Explainable Clustering via Exemplars: Complexity and Efficient Approximation Algorithms

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Abstract Explainable AI (XAI) is an important developing area but remains relatively understudied for clustering. We propose an explainable-by-design clustering approach that not only finds clusters but also exemplars to explain each cluster. The use of exemplars for understanding is supported by the exemplar-based school of concept definition in psychology. We show that finding a small set of exemplars to explain even a single cluster is computationally intractable; hence, the overall problem is challenging. We develop an approximation algorithm that provides provable performance guarantees with respect to clustering quality as well as the number of exemplars used. This basic algorithm explains all the instances in every cluster whilst another approximation algorithm uses a bounded number of exemplars to allow simpler explanations and provably covers a large fraction of all the instances. Experimental results show that our work is useful in domains involving difficult to understand deep embeddings of images and text.

Keywords: Clustering, Explanation, Exemplars, Algorithms, Complexity

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1 Introduction

The area of explainable AI (XAI) tries to make the complex results of an algorithm interpretable by humans. Most work has focused on supervised learning [14], and in particular, instance-level explanations such as which parts of an image resulted in a certain prediction [24]. Our work differs from most XAI work in several ways. Firstly, we explore unsupervised learning, and in particular, clustering. Secondly, we seek higher level explanations of the entire clustering and not just why an instance was placed in a particular cluster. This is not only an understudied problem, but one where explanation is most needed due to the lack of ground truth annotations (i.e., classes) around which explanations can be built.

Existing work in explainable clustering generate explanations in terms of the underlying features used in the clustering [6, 21, 26]. These methods are not suitable for modern settings that use non-interpretable features such as those produced by auto-encoders, word embeddings (e.g., BERT [8]) or graph embeddings (e.g., [13]). Consider two settings which we use to demonstrate our work: clustering of deep embeddings of sentences and images. In this context, the dimensions of the embedded space are completely meaningless to a human. Even if they are eventually understood, the number of dimensions (often hundreds or more) used by deep embedding poses significant challenges.

Core Idea. We address the need for explanation in complex data by creating an exemplar-based approach to clustering that simultaneously finds clusters of points and exemplars that characterize the clusters. We say that an instance $x$ explains another instance $y$ (or instance $x$ serves as an exemplar for instance $y$) if $y$ falls within $\epsilon$ distance of $x$ (i.e., $y$ is within the ball of radius $\epsilon$ centered at $x$).

Exemplars are a natural mechanism for explanation of concepts [23] by enumerating the different variations of the concept. Consider the situation of explaining a cluster of images of a single person, say former French President, Jacques Chirac (center images in Figure 3). One could describe him as ‘balding’, ‘tall’ and with a ‘cherubic face’. But this requires such information to be available for each and every image; moreover, such a description only fits him when he was the President of France after he turned 60. When he was the Prime Minister of France (during his 40’s) he looked very different. Hence, an alternative explanation of “What does Jacques Chirac look like?” is through exemplars of what he looked like over the years and in different poses. The purpose of this work is to choose such exemplars and discover clusters. Cognitive science literature (e.g., [29]) indicates that exemplars are ideal for explaining complex concepts/clusters. Simply increasing $k$ and using the resultant centroids or finding sub-clusters within clusters [31] does not address this challenge as in many situations there is a natural number of clusters (e.g., Figure 2). Further, the variations of the concept need not find dense sub-clusters as shown in Figure 2.

Contributions. Our contributions are as follows.

1. We formulate the novel explainable clustering via exemplars problem [1] and show that even explaining a single cluster is a computationally intractable problem (Theorem 1).

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1 The differences between our approach and density-based clustering (e.g., DBSCAN [10]) and multi-centroid clustering (e.g., [31]) are covered in the related work section.
2. Our setting is naturally a bi-objective clustering problem with respect to cluster quality and explanation quality but we simplify parameter choice by binding both objectives together with the same parameter $\epsilon$.

3. We propose a polynomial time clustering algorithm (Algorithm 1) that provides provable performance guarantees with respect to both the maximum cluster diameter and the minimum number of exemplars. More precisely, the maximum cluster diameter is $2(D^* + \epsilon)$, where $D^*$ is the optimal diameter whilst using at most $O(N^*\log n)$ exemplars, where $N^*$ is the minimum number of exemplars needed for the dataset of size $n$ (Theorem 2).

4. We also provide a relaxed version of the algorithm (see Algorithm 2) that upper bounds the number of exemplars by relaxing the requirement to explain every instance in the cluster. This algorithm provides the same performance guarantee with respect to maximum diameter as our previous algorithm. The number of instances covered by exemplars is at least $(1 - 1/e)Q^*$ (which is $\approx 0.63 Q^*$), where $e$ is the base of the natural logarithm and $Q^*$ is the maximum number of instances that can be covered, given the bound on the number of exemplars (Theorem 3).

5. The algorithms mentioned in Items 3 and 4 are obtained by combining classic approximation algorithms from the literature which are implemented in a variety of packages and platforms. This allows for ease of implementation and scalability (possibly via parallelism) and in the repository of our work we provide Python implementations using standard packages. A novelty of our contribution is that such a combination provides provable worst-case performance guarantees and also shows very good experimental performance.

6. We experimentally evaluate our methods on several domains involving deep embeddings of images (Faces in the wild), text (a Harry Potter novel) and on MNIST digits. We also begin to explore the novel direction of using exemplars for another ML task, namely transfer learning.

Organization. We begin with an overview of our method and then our problem definitions. This is followed by our complexity result and approximation algorithms. Then, we discuss our experimental results and finally conclude.

2 Overview of Our Approach

The input to our method is a collection of instances that we wish to both cluster and explain. Hence, our method is an example of an explainable-by-design clustering algorithm, unlike our previous work that attempts to find an explanation for a given clustering [7]. Further, unlike prior work on conceptual clustering, we do not use the features used to cluster in developing an explanation; for instance, the work discussed in [6] simultaneously builds a clustering and a decision tree using the same features. Here, we instead find a clustering and a suitable subset of the instances (which we call exemplars) within each cluster to explain it. We say an exemplar explains a set of instances that are within $\epsilon$ distance of it. In practice, exemplars are significantly different from cluster centroids; see Figure 1 for an example.
Trading Off Explanation Complexity Against Clustering Quality. We design clustering algorithms that ensure that the maximum diameter of the clustering found is within a small constant factor of the optimal diameter and $\epsilon$ (the radius of an exemplar’s coverage). Hence, the parameter $\epsilon$ provides a natural way to trade off explanation complexity against cluster compactness. If we make $\epsilon$ small, we naturally will require more exemplars but will find more compact clusters. Conversely, if we make $\epsilon$ large, we will create simpler explanations but at the cost of a larger cluster diameter. We present efficient approximation algorithms that provide provable performance guarantees with respect to both the maximum diameter and the number of exemplars used.

Exemplars for Explanation and Their Benefits. Our work can be considered as a quantification of the exemplar-based school of concepts [23] as we are discovering concepts (the clusters) and the exemplars that typify/explain them. This contrasts with a feature based explanation (e.g., using the attributes/properties of the face) as described above. In this paper, we argue that using exemplars has pragmatic and pedagogical benefits. As ML/DM progresses to more complex representations of complex objects, using features as the basis for explanation is no longer always valid, even though there is excellent work in this area [6]. In settings where features are not interpretable (e.g., deep embeddings of image data), one pragmatic explanation mechanism is exemplars. The pedagogical benefit stems from cognitive psychology’s experimentally-verified rich literature on how humans understand and comprehend the world; this literature comes under a topic known as Concept Theory [23,2]. In particular, exemplars are a natural explanation vehicle as they leverage the existing knowledge of humans to make internalizing the explanation easier. For example, the exemplars of Jacques Chirac will be internalized differently by say a French citizen (e.g., “he looks like a taller version of former French President François Mitterrand”) versus an American citizen (e.g., “he is as tall as and looks like the former US President Ronald Reagan”). This direction also presents the opportunity to exploit the literature on how humans organize exemplars into ontologies or hierarchies for more complex explanations [29].

Difficulty of the Problem. Our computational problem inherently has two intertwined tasks: (i) finding compact clusters and (ii) finding a minimal set of exemplars to represent each cluster. This is a challenging problem as the first problem is known to be NP-hard [12] and additionally we show that even for a single cluster, finding a minimal set of exemplars to represent the cluster is NP-hard (Theorem 1). Solving these tasks separately could yield sub-optimal results; instead, we bind them together using a single parameter $\epsilon$ (the exemplar coverage distance) to simultaneously perform clustering and exemplar selection. Our algorithms provide provable performance guarantees.

3 Definitions

3.1 Basic Definitions

Let $X = \{x_1, x_2, \ldots, x_n\}$ be a set of $n$ instances. We assume that for each pair of instances $x_i$ and $x_j$, we have a (symmetric) distance $d(x_i, x_j)$. The distance function $d$ is assumed to be a metric; it may be the distance in some embedding
Explainable Clustering via Exemplars

Fig. 1 An illustrative example of generating clusters (color) and selecting exemplars (stars). The exemplars form a prototypical explanation of a cluster in that they cover all instances in the cluster. Note the exemplars need not be (and rarely) are close to the centroids.

space. We are also given a value $\epsilon > 0$ which is set by a domain expert and naturally trades off explanation complexity against cluster compactness.

**Notion of Explanation.** Given two instances $x_i$ and $x_j$, where $d(x_i, x_j) \leq \epsilon$, we say that $x_i$ covers $x_j$ and that $x_i$ is an exemplar for $x_j$. Since the distance function $d$ is symmetric, it is also true in this case that $x_j$ covers $x_i$ and $x_j$ is an exemplar for $x_i$. For convenience, we will also say that $x_i$ is an $\epsilon$-neighbor of $x_j$ (and vice versa). We now generalize this definition to clusters. Given a subset $Y \subseteq X$ of instances and another subset $E \subseteq X$ of exemplars, we say that $E$ covers $Y$ if for every instance $x_i \in Y$, there is an instance $x_j \in E$ such that $x_j$ covers $x_i$ (i.e., $x_j$ is an exemplar for $x_i$). When a subset $E \subseteq X$ of exemplars covers a set $Y \subseteq X$, we say that $E$ is an exemplar set for $Y$ and that $Y \cup E$ forms a cluster and its explanation.

For any instance $x_i$, let $S_i \subseteq X$ consist of all the instances that are $\epsilon$ neighbors of $x_i$; that is, $d(x_i, x_j) \leq \epsilon$ for each $x_j \in S_i$. We refer to $S_i$ as the $\epsilon$-neighborhood of $x_i$. Note that each subset $S_i$ is nonempty since it includes $x_i$ itself. Further, $x_i$ is an exemplar for all the instances in $S_i$.

**Clustering to Minimize the Maximum Diameter.** For clustering a set $X$ of instances, a common objective is to minimize the maximum diameter [12]. For the reader’s convenience, we provide the associated definitions. The diameter of any cluster is the maximum distance between any pair of instances in that cluster. The diameter of a clustering is the largest cluster diameter. It is known that finding a clustering with $k \geq 3$ clusters that minimizes the maximum diameter is NP-hard [11]. When the distance function is a metric, a well known approximation algorithm due to Gonzalez [12] provides a clustering whose maximum diameter is at most twice the optimal diameter.
3.2 Additional Definitions

**Graph Theoretic Definitions:** We use some graph theoretic concepts and a special class of graphs in proving our results. Given an undirected graph $G(V,E)$, a subset $V'$ of nodes forms a **dominating set** for $G$ if for every node $w \in V - V'$, there is a node $v \in V'$ such that the edge $\{v, w\}$ is in $E$. Given a graph $G(V,E)$, the goal of the **minimum dominating set** (MDS) problem is to find a dominating set of minimum cardinality for $G$.

Given a set of disks (i.e., circles in two-dimensional space) each with the same radius $r$, one can define an associated undirected graph as follows: there is one node for each disk; there is an edge between two nodes if the corresponding disks touch or intersect (i.e., the distance between the centers of the disks is at most $2r$). Such a graph is called a **unit disk graph** [4]. Many optimization problems, including the MDS problem, are known to be **NP-hard** even for unit disk graphs [4,16]. We rely on the NP-hardness of the MDS problem for unit disk graphs in proving Theorem 1.

Unit disk graphs can be defined in three or more dimensions where each object is a ball of unit radius in an appropriate dimension. Each node of the corresponding graph represents a ball with an edge between two nodes if their corresponding balls touch/intersect.

**Minimum Set Cover (MSC) Problem:** In this problem [11], the input consists of a base set $U = \{u_1, u_2, \ldots, u_n\}$, a collection $Y = \{Y_1, Y_2, \ldots, Y_m\}$, where each $Y_j$ is a subset of $U$ ($1 \leq j \leq m$) and an integer bound $\beta \leq m$. The goal is to choose a subcollection $Y'$ of $Y$ with $|Y'| \leq \beta$ such that the union of the sets in $Y'$ is equal to $U$ (i.e., the union covers all the elements in $U$). This problem is **NP-complete** and a natural greedy approximation algorithm (which picks a new set in each iteration such that the set covers as many new elements as possible) is known to give a performance guarantee of $O(\log n)$ for the problem [28]. One of our results (Section 4.3) uses this approximation algorithm.

**Budgeted Maximum Coverage Problem:** We also use a known approximation algorithm for the Budgeted Maximum Coverage (BMC) problem, which is closely related to the Minimum Set Cover (MSC) problem [11]. The input to the BMC problem is a base set $U = \{u_1, u_2, \ldots, u_n\}$, a collection $Y = \{Y_1, Y_2, \ldots, Y_m\}$, where each $Y_j$ is a subset of $U$ ($1 \leq j \leq m$) and a budget $\beta \leq m$. The goal is to choose a subcollection $Y'$ of $Y$ with $|Y'| = \beta$ such that the union of the sets in $Y'$ covers the maximum number of elements of $U$. This problem is also **NP-hard** and a natural greedy approximation algorithm (which picks a new set in each iteration such that the set covers as many new elements as possible) has been shown to give a performance guarantee of $(1 - 1/e)$ for the problem [18], with $e$ being the base of the natural logarithm. One of our results (Section 4.3) uses this result.

3.3 Main Problem Formulations

We now provide rigorous formulations of the problems considered in this paper. We begin with the problem of finding a small set of exemplars for a given set of instances.

(a) **Minimum Set of Exemplars for a Cluster** (MSEC)
Given: A cluster $X = \{x_1, x_2, \ldots, x_n\}$ of $n$ instances, a value $\epsilon > 0$, an integer $\beta \leq |X|$.

Question: Is there a subset $E \subseteq X$, with $|E| \leq \beta$, such that $E$ is an exemplar set for $X$?

We note that the MSEC problem requires an exemplar set for all the instances in the set $X$. We now develop formulations where the set $X$ must be partitioned into clusters and exemplar sets must be found for each cluster. We first provide a formulation where each instance must have an exemplar.

(b) **Simultaneous Construction of Clusters and Exemplars (SCCE)**

Given: A set $X = \{x_1, x_2, \ldots, x_n\}$ of $n$ instances to be clustered, integer $k$, where $2 \leq k \leq n$ (the number of clusters), and a value $\epsilon > 0$.

Requirement: Find a partition of $X$ into $k$ clusters $C_1, C_2, \ldots, C_k$ and an exemplar set $E_j$ for each cluster $C_j$, $1 \leq j \leq k$, such that all the following conditions hold:

- Compactness of Clustering and Explanation: (i) the maximum diameter of the clusters is as small as possible, (ii) $\sum_{j=1}^k |E_j|$ (i.e., the total number of exemplars used) is as small as possible.
- Distinctness of Explanations: (iii) $E_a \cap E_b = \emptyset$ for all $1 \leq a, b \leq k$ and $a \neq b$ (i.e., the exemplar sets are pairwise disjoint), and
- Completeness of Explanations: (iv) for each instance $x \in X$, there is an exemplar $y$ such that $x$ and $y$ are in the same cluster.

We will present an approximation algorithm for SCCE in Section 4. However, this solution may use a large number of exemplars due to the completeness requirement. This can make it difficult for a user to interpret the explanation. To address this, we next explore a relaxed version of the problem where not all instances are explained. (Our approximation algorithm for this problem allows us to analytically bound the number of instances that are not explained.)

(c) **Simultaneous Construction of Clusters and $\beta$-Bounded Exemplars (SCCRB)**

Given: A set $X = \{x_1, x_2, \ldots, x_n\}$ of $n$ instances to be clustered, integer $k$, where $2 \leq k \leq n$ (the number of clusters), a value $\epsilon > 0$ and integer $\beta$ (upper bound the total number of exemplars for all clusters).

Requirement: Find a partition $X$ into at most $k$ clusters $C_1, C_2, \ldots, C_k$ and the corresponding exemplar sets $E_1, E_2, \ldots, E_k$ as in the SCCE problem above with the requirements for compactness of clusters (Condition (i)), distinctness of explanation (Condition (iii)) but now:

- Upper Bound on the Number of Exemplars: (ii) $\sum_{j=1}^k |E_j| \leq \beta$, and
- Relaxing the Condition that Every Instance be Explained: (v) The number of instances which have an exemplar in the same cluster is as large as possible.

We will discuss an approximation algorithm for SCCR in Section 4. Note that compared to SCCE, not every instance will be explained (i.e., covered by an exemplar). Instances which are not explained can be identified; this could be useful in that such instances may represent anomalies.
4 Algorithmic Results

4.1 Finding a Minimum Set of Exemplars For A Single Cluster

We begin with a complexity result for the Minimum Set of Exemplars (MSEC) problem for a single cluster. As can be seen from its proof, this complexity result holds even when the given set of instances \( X \) consists of points in 2D-Euclidean space.

**Theorem 1** The MSE problem is \( \text{NP} \)-hard even when the set of instances \( X \) consists of points in 2D-Euclidean space and the distance between any two points is their Euclidean distance.

**Proof:** The proof is by a reduction from the minimum dominating set (MDS) problem for unit disk graphs discussed in Section 3.2. Let the MDS problem be specified by a unit disk graph \( G(V,E) \), where the radius of each disk is \( r \), and let \( \beta \leq |V| \) be the given upper bound on the size of a dominating set. We construct a set of instances \( X \) for the MSE problem as follows. For the disk corresponding to each vertex \( v_i \), we create an instance \( x_i \in X \), where the coordinates of \( x_i \) are those of the center of the disk corresponding to \( v_i \). The exemplar distance \( \epsilon \) is set to \( 2r \) and the bound on the number of exemplars is set to \( \beta \). Clearly, this construction can be done in polynomial time.

Suppose \( V' \) is a dominating set for \( G \) with at most \( \beta \) nodes. We can show that the instances corresponding to the nodes in \( V' \) form the exemplar set \( E \) for \( X \) as follows. Consider any instance \( x_j \) in \( X \) which is not an exemplar. Since \( V' \) is a dominating set and the node \( v_j \) corresponding to \( x_j \) is not in \( V' \), there is a node \( v_i \in V' \) such that the edge \( \{v_i, v_j\} \) is in \( E \). Since \( G \) is a unit disk graph, the distance between the centers of the disks corresponding to \( v_i \) and \( v_j \) is at most \( 2r \) which is equal to \( \epsilon \) by our construction; that is, the distance between \( x_j \) and the exemplar \( x_i \) is at most \( \epsilon \). Therefore, \( E \) is a set of exemplars of size at most \( \beta \) for \( X \).

Now, suppose \( E \) is a set of exemplars of size at most \( \beta \) for \( X \). Let \( V' \) be the set of nodes of \( G \) corresponding to the instances in \( E \). We claim that \( V' \) is a dominating set for \( G \). To see this, consider any node \( v_j \) which is not in \( V' \). The instance \( x_j \) corresponding to \( v_j \) has an exemplar \( x_i \in E \) and the distance between \( x_i \) and \( x_j \) is at most \( 2r \). Since \( G \) is a unit disk graph, the edge \( \{v_i, v_j\} \) is in \( E \). In other words, \( V' \) is a dominating set for \( G \), and this completes the proof.

4.2 An Approximation Algorithm for SCCE

The SCCE problem requires us to find a clustering where the diameter of each cluster and the number of exemplars are as small as possible. Since each of these problems is computationally intractable, we present an algorithm that provides a provable performance guarantee for each of these measures.

**Overview of the algorithm.** First, the algorithm takes the set \( X \) and produces pairwise disjoint blocks \( B_1, B_2, \ldots, B_k \) to minimize the maximum diameter [12]. It then uses a greedy approximation algorithm for the Minimum Set Cover (MSC) problem [28] to find a near-minimal set of exemplars \( A \) for the set \( X \). For each cluster \( C_j \), the exemplar set \( E_j \) is given by \( E_j = B_j \cap A \), \( 1 \leq j \leq k \). Finally, each
Algorithm 1: Approximation Algorithm for SCCE

Input: A set of instances $X$, the number of clusters $k$ and the exemplar distance bound $\epsilon$.

Output: A clustering of $X$ into $k$ clusters and a set of exemplars for each cluster to satisfy the requirements of the SCCE problem.

1 Block Creation. Use Gonzalez’s approximation algorithm \cite{Gonzalez1969} to obtain $k$ (disjoint) blocks $B_1, B_2, \ldots, B_k$ of $X$.

2 Exemplar Neighborhood Set Construction. For each $x_i \in X$, find $S_i$, the set of all instances $x_j \in X$ such that $d(x_i, x_j) \leq \epsilon$. (Thus, $x_i$ can serve as the exemplar for each instance in $S_i$.)

3 Exemplar Selection. Construct the Minimum Set Cover (MSC) problem consisting of the base set $X$ and the set collection $S = \{S_1, S_2, \ldots, S_n\}$. Use a greedy approximation algorithm for MSC \cite{GareyJohnson1979} to construct a near-optimal set cover given by the subcollection $S_1 \subseteq S$. Obtain the exemplar set $A$ as follows: for each $S_i \in S_1$, add $x_i$ to $A$.

4 Cluster Creation. Create $k$ empty clusters $C_1, C_2, \ldots, C_k$.

5 Exemplar Assignment. For each cluster $C_j$, the set $E_j$ of exemplars is given by $E_j = B_j \cap A$. Add $E_j$ to $C_j$.

6 Non-Exemplar Assignment. Consider each cluster $C_j$. For each exemplar $x_i \in C_j$, add each instance in $S_i - A$ (i.e., each non-exemplar in $S_i$) to $C_j$.

7 Output the set of clusters $C_1, C_2, \ldots, C_k$ and the corresponding exemplars $E_1, E_2, \ldots, E_k$.

This ensures that the exemplars are pairwise disjoint and that each non-exemplar is covered by an exemplar in the same cluster. Note that we only move non-exemplars from their original blocks (i.e., $B_1, B_2, \ldots, B_k$) to new clusters (i.e., $C_1, C_2, \ldots, C_k$). This is crucial to ensure the performance guarantee on the maximum diameter. An outline of our approximation procedure is shown as Algorithm 1. Note that if an instance $x$ is covered by multiple exemplars, it can be assigned to any cluster that has an exemplar for $x$. The following theorem shows the performance guarantee provided by Algorithm 1.

Theorem 2 The solution produced by Algorithm 1 satisfies the following properties:

(i) The diameter of each cluster is at most $2(D^* + \epsilon)$, where $D^*$ is the optimal diameter for a $k$-clustering of $X$ and $\epsilon$ is the exemplar distance. (ii) Every instance in $X$ has an exemplar within the same cluster. (iii) The sets of exemplars for the $k$ clusters are pairwise disjoint. (iv) The total number of exemplars generated by the algorithm is at most $O(N^* \log n)$, where $N^*$ is the minimum number of exemplars needed to cover all the instances in $X$.

Proof: To prove Part (i), we first note that the approximation algorithm used in Step 1 guarantees that the maximum diameter of the clusters produced in that step is at most $2D^*$, where $D^*$ is the optimal solution value for $X$. Step 6 of the algorithm moves only non-exemplars between clusters. We need to show that after these moves, the maximum diameter is at most $2(D^* + \epsilon)$. To see this, consider any cluster $C_i$ and any pair of instances $x_a$ and $x_b$ in $C_i$. There are three cases to consider.

Case 1: Both $x_a$ and $x_b$ are exemplars. In this case, both $x_a$ and $x_b$ must be in $B_i$ since we chose $E_i = B_i \cap A$. Thus, at the end of Step 1, $d(x_a, x_b) \leq 2D^*$. 


Case 2: One of them, say \( x_a \), is an exemplar and the other (i.e., \( x_b \)) is a non-exemplar that got moved into \( C_i \). In this case, \( C_i \) contains an exemplar \( x_q \) at a distance of at most \( \epsilon \) from \( x_b \). Since \( d(x_a, x_q) \leq 2D^* \) and \( d(x_q, x_b) \leq \epsilon \), it follows from triangle inequality that \( d(x_a, x_b) \leq 2D^* + \epsilon \).

Case 3: Both \( x_a \) and \( x_b \) are non-exemplars which were moved into \( C_i \). In this case, \( C_i \) contains exemplars \( x_p \) and \( x_q \) such that \( d(x_a, x_p) \leq \epsilon \) and \( d(x_b, x_q) \leq \epsilon \). Further, \( d(x_p, x_q) \leq 2D^* \). Now, using triangle inequality, it follows that \( d(x_a, x_b) \leq 2(D^* + \epsilon) \), and this completes our proof of Part (i).

The result in Part (ii) follows since the set \( A \) constructed in Step 3 is an exemplar set for \( X \) and each non-exemplar instance \( x_j \) gets moved (in Step 6) to a cluster containing an exemplar for \( x_j \). Since the blocks constructed in Step 1 are pairwise disjoint, so are the exemplar sets constructed in Step 5; this proves Part (iii). Since Step 3 uses the greedy approximation algorithm for MSC and this algorithm provides a performance guarantee of \( O(\log n) \) [25], the total number of exemplars produced in Step 3 is at most \( O(N^* \log n) \), where \( N^* \) is the minimum number of exemplars needed to cover all instances in \( X \). This establishes Part (iv) and the theorem follows.

Remark: Since Step 3 in Algorithm [1] uses an approximation algorithm for MSC, the performance guarantee with respect to the number of exemplars is \( O(\log n) \), where \( n = |X| \). Theoretically, one can get a better approximation by transforming the Exemplar Selection steps (i.e., Steps 2 and 3 of the algorithm) into that of finding a near-optimal dominating set for unit disk graphs in an Euclidean space whose dimension \( \ell \) is the same as that of the points in \( X \). This is done by placing an \( \ell \)-dimensional ball of radius \( \epsilon/2 \) at each instance in \( X \). The corresponding unit disk graph has a node for each instance in \( X \) and there is an edge between two nodes if the corresponding balls intersect or touch. It can be verified that any dominating set for this graph provides the necessary set of exemplars. An approximation scheme which provides a performance guarantee of \( (1 + \delta) \) for any fixed \( \delta > 0 \) is known for the minimum dominating set problem for such graphs [16]. Thus, one can obtain a performance guarantee of \( (1 + \delta) \) for any fixed \( \delta > 0 \) with respect to the number of exemplars. However, this approximation scheme is impractical even for data sets of moderate size since its running time has the factor \( O(n^{(1/\delta)^2}) \). (Thus, even when \( \delta = 0.5 \), the running time has the factor \( O(n^4) \).) For this reason, we decided to use the MSC-based approximation algorithm in our experiments.

Running time of Algorithm [1] We can estimate the asymptotic running time this approximation algorithm as follows. Step 1 uses Gonzalez’s algorithm which has a running time of \( O(nk) \), where \( n \) is the number of instances and \( k \) is the number of clusters [12]. Step 2 constructs the neighborhood set for each instance and can be done in time \( O(n^2) \). Step 3 runs the greedy set cover heuristic for which the running time is \( O(W) \), where \( W \) is the sum of the sizes of all the sets [3]. In our case, since there are \( n \) sets and each set is of size at most \( n \), \( W \leq n^2 \); that is, Step 3 runs in time \( O(n^2) \). Step 4 runs in \( O(k) \) time. Using a bit vector representation for each set, Steps 5 and 6 can be implemented to run in time \( O(nk) \). Since \( k \leq n \), the overall running time of Algorithm [1] is \( O(n^2) \).
Algorithm 2: Approximation Algorithm for SCCRB

**Input:** A set of instances $X$, the number of clusters $k$, the exemplar distance bound $\epsilon$ and an upper bound $\beta$ on the total number of exemplars for all clusters.

**Output:** A clustering of $X$ into $k$ clusters and a set of exemplars for each cluster to satisfy the requirements of the SCCRB problem.

1. **Block Creation.** Use Gonzalez’s approximation algorithm \cite{12} to obtain $k$ (pairwise disjoint) blocks $B_1, B_2, \ldots, B_k$ of $X$.

2. **Exemplar Neighborhood Set Construction.** For each $x_i \in X$, find $S_i$, the set of all instances $x_j \in X$ such that $d(x_i, x_j) \leq \epsilon$. (Thus, $x_i$ can serve as the exemplar for each instance in $S_i$.)

3. **Exemplar Selection.** Construct the Budgeted Maximum Coverage (BMC) problem consisting of the base set $X$, the set collection $S = \{S_1, S_2, \ldots, S_n\}$ and the budget $\beta$. Use the greedy approximation algorithm for BMC \cite{18} to construct a subcollection $S_1 \subseteq S$. Obtain the exemplar set $A$ as follows: for each $S_i \in S_1$, add $x_i$ to $A$.

4. **Cluster Creation.** Create $k$ empty clusters $C_1, C_2, \ldots, C_k$.

5. **Exemplar Assignment.** For each cluster $C_j$, the set $E_j$ of exemplars is given by $E_j = B_j \cap A$. Add $E_j$ to $C_j$.

6. **Non-Exemplar Assignment.** Consider each cluster $C_j$. For each exemplar $x_i \in C_j$, add each instance in $S_i - A$ (i.e., each non-exemplar in $S_i$) to $C_j$. The set of instances $X'$ which don’t have exemplars is given by $X' = X - \bigcup_{S_i \in S_1} S_i$.

7. Output the set of clusters $C_1, C_2, \ldots, C_k$ and the corresponding exemplars $E_1, E_2, \ldots, E_k$.

4.3 An Approximation Algorithm for SCCRB

When $\epsilon$ is small, our approximation algorithm for SCCE generates a solution with a small cluster diameter; however, it may yield a large number of exemplars leading to an overly complicated explanation. The goal of SCCRB is also to find a clustering with a small maximum diameter but we relax the requirement to have exemplars for all the instances. Instead, we are given an upper bound on the total number of exemplars for all clusters, and we want to maximize the number of instances with exemplars subject to the bound on the number of exemplars.

We now present an approximation algorithm that provides a provable performance guarantee for the diameter as well as the number of instances covered by exemplars in each cluster. This algorithm is similar to the one for the SCCE problem (Algorithm 1) except that it uses a known approximation algorithm for the Budgeted Maximum Coverage (BMC) problem \cite{18} in Step 3 instead of the approximation algorithm for the MSC problem. The steps of this approximation algorithm are shown as Algorithm 2. The following theorem establishes the performance guarantee provided by the Algorithm 2.

**Theorem 3** The solution produced by Algorithm 2 satisfies the following properties: (i) The diameter of each cluster is at most $2(D^* + \epsilon)$, where $D^*$ is the optimal diameter for a $k$-clustering of $X$ and $\epsilon$ is the exemplar distance. (ii) The sets of exemplars for the $k$ clusters are pairwise disjoint. (iii) The total number of instances with exemplars is at least $(1 - 1/e)Q^*$, where $e$ is the base of the natural logarithm and $Q^*$ is the maximum number of instances in $X$ that can have exemplars under the constraint that the total number of exemplars is at most $\beta$. 
**Proof:** The proofs of Parts (i) and (ii) of the theorem are identical to the ones given in the proof of Theorem 2. Part (iii) follows from [18] that the greedy approximation algorithm for BMC covers at least \((1 - 1/e)Q^*\) elements, where \(Q^*\) is the maximum number of elements that can be covered using at most \(\beta\) sets.

**Running time of Algorithm 2** The estimation of the asymptotic running time of Algorithm 2 is similar to that of Algorithm 1. The main difference between the two algorithms is that while Algorithm 2 uses the greedy algorithm for the BMC problem in Step 3 while Algorithm 1 uses the greedy algorithm for the Minimum Set Cover (MSC) problem. However, the asymptotic running time of the greedy algorithm for BMC is also the same as that of the greedy algorithm for MSC [18]. Therefore, the running time of Algorithm 2 is also \(O(n^2)\).

5 Experiments

Code and data to reproduce and document the experiments are available\(^2\) with the exception of the Harry Potter novel data which is not in the public domain but is freely available. We have tried to quantitatively and qualitatively evaluate our approach’s usefulness for explanation to a human. We explore several directions including generating summaries of a novel which we compare against human written summaries. Similarly, we explore quantitative measures on human faces in the wild data, and for completeness, a qualitative analysis of a standard digit data set. Finally, in an emerging direction of using explanation for machines (not humans), we explore using exemplars for SVM transfer learning.

**Time Complexity.** Our approximation algorithms run in polynomial time (more precisely, in \(O(n^2)\) time in the worst-case) and have strong performance guarantees in terms of clustering quality and explanation complexity. The run times for our algorithms are as expected not as fast as simple \(k\)-means style algorithms but our work comes with performance guarantees with respect to optimal solutions and are much faster than state of the art domain specific methods. For example in our work on explaining deep embeddings for text (Section 5.2), our SCCE and SCCRB algorithms took 93 and 96 seconds respectively whilst the state of the art method took 700+ seconds and \(k\)-means style algorithms (which lack explanation) took under 10 seconds. Our algorithm has just two parameters, namely \(k\) and \(\epsilon\), where the latter parameter naturally trades off clustering quality and explanation complexity.

5.1 Qualitative Experiments on Digits Data

Here, we take the standard MNIST data set consisting of 10,000 written digits. We embed them using tSNE [20] and use our algorithm to cluster them and generate exemplars. Our hope is that the exemplars will be a varied representation of the different ways of writing each digit. Through experiments, we empirically verify how useful exemplars from text and images are from a predictive perspective, but here visually inspect them for usefulness. The clusters found by our methods and

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\(^2\) URL: [www.cs.ucdavis.edu/~davidson/SCCE-DMKD-main.zip](http://www.cs.ucdavis.edu/~davidson/SCCE-DMKD-main.zip) All code and public data are located at the site.
Fig. 2 Clusters and centroids (not exemplars) found by our method when applied to the MNIST dataset. A larger version of the figure is given in Section 8.2 of the Appendix.

Table 1 The clusters and exemplars found by our method on the MNIST data set. Note that the exemplars provide a variety of ways that the digits are written and most importantly are quite different from the centroids shown in Figure 2.

| Cluster | Exemplars |
|---------|------------|
| 0       | 0 0 0 0 0 |
| 1       | 2 1 1 2 1 1 1 2 1 |
| 2       | 2 2 2 2 2 1 |
| 3       | 3 3 3 3 |
| 4       | 4 4 4 4 |
| 5       | 5 5 5 5 |
| 6       | 6 6 0 6 6 6 6 6 6 |
| 7       | 7 7 7 7 7 |
| 8       | 8 8 8 8 |
| 9       | 9 9 9 9 9 |

approximate centroids (not exemplars) are shown in Figure 2. (A larger version of the figure is given in Section 8.2 of the Appendix.) For each cluster, we present the exemplars found in Table 1. Of course, the clustering does not have 100% accuracy but we see that for well separated clusters (0, 5, 6, 7, 8 and 9), the exemplars do indeed capture a variety of ways that the digits are written. Quite surprisingly, many are fundamentally different from the centroid. Take for example the digit 7. The centroid has the top line pointing downwards but the exemplars show examples where the top line is up and the vertical line is crossed. The exemplars vary by their form and also in the pressure applied to the pen.
5.2 Quantitative Experiments on Textual Data

In this section, we evaluate the ability of exemplars to simplify a corpus by summarizing content. In particular, we take the sentences in the first Harry Potter (HP) book, embed them using deep learning, apply Algorithms 1 and 2 and concatenate the resultant exemplars to form a summary. This is compared with a ranking based approach [9,22] which can be viewed as choosing exemplars from a list based on importance. These ranking methods are known to produce superior results for HP books [15] compared to recent methods. We measure results by comparing against four human written summaries. Results (Table 2) show that our method performs better than these ranking method by 12.8% and the baseline of random selection of sentences by over 20%. Most importantly, our method’s summary score is almost comparable (on average) to the similarity between the human summaries themselves (Table 3).

We measure performance using the ROUGE score [19] which is a standard method of evaluating the similarities between computer generated summaries and human written summaries. We represent each sentence in the first HP book using the state-of-the-art language model BERT [8]. Hence, the exemplars generated by our method will be sentences in the book. Specifically, we fine-tune a pre-trained BERT-base model (https://huggingface.co/) in two steps. First, we add to the vocabulary terms words that are unique to the Harry Potter universe (e.g., “quidditch”) and train the model with a very low learning rate. Then, we fine-tune the model to produce a relevant sentence embedding using the Sentence-BERT architecture [24] to create a HP Specific BERT model. It is important to note that all methods and baselines use this embedding scheme.

We compare our two methods against two approaches. The first one is a random subset of sentences used as a control. We repeat this random selection process 20 times. The second baseline is the widely used ranking approach for extracting summaries [22,9]. These methods require a graph which we construct from pairwise cosine similarities using the sentence embedding obtained with our fine-tuned BERT model. This is a time tested method with thousands of citations and in 2020 still produces state of the art results for the HP literature [15]. For all methods except for SCCE, we fix the number of sentences extracted to be equal to the number of sentences in the ground truth summaries. We use 6 clusters chosen after hyper-parameter tuning to find the stablest clusters. An example summary is shown in Section 8.1 of the Appendix.

5.3 Quantitative Experiments on Facial Data

One way to determine whether an explanation is useful is to check if it helps a human to understand the underlying concepts which are the clusters. A typical test of exemplar theory given to humans [23] is the task of identifying several people they have never seen before using only a small set of exemplars of the people. We make the task challenging by choosing three similar men (Gerhard Schröder, Jacques Chirac and Tony Blair) and use just 40 images of each person, with half used for clustering and half for testing.
Explainable Clustering via Exemplars

Table 2 The ROUGE-1 F1-scores (the larger the better) measuring the similarity of our two methods, one state of the art (Ranking), one baseline (Random) to four human written summaries (one per row) of the first Harry Potter novel. For each summary, we also report the the average similarity to the remaining three summaries (Human Summaries). Each computational method (except SCCE) generates the same number of sentences as the summary against which it is compared.

| Summary | SCCE (Ours) | SCCE (Ours) | Ranking | Random | Other Summaries | Relative Performance To Ranking | Relative Performance To Other Summaries |
|---------|-------------|-------------|---------|--------|----------------|-------------------------------|--------------------------------------|
| Sum-1   | 31.65       | 33.81       | 28.86   | 23.69  | 38.09          | +17%                          | -11%                                 |
| Sum-2   | 29.58       | 31.26       | 28.73   | 25.89  | 25.82          | +9%                           | +21.1%                               |
| Sum-3   | 27.08       | 28.78       | 25.58   | 22.68  | 31.32          | +8.3%                         | -8.1%                                |
| Sum-4   | 33.33       | 34.11       | 28.31   | 24.29  | 36.08          | +17%                          | -5.5%                                |

Table 3 Measuring the effectiveness of exemplars to explain/predict a person from images. Competing methods use the same clustering we find but instead use $k$-Nearest-Neighbor for prediction with different aspects/artifacts of the cluster. The value $\epsilon$ is tuned and set to 0.6 to maximize the stability of clusters.

| Clustering Artifact Used | Accuracy |
|--------------------------|----------|
| Exemplars                | 48.33    |
| Cluster centers          | 44.00    |
| All Points               | 42.00    |
| Random Points in cluster | 44.66    |

Fig. 3 Faces in the Wild Experiments. Exemplars found for our three clusters correspond to the three people used in this experiment, Gerhard Schröder (left), Jacques Chirac (middle) and Tony Blair (right). Note the exemplars of the same person differ mainly by the position of the mouth.

For reproducibility, we simulate a person by the most simple learning algorithm, namely $k$-nearest neighbor ($k$-NN). We cluster images of three well-represented individuals from the Labeled Faces in the Wild dataset [17] using our method. Images are first processed into embeddings via FaceNet, a deep embedding network. After clustering using our method, each cluster was assigned the label of its most well-represented individual.

We created three baselines to predict the person in the hold out image: 1) Using a nearest centroid approach, 2) Using a $k$-NN approach with all points and 3) Using a $k$-NN approach but with random 20% of points from each cluster. After conducting this experiment five times with five different training/testing splits, we obtained the results summarized in Table 3. This experiment demonstrates that exemplars produced by our method are more useful than other artifacts of the very same clustering namely centroids, all points and random subsets of points. A possible reason for the improvement is that our method chooses a more diverse collection of instances (Figure 3).
Table 4: Accuracy for Transfer Learning. 350 training instances of each digit were randomly chosen for both source and target problems. The 3rd column shows transferring the support vectors and the 4th column shows transferring the exemplars from our work. Results are averaged over 100 random trials. Results above (below) the double lines use all 8 pairs (first 4 pairs) of coordinates. Using just half the features produces nearly twice as many support vectors.

5.4 Exemplars for Instance Transfer Learning

Our exemplar and clustering discovery method can also help to explain a problem to a machine. Essentially, our method identifies clusters of points and important examples of each cluster. Here we use those important points to do instance transfer learning for support vector machines (SVMs). Transfer learning uses a source task to help a target task. We use the well known pendigits dataset [1] to transfer the task of predicting between two digits to help another task of predicting between two very similar digits. For example, we can learn the source task of \(1 \text{ vs } 9\) and transfer it to help the \(1 \text{ vs } 7\) task as shown in Table 4.

Recall that with a SVM the vector \(w\) implicitly defines the hyperplane and a constraint to separate the two classes is defined as shown below in equation 1.

A common method of performing SVM transfer learning is to add an additional constraint to the problem that requires the hyperplane to also separate the classes in the source problem. Note the last constraint in equation 1 contains the transfer as \((x^s_i, y^s_i)\) are the support vectors from the previously solved SVM for the source problem. In our experiments, rather than transferring over these support vectors, we can instead transfer the exemplars. We use the bounded version of our formulation to transfer over the same number of instances as support vectors in the source problem. Results in Table 4 show promise and a future direction of exemplars augmenting existing ML tasks.

\[
\arg\min_w, w_0 \frac{1}{2} ||w||^2
\]

\[
\text{s.t. } y_i(w^T x_i + w_0) \geq +1 \ \forall i \ \text{and} \ \\
y^s_j(w^T x^s_j + w_0) \geq +1 \ \forall j
\]
6 Related Work

Explanation and Clustering. The machine learning community has studied explaining clusters from two perspectives. The one-view approach of conceptual clustering [21,6,26] proposes a task that is similar to our own (i.e., finding a clustering and its description), but requires that the features used to perform clustering are human interpretable. This work can be seen as expounding the definition-based theory of concepts [23] as it defines the concept explicitly using an underlying language. Two-view work attempts to find a clustering using one set of features and a description using another set of features (typically human interpretable tags) such as our own [5]. This work again takes a descriptive (non-exemplar) based approach to explanation and most importantly does not scale beyond a few hundred points as it performs Pareto optimization. In contrast, the work presented in this paper scales to hundreds of thousands of points; all our experiments run on standard laptops in under a minute. More recent work [7,24] has explored explaining a given clustering using a set of auxiliary tags; it does not find a clustering itself.

Concept Theory. A motivation for our work comes from human psychology and philosophy, and in particular, the large body of work known as theories of concepts [23]. This field defines the building blocks of knowledge as concepts but there are several different definitions of concepts. Our work falls under the exemplar based theory which defines a concept by exemplars of that concept whilst the competing classical definition theory requires defining properties of the concept (e.g., “Jaques Chirac is tall, bald and cherubic faced”). However, this classic definition requires the instances to be described using an understandable set of features which is not the case for deep embeddings or most complex domains. Though exemplar based theories suggest how to define a concept, the problem of finding/choosing those exemplars is not well posited by the psychology community. Our work can be seen as formalizing and extending this theory by formulating simultaneous concept and exemplar discovery as a combinatorial optimization problem.

Comparison to DBSCAN and Other Density Based Clustering Methods. Superficially, our method may seem to be similar to DBSCAN [10] and other similar algorithms as it uses notions such as $\epsilon$-neighbors. However, there are several fundamental differences. Firstly, our method is guaranteed to use the specified number or near-minimum number of exemplars, where as DBSCAN, while being a very useful method, does not provide such guarantees. Similarly, our method has an explicit clustering objective (i.e., to minimize the maximum cluster diameter) where as DBSCAN does not. Finally, DBSCAN is not designed so that the core points can be considered explanations of the clusters. As a consequence, it is not meaningful to compare our method with DBSCAN.

Comparison to Multiple Centroid Methods. An area that is superficially similar to our own work is finding multiple centroids per cluster; these centroids are sometimes referred to as exemplars. However, there are significant differences with respect to the definition of an exemplar, the purpose of the exemplars and the efficiency of the algorithms.

The multi-centroid/exemplar methods are specifically focused on identifying multiple centroids in each cluster, where each centroid specifies a new sub-cluster (e.g., [30,31]). While these methods allow a user to specify the number of clusters
$k$, the algorithms may find more clusters, that is, possible sub-clusters within each cluster \cite{31}. One can view these as finding a one layer hierarchy within each cluster and experimental results typically compare these algorithms against hierarchical clustering methods.

In our work, an exemplar has a very precise definition: namely a point $x$ is an exemplar for another point $y$ if and only if $x$ is within a certain distance from $y$. The work on multiple centroid clustering has no such definition. Further, the exemplars generated by our methods are motivated by the need to explain clusters rather than to identify sub-clusters and hence yield fundamentally different results. As an illustrative example, consider a cluster with points uniformly distributed throughout it. Methods such as MEAP and K-MEAP \cite{30,31} will return just one exemplar for the entire cluster, as there are no distinct sub-clusters. However, our methods will return multiple exemplars when $\epsilon$ is small enough. Figure 2 provides such an example where the clusters are tightly defined with no sub-clusters. Finally, while the methods in \cite{30,31} provide no formal performance guarantees with respect to either of the two objectives considered in our work (i.e., the cluster quality and the number of exemplars chosen), our methods have provable performance guarantees for both of the objectives.

7 Future Work and Conclusions

XAI for clustering is an under-studied problem compared to supervised learning. Here we explore a style of explainable-by-design algorithm that simultaneously finds clusters and exemplars to describe those clusters. The idea of using exemplars has several benefits. Firstly, it has pedagogic benefits in that humans are known to naturally understand concepts in terms of exemplars \cite{23}. How humans naturally cluster and then organize these exemplars into hierarchical structures will motivate future work. Secondly, the use of exemplars is perhaps the only way to explain data when it is clustered in high dimensional uninterpretable spaces such as deep embeddings. We show that finding a small set of exemplars for just one cluster is \textit{NP}-hard and design approximation algorithms with provable performance guarantees. We demonstrate their usefulness in four tasks: (i) to generate a summary of a book which is compared to a human summary, (ii) to generate exemplars for the classic MNIST data set, (iii) to generate exemplars that can be used to identify people and (iv) to perform instance transfer learning. Our approach is based on classic computations (e.g., minimum set cover) but the combination of the methods is novel. This has the advantage of being able to leverage known results and implementations of these classic algorithms; see code in the following repository: \url{www.cs.ucdavis.edu/~davidson/SCCE-DMKD-main.zip} This has other advantages such as ease of parallel implementation. Like most ML methods, our methods also need parameter tuning. Most clustering algorithms need to tune $k$ (the number of clusters) and our method adds another parameter $\epsilon$ (the coverage of an exemplar). The relationship between $\epsilon$ and the number of exemplars allows for a natural trade off between the complexity of the explanation and cluster compactness as per our bounds. If the data to be clustered is human interpretable, then other methods of explanation are also suitable \cite{6,21} but exemplars are a natural and pragmatic way to explain complex data.
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Appendix

8 Additional Material for Section 5

8.1 Harry Potter Explanations By Our Method

Here we present the explanation generated by our approach. We color code the exemplars by the cluster they belong to.

At that moment the telephone rang and Aunt Petunia went to answer it while Harry and Uncle Vernon watched Dudley unwrap the racing bike a video camera a remote control airplane sixteen new computer games and a VCR. One small hand closed on the letter beside him and he slept on not knowing he was special not knowing he was famous not knowing he would be woken in a few hours’ time by Mrs Dursley’s scream as she opened the front door to put out the milk bottles nor that he would spend the next few weeks being prodded and pinched by his cousin Dudley. Harry didn’t sleep all night. Perhaps it was because he was now so busy what with Quidditch practice three evenings a week on top of all his homework but Harry could hardly believe it when he realized that he’d already been at Hogwarts two months. Don’t mention it said Hagrid gruffly. Hagrid grinned at Harry. I was allowed ter do a bit ter follow yeh an’ get yer letters to yeh an’ stuff. There was only one room inside. He leapt to his feet and ran to the window. It got to its feet and came swiftly toward Harry. But he couldn’t do it. He sat up and felt around his eyes not used to the gloom. But he never wanted you dead. Hermione had now started making study schedules for Harry and Ron too. The Chasers throw the Quaffle and put it through the hoops to score Harry recited

8.2 Larger Versions of a Figure

A larger version of the clustering of digits shown in Figure 2 is shown on the next page.
Fig. 4. Clusters and centroids (not exemplars) found by our method when applied to the MNIST dataset.