphs illustrate the effort (join attempts) required to build a dendrogram as a multiple of the number of initial clusters less one. Since at each level of the dendrogram a join must be between two clusters that will not violate any constraint, more potential join calculations are required than for unconstrained dendrogram con-

Dataset	Difficult - Easy Iterations	Difficult - Easy Error
Breast-MPKM	2.21 (0.43)	3.06 (1.77)
Breast-PKM	2.89 (0.78)	4.22 (2.68)
Ion.-MPKM	2.08 (1.33)	1.66 (0.99)
Ion.-PKM	2.31 (1.78)	2.36 (1.43)
Iris-MPKM	0.41 (0.23)	1.21 (0.60)
Iris-PKM	0.12 (0.04)	0.84 (0.57)
Pima-MPKM	0.47 (0.41)	1.96 (1.42)
Pima-PKM	0.47 (0.40)	1.97 (1.56)
Wine-MPKM	3.26 (1.09)	2.01 (1.17)
Wine-PKM	1.87 (1.04)	2.31 (1.69)
Vote-PKM	1.01 (0.86)	1.37 (0.78)
Vote-MPKM	1.22 (1.01)	1.42 (1.11)

Table 1: Mean difference in performance of various techniques on standard UCI data sets for approximately equal number of easy and non-easy sets of CL constraints. Results are averaged over 500 constraint sets. P values are shown in parenthesis at 99% confidence level

Figure 4: Graph of the mean effort for the CHC algorithm to build a dendrogram and its size over 500 randomly generated ML and CL constraint sets. The solid line is for difficult problems, dashed line for easy problems.



struction (just the number of initial clusters less one). We see that on average whenever the constraint set is easy results in less computational effort regardless of the number of constraints. Similarly, the second row of graphs show how large the dendrogram that can be constructed as a fraction of the unconstrained dendrogram height. We see again when the constraint set is **not** easy that the dendrogram prematurely terminates compared to when the constraint set is easy. The notion of premature termination of dendrogram construction is essentially that the constraint set along with the distance measure causes a series of joins that dead-ends at a dendrogram height that is sub-optimal in that another series of joins could have built a taller/fuller dendrogram. The notion of premature termination for hierarchical clustering under constraints is discussed extensively in (Davidson & Ravi, 2005b).

Sufficient Conditions for Easiness

Our previous sections have shown that there are easy constraint sets and that using easy constraint sets leads to better empirical results. In this section we outline two conditions of the properties of the constraint graph (see Figure 1 for an example) that are sufficient (but not necessary) for identifying *Cop-k-means*-easy constraint sets. The first condition is a set theoretic property of the constraints regardless of the data set ordering. The second incorporates the data set ordering. In a later section we illustrate how to use these conditions to generate a set of constraints that are easy to satisfy.

Brooks's Theorem

To explain the phenomenon observed in Figures 2 and 3, we will use Brooks's theorem (West, 2001) and the notion of *entailed constraints*. Brooks's theorem points out that if the maximum node degree of a graph G is Δ and $k \geq \Delta + 1$, then the coloring problem is easy; that is, graph G can always be colored using k colors. Such a coloring can be obtained using *any* linear ordering of the nodes. An example of such an algorithm is to assign to the current node v a color that has not been used for any of the neighbors of v which have already been colored.

The COP-k-means style of greedy clustering under constraints can be viewed as a greedy type of graph coloring to find a feasible solution that also minimizes the algorithm's objective function. The centroids tessellate the instance space into regions and the COP-k-means strategy is to assign each node a color according to this tessellation. Brooks's theorem gives us a sufficient condition to identify when greedy coloring algorithms will always converge and when they won't. In easy instances of the feasibility problem, the value of Δ (the maximum degree of the constraint graph) is less than k, and the coloring algorithm based on Brooks's theorem will *always* succeed. Informally, if the maximum number of CL-constraints involving the same point is at most $k - 1$, then the feasibility problem is easy; otherwise, the feasibility problem will be difficult (i.e., the nearest-feasible-centroid assignment approach will fail in general). As the number of constraints increases, the proportion of easy constraint sets diminishes since the chance of a node being encountered in k or more constraints increases. In figure 2 the crossed-line plots the proportion of times the maximum degree of the graph is less than k. Since Brooks's theorem is a *sufficient* condition for easy problems, the occurrence of the sufficient condition always under-estimates how often the problem is easy in practice.

Explaining the results for both ML and CL constraints requires more effort and the use of the transitivity and entailment properties of ML and CL constraints respectively. When the number of constraints is small, the number of connected components in the graph representing the clustering problem would also be small. So, the chance of any node being part of more than k CL constraints is small. Thus, the problem is easy. Conversely, when the number of constraints is large, the number of connected components will be typically the number of extrinsic labels (due to the transitive

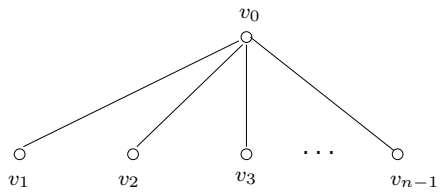


Figure 5: A Star Graph with n nodes.

nature of ML-constraints), and hence the maximum degree of the graph is $k-1$ (i.e., there is a CL-constraint between each pair of connected components). Thus, the maximum node degree Δ and k satisfy the condition $k \geq \Delta + 1$, and again the problem is easy. However, when the number of constraints is not too large, the number of connected components is typically much greater than k. This is because many points with the same extrinsic label have not had the opportunity to combine and form a single connected component. Furthermore, the chance of a CL-constraint between two connected components is large due to the entailed constraint property. Figure 3 (crossed-line) shows the number of connected components (normalized to fit on the same axes) which is maximum when the constraint sets are difficult.

The above discussion points out at least two ways of making the constrained clustering problem easy. Firstly, we can make a point part of only one ML or CL constraint. This, is achieved by sampling the points *without* replacement while generating constraints. Alternatively, we can make k larger than Δ. However, these are less than desirable approaches since they limit how we can use our clustering algorithm and constraints. Instead we may generate constraint sets so that the maximum degree of the constraint graph is less than k. This is achieved by ensuring that each instance is part of $k-1$ or fewer constraints. Note that Brooks's theorem states a $\Delta + 1$ coloring is possible regardless of the order in which nodes are considered. The notion of *inductiveness* of a graph, explored in the next section removes this requirement by providing a particular ordering and hence can significantly reduce the number of colors needed.

Inductiveness of Graphs

When the maximum node degree of a graph is Δ, Brooks's theorem shows how the graph can be colored using at most $\Delta + 1$ colors. However, there may be ways to color the graph using far fewer colors. Consider our simple example in Figure 1 which according to Brooks's theorem is four-colorable but is clearly two-colorable. Here, we examine another graph property which generalizes Brooks's result to give a stronger bound on the number of colors and most importantly can be used to order the instances in the training data set to make the feasibility problem easy. The following definition is from (Irani, 1994).

Definition 3. *Let q be a positive integer. An undirected graph $G(V, E)$ is q-**inductive** if the nodes of G can be assigned distinct integer values in such a way that each node has an edge to at most q nodes with higher assigned values.*

To illustrate this definition, consider the star graph $G(V, E)$ shown in Figure 5. Let us assign the integer 1 to node v_1, 2 to node v_2, ..., $n-1$ to node v_{n-1} and n to node v_0. This creates the following linear ordering of the nodes: $\langle v_1, v_2, \ldots, v_n, v_0 \rangle$. Examining the nodes in this order, it can be seen that each node has an edge to *at most one* node with a higher assigned value (each node v_i, $i \neq 0$, has one edge to v_0). Thus, the star graph is 1-inductive. It is known that all trees are 1-inductive and all planar graphs are 5-inductive (Irani, 1994). The usefulness of q-inductiveness is shown in the following theorem from (Irani, 1994). We have included the proof below since the proof directly leads to an algorithm we shall use.

Theorem 1. *Suppose $G(V, E)$ is q-inductive. G can be colored using at most $q+1$ colors.*

Proof: Let $n = |V|$. Without loss of generality, let $\langle v_1, v_2, \ldots, v_n \rangle$ denote the ordering of the nodes which guarantees the q-inductiveness property. We color the nodes in *reverse* order. To begin with, assign the color 1 to node v_n. To proceed by backward induction, assume that for some $j \geq 2$, nodes v_j through v_n have been colored using at most $q+1$ colors. Now, node v_{j-1} can be colored using one of the colors from the set $\{1, 2, \ldots, q+1\}$ as follows. Since G is q-inductive, node v_{j-1} is adjacent to at most q of the nodes in the set $V_j = \{v_j, \ldots, v_n\}$. Thus, among the $q+1$ colors used for the nodes in V_j, there is at least one color, say α, that has not been used for any neighbor of v_{j-1}. Thus, we can use α as the color for v_{j-1}. Continuing in this fashion, we can obtain a $(q+1)$-coloring of G. ■

The advantage of Theorem 1 over Brooks's theorem is that many graphs which have nodes of high degree, are q-inductive for a small integer q.

We shall use the notion of *q-inductiveness* to present an ordering of the training instances so that satisfying all constraints can be easily obtained by processing the instances in that particular ordering. One approach to obtain such an inductive ordering of the nodes is shown in Figure 6. The idea is to repeatedly choose a node of minimum degree from G, output that node and delete it from the graph. (The degrees of nodes must be updated after each deletion.) Suppose during this iterative process, we keep track of the degrees of the nodes chosen for deletion at each stage, and q denotes the maximum of these degrees. Since the insertion (step b) is at the end of the list this creates an ordering of instances from the largest degree (most constrained) to the smallest degree (least constrained). It is straightforward to verify that the resulting ordering establishes the q-inductiveness of G. As an example, for the graph in Figure 1, the following is a 1-inductive ordering: $\langle fg, abc, l, de, jk, hi \rangle$.

In the worst-case, the algorithm in Figure 6 will output an ordering for which $q = \Delta$, the maximum node degree. However, for special classes of graphs, the algorithm will do much better. For example, it can be seen that for trees, the algorithm will find a 1-inductive ordering, likewise, the algorithm will output a 5-inductive ordering for planar graphs.

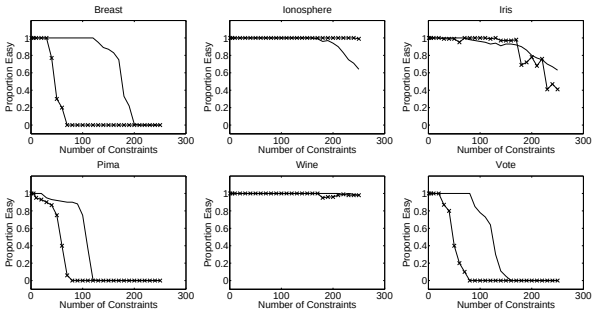
Input: Undirected graph $G(V, E)$.
Output: An ordering $\langle v_{i_1}, v_{i_2}, \ldots, v_{i_n} \rangle$ of the nodes of G such that G is q-inductive for with respect to this ordering.

1. Set list L to empty. (L will give the node ordering.)
2. For each node $v \in V$, find the degree of v in G.
3. **while** $V \neq \emptyset$ **do**
   (a) Find a node $x \in V$ of minimum degree.
   (b) Insert x at the end of list L.
   (c) Delete node x from V and all nodes incident to x from E.
   (d) For each node y which had an edge to x, decrement the degree of y by 1.
4. Output the nodes in the (left to right) order given by L.

Figure 6: An Algorithm for Inductive Ordering of Nodes

Figure 7: For training sets reordered according to the q-inductiveness of the graph (solid line) and constraint sets that attempt to minimize the maximum degree of the constraint graph (crossed line): the proportion of the 500 constraint sets that are easy. Compare with Figure 2

.



Generating Easy Sets of Constraints

One obvious method of using our sufficient conditions is to generate a set of constraints from the labeled data randomly as before and test if they are easy or not. If not, then generating another set of constraints is suggested. In this section we shall explore approaches that use our sufficient conditions to generate large and easy to satisfy sets of constraints.

We begin this section by using the result of Brooks's theorem so as to generate constraint graphs that *attempts* to create no node with a degree greater than $k - 1$. In essence our constraint generation approach tries to distribute the number of CL constraints amongst as many instances as possible so that no node is involved in significantly more CL constraints than any other. We then ran the previous experiments reported in Figure 2 except using our new constraint generation approach. The results for this new experiment are shown in Figure 7 crossed line. Comparing these results to Figure 2 we see that we can generate constraint sets with nearly twice as many constraints before the problem becomes over-constrained. This has significant practical benefit as it has been previously shown that more constraints lead to improved clustering quality (Wagstaff et al. 2001; Bilenko et al. 2004; Davidson & Ravi, 2005a). The results for making use of Brooks's theorem seem almost too good to believe. However, upon careful examination of the labeled data the results hold up to scrutiny. Take the Iris data set which contains 150 instances with 50 each of one of the three extrinsic classes. Clustering with $k = 3$ it is possible purposefully create 75 constraints and create a constraint graph with a degree of at most one and 150 constraints with a maximum degree at most 2. Above 150 constraints the maximum degree of the graph must be three and the problem becomes difficult. Looking at our graph it is around the 150 constraint mark that the problem starts to become difficult.

Next we use the algorithm in Figure 6 to reorder constrained instances so that they form an easy constraint set. Note that this algorithm may create a different instance ordering for each constraint set. We then ran the previous experiments reported in Figure 2 with the *exact same constraint sets* except that the instances were re-ordered. The results for this new experiment but with reordered instances is shown in Figure 7 (solid line). We see that the transition point from when the randomly generated constraint sets become consistently (proportion close to 0) difficult has shifted approximately 100 constraints to the right. This essentially means that this approach of generating easy constraint sets allows us to use nearly ten times as many cannot link constraints before over-constraining the problem.

Conclusion

We have shown that despite worst case results the difficulty landscape for randomly generated sets of constraints contains many easy (under-constrained) problem instances. Furthermore, our empirical results show that for equally size easy and difficult constraint sets, the easy sets produce significantly better performance results. We then presented two sufficient conditions to identify easy constraint sets and approaches to create constraint sets that attempt to satisfy the conditions. Our empirical results indicate that creating constraint sets in this purposeful manner (rather than randomly) can lead to using up to ten times as many constraints before the problems becomes difficult (over-constrained).

References

Bilenko, M., Basu, S., & Mooney, R. J. (2004). Integrating constraints and metric learning in semi-supervised clustering. *Proc. of 21st Intl Conf. on Machine Learning*.

Davidson, I., & Ravi, S. S. (2005a). Clustering with constraints: Feasibility issues and the k-means algorithm. *Proc. of SIAM Intl. Conf. on Data Mining*.

Davidson, I., & Ravi, S. S. (2005b). Hierarchical clustering with constraints: Theory and practice. *ECML/PKDD 2005*.

S. Irani, "Coloring Inductive Graphs Online", *Algorithmica*, Vol. 11, No. 1, Jan. 1994, pp. 53–72.

Wagstaff, K., Cardie, C., Rogers, S., & Schroedl, S. (2001). Constrained k-means clustering with background knowledge. *Proc. of 18th Intl. Conf. on Machine Learning*.

D. B. West, *Introduction to Graph Theory*, Second Edition, Prentice Hall, Inc., Englewood Cliffs, NJ, 2001.

Xing, E. P., Ng, A. Y., Jordan, M. I., & Russell, S. (2003). Distance metric learning, with application to clustering with side-information. *NIPS 15*.