Compositional Affinity Propagation: When Clusters Can Have Compositional Structure

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Abstract

We consider a new kind of clustering problem in which clusters need not be independent of each other, but rather can have compositional relationships with other clusters (e.g., an image set consists of rectangles, circles, as well as combinations of rectangles and circles). This task is motivated by recent work in few-shot learning on compositional embedding models (Alfassy et al. 2019), (Li, Mozer, and Whitehill 2021) that structure the embedding space to distinguish the label sets, not just the individual labels, assigned to the examples. To tackle this clustering problem, we propose a new algorithm called Compositional Affinity Propagation (CAP). In contrast to standard Affinity Propagation (Frey and Dueck 2007) as well as other algorithms for multi-view and hierarchical clustering, CAP can deduce compositionality among clusters automatically. We show promising results, compared to several existing clustering algorithms, on the MultiMNIST, Omniglot, and LibriSpeech datasets. Our work has applications to multi-object image recognition and speaker diarization with simultaneous speech from multiple speakers.

1 Introduction

We consider a new kind of clustering problem in which clusters have compositional structure, in the sense that each example in one cluster may exhibit the union of the properties found in another set of clusters. The goal is not just to partition the data into distinct and coherent groups, but also to infer the compositional relationships among the groups. This scenario arises in speaker diarization (i.e., infer who is speaking when from an audio file) in the presence of simultaneous speech from multiple speakers (Bullock, Bredin, and Garcia-Perera 2020). The audio at each time $t$ is generated as a composition of the voices of all the people speaking at time $t$, and the goal is to cluster the audio samples, over all timesteps, into sets of speakers. Hence, if there are 2 people who sometimes speak by themselves and sometimes speak simultaneously, then the clusters would correspond to the speaker sets $\{1\}$, $\{2\}$, and $\{1, 2\}$. An analogous scenario arises in multi-object image recognition when clustering images such that each image may contain multiple objects from a fixed set (see Figure 1). In some scenarios the composition function that specifies how examples are generated from other examples might be as simple as superposition by element-wise maximum or addition. However, a more powerful form of composition – and the main motivation for our work – is enabled by compositional embedding models, which are a new technique for few-shot learning.

Compositional embedding models: Standard (non-compositional) embedding models such as FaceNet (Schroff, Kalenichenko, and Philbin 2015) and x-vector (Snyder et al. 2018) have an embedding function $f^{\text{emb}}$ (typically a neural network) that maps each example (e.g., image, audio clip) into an embedding space so that examples with the same label are mapped close together, and examples with different labels are mapped far apart. Compositional embeddings (Alfassy et al. 2019), (Li, Mozer, and Whitehill 2021) go a step further and separate not just individual labels, but entire sets of labels. As an example, suppose an image collection contains some images of rectangles, some of circles, and some of both (see Figure 1). Then the embedding function $f^{\text{emb}}$ would induce three clusters in the embedding space corresponding to \{rectangle\}, \{circle\} and \{rectangle, circle\}. In addition to $f^{\text{emb}}$, compositional embedding models have a composition function $g$ that takes the embedding vectors $x_a, x_b$ of two examples and computes a set relationship between them. For instance, $g(x_a, x_b)$ might return another vector in the same embedding space corresponding to where an example containing the union of the labels in the two inputs would lie – see Figure 1 (lower left). At test time, $f^{\text{emb}}$ and $g$ are used together (along with a support set of few-shot examples) to infer the set of labels in an example.

Compositional Affinity Propagation: In this paper we propose a new algorithm to tackle the clustering problem described above; we call it Compositional Affinity Propagation (CAP). CAP generalizes the widely used Affinity Propagation (AP) algorithm (Frey and Dueck 2007), which assigns to each data point $x_i \in X$ the index $c_i$ of an “exemplar” in $X$ that represents the cluster to which $x_i$ belongs. CAP extends AP by allowing each $c_i$ to denote a set of exemplars rather than just a single exemplar. In this paper, we define the CAP model and derive an efficient algorithm to perform inference in time $O(nd_n^{d+1})$ per iteration, where $n$ is the number of examples in the dataset and $d$ is the size of the largest composition (e.g., number of simultaneous speakers) under consideration. By modeling the compositionality of the data,
Compositional Affinity Propagation (Frey & Dueck 2007).

Affinity Propagation (Frey & Dueck 2007).

Composition inference from the first two clusters. Scenario (b) in the figure shows how modeling compositionality yields purer clusters by not lumping the two sets of images (some with triangles, and some with rectangles & circles) together.

Figure 1: Overview of Compositional Affinity Propagation: Scenario (a) shows clusters of images (containing rectangles, circles, or both) and their exemplars ($x_a$, $x_b$, etc.). Each arrow represents the assignment of an example to its cluster exemplar. Standard Affinity Propagation detects 3 clusters that are independent of each other. Compositional Affinity Propagation infers that each example in the bottom cluster is composed (via $g$) of examples from clusters $a$ & $b$. Scenario (b) illustrates how modeling compositionality yields purer clusters by not lumping the two sets of images (some with triangles, and some with rectangles & circles) together.

CAP can both provide richer information about the clusters and also potentially partition the data more accurately.

As a conceptual illustration, see Figure 1. In scenario (a) (left half of the figure), there are three sets of images – some contain circles, some contain rectangles, and some contain both. Both standard AP and CAP (as well as various other clustering algorithms) can separate the data correctly into three clusters. However, CAP can also infer that the cluster shown in purple in the bottom-left is actually a compositional cluster in which each example contains both objects from the first two clusters. Scenario (b) in the figure shows how modeling the compositionality can yield a more accurate partition: whereas standard AP lumps together the images containing triangles with those containing a composition of rectangles and circles, CAP identifies this relationship automatically and thereby obtains purer clusters.

2 Related Work

To our best knowledge, no currently used clustering algorithms exist that can both cluster a dataset and infer the compositionality among clusters. Below we describe the most relevant techniques within the clustering literature and describe how they differ from our proposed method.

Mixture models, such as the Mixture of Gaussians fit using Expectation-Maximization, or the Dirichlet mixture process (Blei and Jordan 2006), extend the standard $k$-means algorithm by “softly” assigning each data point to a probability distribution over the mixture components instead of giving a “hard” assignment like in $k$-means. Importantly, these approaches assume that each data point is generated by a single cluster, and the probability distribution expresses the uncertainty over which cluster it is. These models do not capture compositionality between clusters, and they cannot distinguish between an example that is unconfidently assigned to a single cluster (thus resulting in high entropy over the mixture components for that example), from an example that is confidently assigned to multiple clusters.

Hierarchical clustering algorithms create a tree (dendrogram) such that the $n$ leaf nodes correspond 1-to-1 to the examples in the dataset, and each internal node $i$ represents a cluster whose members consist of all the leaf nodes descending from $i$. Internal nodes closer to the root correspond to higher-level abstractions of the data. Hierarchical clustering algorithms can work either top-down by splitting clusters or bottom-up by merging clusters, until some clustering criterion is reached. One popular variant is agglomerative clustering using the Ward Jr (1963) criterion, which seeks to minimize the variance within each cluster. In all cases, hierarchical clustering algorithms assign each example to a sequence of clusters of increasing generality, starting from the internal node just above the leaf all the way up to the root node, such that each parent cluster captures the intersection of the characteristics of the child clusters. In contrast, our proposed method can assign each example to the union of the properties in multiple clusters; this is tantamount to a dendrogram where each example is connected by an edge to multiple parent nodes, thus yielding a directed acyclic graph rather than a tree.

Multi-view clustering algorithms (e.g., Bickel and Scheffer (2004)) partition the feature space into multiple subsets, each corresponding to a different “view” of the data. For instance, each example might be a video and thus have both auditory and visual features associated with it. The structure of the ta from one view can provide implicit supervision when clustering using the other views. These methods do not have any inherent ability to model compositionality. Franklin and Frank (2018) recently proposed a method for “compositional clustering in task structure learning”, but their method is more akin to multi-view clustering, and the compositionality pertains to how they tackled a control problem (separately addressing the reward and transition functions), not the clustering problem itself.

Exemplar-based clustering algorithms differ from centroid-based algorithms in how clusters are represented: In the former, each cluster is represented by a specific example in the dataset; in contrast, the latter (e.g., $k$-means) may compute a function of the examples (e.g., the mean) to represent the cluster. One of the mostly widely used exemplar-based clustering algorithms is Affinity Propagation (Frey and Dueck 2007).

3 Model

Before presenting our method, Compositional Affinity Propagation, we first review standard AP (Frey and Dueck 2007).
3.1 Review of Affinity Propagation

Let $\mathcal{X} = \{x_1, \ldots, x_n\} \subset \mathbb{R}^p$ be a dataset, and let $\mathcal{C} = \{1, \ldots, n\} \cong [n]$ be the set of indices of the examples in $\mathcal{X}$. Next, let $c_1, \ldots, c_n \in \mathcal{C}$ be the cluster assignments: Each $c_i$ denotes the exemplar representing the cluster to which example $i$ belongs; if example $i$ itself is the exemplar for some other example $j \neq i$, then we require $c_i = i$. For instance, if $\mathcal{X}$ contains $n = 3$ examples, the first two of which belong to the same cluster and the third of which belongs to its own cluster, then we might have $c_1 = 2, c_2 = 2, c_3 = 3$ (or possibly $c_1 = 1, c_2 = 1, c_3 = 3$). Let $f : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}_{\geq 0} \cup \{-\infty\}$ map from a pair of examples to the distance between them (or, alternatively, the negative log-likelihood that example $i$ belongs to cluster $j$). Next, define function $S : \mathcal{C} \times \mathcal{C} \rightarrow [-\infty, 0]$; for each $i \neq j$, we define $S(i, j) = -f(x_i, x_j)$, and we define each $S(i, i) = \gamma$ as the “preference” (a hyperparameter) that $x_i$ is an exemplar, where larger negative values discourage those examples from becoming exemplars. From these definitions, we can formulate the following constrained optimization problem:

$$\arg\max_{c_1, \ldots, c_n \in \mathcal{C}} \sum_{i=1}^{n} S(i, c_i) \quad \text{s.t.} \quad (\exists i : c_i = k) \implies c_k = k$$

The objective is the sum of the distances between each point and its assigned exemplar, and the constraints enforce consistency that examples used by others as exemplars also designate themselves as exemplars. The optimization process has to weigh the cost $\gamma$ of creating a new cluster against assigning examples to existing exemplars that are farther away.

Illustration: Given an appropriate choice for the $\gamma$, Affinity Propagation would yield the results shown in the top half of Figure 1. In particular, in scenario (a), the cluster shown in purple would be identified as an independent cluster with exemplar $x_c$, and in scenario (b), the cluster shown in purple would contain the images with triangles as well as those composed of rectangles and circles.

Inference: Frey and Dueck (2007) showed a procedure to approximate the solutions by defining a factor graph (see Figure 2) to represent the variables and constraints, where $S$ is interpreted as containing log-likelihoods, and then applying loopy belief propagation. This results in a new optimization problem where the goal is to find maximum posteriori (MAP) solutions to $\arg\max_{c_1, \ldots, c_n \in \mathcal{C}} P(c_1, \ldots, c_n \mid S)$, where probability distribution $P$ is understood to encode the constraints. Specifically, the factor graph contains variable nodes to represent $c_1, \ldots, c_n$ and factor nodes to represent both the log-likelihoods $S(1, \cdot), \ldots, S(n, \cdot)$ and a set of constraints $\delta_1, \ldots, \delta_n$. Each $\delta_k$ encodes whether $c_k$ is compatible with the other $c_{k'} \neq k$:

$$\delta_k(c_1, \ldots, c_n) = \begin{cases} -\infty & \text{if } \exists i : (c_i = k) \land (c_k \neq k) \\ 0 & \text{otherwise} \end{cases}$$

Given the factor graph, a sequence of “messages” (functions $\alpha, \rho : [n] \times [n] \times \mathcal{C} \rightarrow \mathbb{R}_{\geq 0} \cup \{-\infty\}$) is passed back and forth between the variable and factor nodes. Each variable $i$ sends a message $\rho_{i \rightarrow k}(c_i)$ to constraint $k$, and each constraint $k$ sends a message $\alpha_{i \leftarrow k}(c_i)$ to variable $i$, about the likelihood of each possible value of $c_i$. The values of $\alpha$ and $\rho$ are determined by the max-product algorithm for loopy belief propagation (Weiss and Freeman, 2001) applied to the factor graph (see the Technical Appendix). To find an approximate MAP estimate for all the $c_i$, we alternate between computing the $\alpha$s and the $\rho$s. Finally, after any number of iterations, we compute:

$$c_i^{MAP} = \arg\max_{c_i} \left[ \sum_k \alpha_{i \leftarrow k}(c_i) + S(i, c_i) \right]$$

Frey and Dueck (2007) also presented an efficient $(O(n^2))$ method to calculate all the messages for each iteration.

3.2 Compositional Affinity Propagation

Here we describe our proposed model. Let $\mathcal{X} = \{x_1, \ldots, x_n\} \subset \mathbb{R}^p$ be a dataset. Let $\mathcal{C} \subset 2^{[n]} \setminus \emptyset$ be the set of compositions of examples in $\mathcal{X}$ under consideration, where we assume $\mathcal{C}$ contains all the singleton sets, i.e., $\{i\} \in \mathcal{C}, i = 1, \ldots, n$. Let $d = \max_{c \in \mathcal{C}} |c|$, i.e., the size of the largest composition under consideration. To identify which compositions contain (or do not contain) each example $k$, define functions $\phi, \overline{\phi} : [n] \rightarrow 2^\mathcal{C}$ such that $\phi(k) = \{c \in \mathcal{C} : c \ni k\}$ and $\overline{\phi}(k) = \mathcal{C} \setminus \phi(k)$.

Let $f$ be defined as in standard Affinity Propagation. We further assume there is a function $g : 2^\mathcal{X} \setminus \emptyset \rightarrow \mathbb{R}^p$ that satisfies a set of examples and produces another vector representing their composition; for singleton sets, we set $g$ to be the identity function, i.e., $g(\{x\}) = x$. For instance, $g$ could be the element-wise maximum to perform pixel-wise superposition of the images; for word embeddings, it could be element-wise addition (Allen and Hospedales, 2019); or it could be a trained neural network within a compositional embedding model. We define $S : [n] \times \mathcal{C} \rightarrow [-\infty, 0]$ to measure the distance between each example and each composition: $S(i, c) = -f(x_i, g(\{x_k : k \in c\}))$ for $c \neq \{i\}$, and $S(i, \{\}) = \gamma$ is a hyperparameter for each example. Finally, define $c_1, \ldots, c_n \in \mathcal{C}$ as the assignment of which example belongs to which cluster. If $c_i = \{k\}$ (i.e., a singleton), then example $i$ belongs to a primitive cluster with exemplar $x_k$. If $|c_i| \geq 2$, then example $i$ belongs to the cluster with a compositional exemplar $g(\{x_k : k \in c_i\})$, i.e., the composition of all the examples in $c_i$. Note that, in general, compositional exemplars are not members of $\mathcal{X}$. In CAP, we require that, whenever some example $i$ designates its exemplar either to be example $k$ ($c_i = \{k\}$), or to include example $k$ ($c_i \ni k$), then example $k$ must designate itself as...
an exemplar \(c_k = \{k\}\). Example: if \(X = \{x_1, x_2, x_3, x_4\}\) and we allow compositions of size at most 2, then \(C = \{\{1\}, \{2\}, \{3\}, \{4\}, \{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}, \{2, 4\}, \{3, 4\}\};\) if \(x_1\) and \(x_2\) each constitutes its own cluster and the last two examples are both assigned to the composition of the first two clusters, then we would have \(c_1 = \{1\}, c_2 = \{2\}, c_3 = c_4 = \{1, 2\}\).

Our new constrained optimization problem is thus:

\[
\arg\max_{c_1, \ldots, c_n \in C} \sum_{i=1}^{n} S(i, c_i) \quad \text{s.t.} \quad (\exists i: c_i \ni k) \implies c_k = \{k\}
\]

Importantly, the optimization objective incurs no additional cost when an example is assigned to a compositional exemplar \(c_k\) as long as all of the examples \(k' \in c_k\) have themselves already been designated as exemplars.

Illustration: Given an appropriate choice for \(\gamma\), \(\text{CAP}\) would yield the results shown in the bottom half of Figure [1].

In scenario (a), the cluster shown in purple would be identified as a cluster with a compositional exemplar \(g(x_a, x_b)\). In scenario (b), the compositional structure identified by the algorithm could help it to separate the images containing triangles from those containing both a rectangle and a circle.

Inference. As with standard Affinity Propagation, we find a MAP estimate for each \(c_i\) by defining a factor graph and computing and passing messages between the variables and the factors. We adjust the definition of \(\delta_k\) to be:

\[
\delta_k(c_1, \ldots, c_n) = \begin{cases} 
-\infty & \text{if } (\exists i: (c_i \ni k) \land (c_k \neq \{k\})) \\
0 & \text{otherwise}
\end{cases}
\]

In the Technical Appendix, we derive an algorithm to compute all the messages \(\alpha, \rho\) efficiently; the result is shown in Algorithm [1]. The \(\arg\max_{c_1, c_2}^{1, 2}\) called in \(\text{FindAllMaxes}\) returns the \(c_1, c_2\) that give the largest and second-largest values of the specified function, where \(c_2 = \emptyset\) if the input set is of size 1, and \(c_1 = c_2 = \emptyset\) if the input set is empty.

Theorem 1. Let \(n\) be the number of examples in a dataset \(X\), and let \(d\) be the largest element in the set \(C\) containing all compositions under consideration. Then Algorithm 1 implements message passing (i.e., computation of sufficient statistics of \(\alpha\) and \(\rho\)) for Compositional Affinity Propagation and operates in time \(O(dn^2+1)\) per iteration.

Proof. See Technical Appendix in the Supp. Materials. \(\square\)

Python+numpy code for \(\text{CAP}\) is in the Supp. Materials.

3.3 \(\text{CAP} \subset\): An Approximation to \(\text{CAP}\)

To improve the scalability of \(\text{CAP}\), we can apply it to a randomly selected subset of examples \(X' \subset X\) and infer the cluster assignments \(\tilde{c}_1, \ldots, \tilde{c}_{|X'|}\). Let \(E = \{\tilde{c}_i\}_{i=1}^{|X'|} \subset C\) be the set of unique exemplars (primitive or compositional) inferred for \(X'\). Then, for each example \(x_i\) in the original dataset \(X\), we designate its exemplar to be the \(\tilde{c}_i \in E\) that is closest to it \(x_i\) according to \(f\). Specifically, we assign \(c_i = \arg\min_{\tilde{c}_i \in E} f(x_i, g(\{x_j : j \in \tilde{c}_i\}))\). We call this method \(\text{CAP} \subset\).

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**Algorithm 1: Compositional Affinity Propagation (CAP)**

1. **CAP(S, C):**
   - \(\phi(k) \leftarrow \{c \in C : c \ni k\} \quad \forall k\)
   - \(\hat{\phi}(k) \leftarrow C \setminus \phi(k) \quad \forall k\)
   - \(q(i, c_i) = 0 \quad \forall i, c_i\)
   - \(a(i, k) = 0 \quad \forall i, k\)
   - \(\pi(i, k) = 0 \quad \forall i, k\)

   while not converged do
     - ComputeRhoStats(S, C, \(\phi, \hat{\phi}, a, \pi, q\))
     - ComputeAlphaStats(C, b, \(\tilde{b}, h\))

   return \(\arg\max_{c_i} (q(i, c_i) + S(i, c_i)) \quad \forall i\)

2. **ComputeRhoStats(S, C, \(\phi, \hat{\phi}, a, \pi, q\):**
   - for \(i = 1, \ldots, n\) do
     - \(r, s \leftarrow \text{FindAllMaxes}(S(i, \cdot) + q(i, \cdot), C, \phi, \hat{\phi})\)
   - for \(k = 1, \ldots, n\) do
     - \(b(i, k) \leftarrow \max(r(k) - a(i, k), s(k) - \pi(i, k))\)
     - \(\tilde{b}(i, k) \leftarrow s(k) - \pi(i, k)\)
   - for \(k = 1, \ldots, n\) do
     - \(h(k) \leftarrow S(k, \{k\}) + q_k(\{k\}) - a(k, k)\)
   - return \(b, \tilde{b}, h\)

3. **ComputeAlphaStats(C, b, \(\tilde{b}, h\):**
   - for \(k = 1, \ldots, n\) do
     - \(e(k) \leftarrow \sum_{i \neq k} b(i', k)\)
     - \(\rho(k) \leftarrow \sum_{i \neq k} \tilde{b}(i', k)\)
   - for \(i = 1, \ldots, n\) do
     - \(q^*(i) \leftarrow \sum_{k \in C} \pi(i, k')\)
   - for \(c_i \in C\) do
     - \(q(i, c_i) \leftarrow q^*(i) + \sum_{k' \in c_i} (a(i, k') - \pi(i, k'))\)
   - return \(a, \pi, q\)

4. **FindAllMaxes(q, C, \(\phi, \hat{\phi}\):**
   - \(r(k) \leftarrow \max q(\phi(k)) \quad \forall k\)
   - \(s(k) \leftarrow -\infty \quad \forall k\)
   - for \(j = 1, \ldots, d\) do
     - for \(r \in \{\frac{t_1, \ldots, t_{j-1}}{t_j, t_{j+1}} : t_j \in C\}\) do
       - \(\psi_r \leftarrow \{\{t_1, \ldots, t_{j-1}, t_j\}, t_j > t_{j+1} \cap C\}\)
       - \(c_1, c_2 \leftarrow \arg\max_{c_1, c_2}^{1, 2}(c, q(c))\)
       - for \(k = 1, \ldots, n\) do
         - if \(c_1 \in \hat{\phi}(k)\) then
           - \(s(k) \leftarrow \max s(k), q(c_1)\)
         - else if \(c_2 \in \hat{\phi}(k)\) then
           - \(s(k) \leftarrow \max s(k), q(c_2)\)
       - return \(r, s\)
4 Experiments

Before describing our experiments on MultiMNIST, LibriSpeech, and OmniGlot, we first define the evaluation metric and describe the baseline methods for comparison.

4.1 Compositional Rand Index (CRI)

Suppose that the examples in $\mathcal{X}$ are compositions of examples from $l$ primitive clusters (i.e., exemplars that are singletons). Then $\mathcal{Y} = 2^{|\mathcal{I}|}$ \( \mathcal{Y} \neq \emptyset \) is the set of all possible compositional cluster labels, and $y_1, \ldots, y_n \in \mathcal{Y}$ are the ground-truth cluster assignments. A sensible evaluation criterion of some inferred labels $c_1, \ldots, c_n$ w.r.t. the ground-truth should capture the number of clusters, their purity, and the compositional relationships between them. It should not depend on the particular naming of cluster labels (the identifiability issue). With these goals in mind, we define the Compositional Rand Index (CRI) to compute the probability, over all pairs $i \neq j$, that the inferred labels agree with the ground-truth about whether the cluster assignment of example $i$ subsumes the cluster assignment of example $j$:

$$
\text{CRI}(c_1, \ldots, c_n, y_1, \ldots, y_n) = \frac{1}{n(n-1)} \sum_{i \neq j} \mathbb{I}(c_i \supseteq c_j) \cdot (y_i \supseteq y_j)
$$

where $\mathbb{I}[\cdot]$ is a 0-1 indicator function. For datasets without compositionality (i.e., $\mathcal{Y} = \{[l]\}$), CRI is equivalent to the standard Rand Index (Rand 1971).

4.2 Baseline Methods

Since this clustering problem is new, we must select a reasonable baseline to tackle this clustering problem without CAP. Probably the simplest way is to use any exemplar-based method to cluster the examples; then, we can use the distance function $f$ and composition function $g$ to find the optimal “remapping” of the inferred clusters so that some of them are considered to be compositions of others. Specifically, we first obtain a set of $l$ primitive clusters with associated exemplar indices $\mathcal{E} \subset [n]$. Then we iterate over every possible subset $\tilde{\mathcal{E}} \subseteq \mathcal{E}$; these represent the compositional clusters. For each $\tilde{\mathcal{E}}$, we conduct an inner-loop to iterate over every possible 1-to-1 mapping from $\tilde{\mathcal{E}}$ to the set of combinations of $\mathcal{E} \setminus \tilde{\mathcal{E}}$; these are the primitive clusters. We select $\tilde{\mathcal{E}}$ and its remapping so as to minimize the sum of distances, according to $f$ and $g$, of all the examples according to the updated clustering (see the Technical Appendix).

Using this post-hoc heuristic remapping, we implement two strong baselines on top of standard Affinity Propagation (AP+Heur) and Agglomerative Clustering using the Ward criterion (AC+Heur). We note that these are practically only for small $\mathcal{E}$, as the cost of the remapping grows factorially with $|\mathcal{E}|$ (e.g., for $|\mathcal{E}| = 15$ and $d = 2$, there are 107770296705436 possibilities). Hence, we also use two more baselines consisting of just AP and AC by themselves.

4.3 MultiMNIST

Here we apply CAP to a dataset without training a compositional embedding model. The goal is to cluster MultiMNIST images containing either a single or a combination of 2 hand-written digits; this is similar to the dataset by Frosst, Panayotov, and Hinton (2017). For $n \in \{100, 500, 1000\}$, and for either $l = 3$ or $l = 5$ primitive clusters (digit classes), we randomly sampled the ground-truth exemplar $y_i$ for example $i$ from either $C_3$ or $C_5$, which contains all singletons and pairs from the sets $\{0, 1, 3\}$ and $\{0, 1, 3, 5, 8\}$, respectively. These sets of digits were heuristically chosen so that the images of the primitive exemplars and their compositions were somewhat distinctive. We then generated each $x_i \in \mathcal{X}$ by randomly picking an MNIST image from each digit class $k \in y_i$, and then composing them using pixel-wise maximum as the composition $g$. We note that this $g$ is very weak since it has no ability to account for rotation, translation, etc. The distance function $f$ is the squared Euclidean distance. Some examples are shown in Figure 3 (right). For each value of $n$ and $l$, we conducted 10 trials by sampling the MultiMNIST data and then clustering the data using either CAP, CAP⊂ (subset of 50 examples for $n = 100$), and subset of 100 for $n \in \{500, 1000\}$, or the four baselines. We ran the full CAP only for $n = 100$ since it is slow for $n \geq 500$. We ran AP+Heur and AC+Heur only for $l = 3$ due to the computational cost.

Hyperparameters: CAP, CAP⊂, AP, and AP+Heur have one hyperparameter, which is the cost $\gamma$ of creating a new primitive cluster. AC and AC+Heur use a distance threshold hyperparameter that determines whether to merge two clusters. The hyperparameter sets were chosen heuristically for each method, based on pilot exploration, to give each method a good chance of succeeding. The hyperparameter values were then optimized independently for each method so as to maximize the average (over the 10 trials) accuracy (see Technical Appendix). Experiments were conducted using the Python/numpy code in the Supp. Materials and the sklearn implementations of AgglomerativeClustering and standard AffinityPropagation.

Results (mean CRI % and standard error) are shown in Figure 3 (left). For $l = 3$, either CAP or CAP⊂ always did best. For $l = 5$, the CAP and CAP⊂ results were not as consistent, likely because the weak $g$ function caused problems for inferring compositionality. Figure 4 shows some clustering results (for $l = 3$) of the 6 different methods; in each plot (generated using PCA applied to $\mathcal{X}$), circles and plusses represent examples from primary and compositional clusters, respectively. (To avoid clutter, the inferred relationships of which clusters are composed to yield other clusters are not shown.) CAP and CAP⊂ are largely successful in inferring both the clusters and their compositionality. AP and AC can approximately infer the clusters but sometimes lump groups of examples together that actually come from distinct clusters. AP+Heur and AC+Heur do manage to infer some compositionality correctly, but not as well as CAP or CAP⊂.

4.4 LibriSpeech

We used the LibriSpeech (Panayotov et al. 2015) dataset to explore how well each method can cluster speech samples into speaker sets and infer the compositional relationships between sets. While LibriSpeech contains only indi-
We presented a new algorithm — Compositional Affinity Propagation (CAP) — that can both cluster data and infer the compositional relationships between clusters. Experiments on MultiMNIST, LibriSpeech, and Omniglot showed promising results, especially when used in conjunction with a compositional embedding model. While no clustering algorithm always outperforms all others, our experience with CAP suggests that modeling compositionality explicitly is useful. CAP likely has the strongest advantage when the clusters have moderate (neither huge nor tiny) overlap, so that modeling compositionality during the inference process can yield purer clusters than attempting to account for it post-hoc. 

**Future work** can extend other clustering algorithms (e.g., agglomerative clustering, Dirichlet mixture models) to infer compositionality.

## 5 Conclusions

Table 1: LibriSpeech results (mean CRI% and s.e.).

| Method  | n = 120 | n = 150 | n = 495 |
|---------|--------|---------|--------|
| CAP     | 76.3 (1.3) | 77.2 (0.6) | 91.0 (0.9) |
| CAP⊂    | 74.8 (1.2) | 69.2 (0.2) | 88.5 (0.2) |
| AP      | 69.6 (0.3) | 71.1 (1.1) | 87.0 (0.2) |
| AP+Heur | 71.2 (0.7) | 71.1 (1.1) | 96.5 (1.3) |
| AC      | 72.0 (1.0) | 71.1 (1.1) | 95.9 (0.8) |

Figure 3: Left: MultiMNIST clustering accuracy (mean CRI% and s.e.). Right: Some representative examples for l = 3 primitive clusters, as well as 3 compositional clusters (for d = 2), from the label set \{0, 1, 3\}.

Table 2: Omniglot results (mean CRI% and s.e.).

| Method  | n = 120 | n = 150 | n = 495 |
|---------|--------|---------|--------|
| CAP     | 92.4 (1.7) | 91.0 (0.9) | 90.8 (1.1) |
| CAP⊂    | 80.9 (0.6) | 88.3 (0.3) | 88.1 (0.2) |
| AP      | 87.8 (2.2) | 88.5 (0.2) | 87.8 (0.1) |
| AP+Heur | 91.5 (1.3) | 91.0 (0.9) | 90.8 (1.1) |

4.5 Omniglot

This experiment was conducted on Omniglot (Lake, Salakhutdinov, and Tenenbaum 2015). All characters are augmented with random scaling and shifting, and random Gaussian noise is added to the background. We pre-trained a compositional embedding model f_{emb} using a ResNet18 (He et al. 2016) network; the composition function g is the same as for LibriSpeech (see Technical Appendix). The procedures and scenarios are analogous to Section 4.4.

**Results** (mean CRI% and s.e.) are in Table 2. CAP or CAP⊂ did best for scenarios (b) and (c); for scenario (a), CAP was worse than AC+Heur but still second best. Manual inspection of some clusterings revealed that AC often recovered the clusters perfectly whereas AP did not; thus, it is not surprising that CAP was also worse than AC+Heur.

...individual speakers, we can synthesize simultaneous speech using element-wise addition of the waveforms. To make the raw speech more separable, we first trained (on a separate dataset) a compositional embedding model (f_{emb} and g) for speaker verification using an LSTM neural network on top of MFCC audio features (see Technical Appendix). Then we conducted 10 clustering experiments each in three scenarios: (a) n = 120, l = 3; here, we used f_{emb} to extract embeddings from 20 speech samples (2s long) each from a random set of 3 LibriSpeech speakers either in isolation or in combinations of 2 (thus yielding a total of 6 sets: \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}); (b) n = 150, l = 5, with 10 samples each from 5 random speakers (yielding \binom{5}{i} + \binom{5}{j} = 15 different label sets); and (c) n = 495, l = 5 with 33 samples each from 5 random speakers. In scenarios (a) and (b), we used the full CAP; in (c), we used CAP⊂ (subset of 150). For all methods, we optimized hyperparameters using a validation set for l = 3 and l = 5 separately.

**Results** (mean CRI% and s.e.) are in Table 1. Either the CAP or CAP⊂ did best in all three scenarios.
References
Alfassy, A.; Karlinsky, L.; Aides, A.; Shtok, J.; Harary, S.; Feris, R.; Giryes, R.; and Bronstein, A. M. 2019. Loso: Label-set operations networks for multi-label few-shot learning. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, 6548–6557.
Allen, C.; and Hospedales, T. 2019. Analogies explained: Towards understanding word embeddings. In International Conference on Machine Learning, 223–231. PMLR.
Bickel, S.; and Scheffer, T. 2004. Multi-view clustering. In ICDM, volume 4, 19–26. Citeseer.
Blei, D. M.; and Jordan, M. I. 2006. Variational inference for Dirichlet process mixtures. *Bayesian analysis*, 1(1): 121–143.
Bullock, L.; Bredin, H.; and García-Perera, L. P. 2020. Overlap-aware diarization: Resegmentation using neural end-to-end overlapped speech detection. In ICASSP 2020-2020 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), 7114–7118. IEEE.
Franklin, N. T.; and Frank, M. J. 2018. Compositional clustering in task structure learning. *Proceedings of the IEEE conference on computer vision and pattern recognition*, 296–304.
Lake, B. M.; Salakhutdinov, R.; and Tenenbaum, J. B. 2015. Human-level concept learning through probabilistic program induction. *Science*, 350(6266): 1332–1338.
Li, Z.; Mozer, M.; and Whitehill, J. 2021. Compositional embeddings for multi-label one-shot learning. In Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision.
Panayotov, V.; Chen, G.; Povey, D.; and Khudanpur, S. 2015. Librispeech: an asr corpus based on public domain audio books. In 2015 IEEE international conference on acoustics, speech and signal processing (ICASSP), 5206–5210. IEEE.
Rand, W. M. 1971. Objective criteria for the evaluation of clustering methods. *Journal of the American statistical association*, 66(336): 846–850.
Salbaut, S.; Froest, N.; and Hinton, G. E. 2017. Dynamic routing between capsules. *arXiv preprint arXiv:1710.09829*.
Schroff, F.; Kalenichenko, D.; and Philbin, J. 2015. Facenet: A unified embedding for face recognition and clustering. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, 815–823.
Snyder, D.; Garcia-Romero, D.; Sell, G.; Povey, D.; and Khudanpur, S. 2018. X-vectors: Robust dnn embeddings for speaker recognition. In *2018 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, 5329–5333. IEEE.
Ward Jr, J. H. 1963. Hierarchical grouping to optimize an objective function. *Journal of the American statistical association*, 58(301): 236–244.
Weiss, Y.; and Freeman, W. T. 2001. On the optimality of solutions of the max-product belief-propagation algorithm in arbitrary graphs. *IEEE Transactions on Information Theory*, 47(2): 736–744.

A Loopy Belief Propagation for Standard Affinity Propagation
When applying the max-product algorithm (a technique to find MAP estimates using loopy belief propagation) to the factor graph shown in the main paper for standard Affinity Propagation, a sequence of “messages” (functions \( \alpha, \rho : [n] \times [n] \times C \to \mathbb{R}_{\leq 0} \cup \{-\infty\} \)) is passed back and forth between the variable and factor nodes. Each variable \( i \) sends a message \( \rho_{i \to k}(c_i) \) to constraint \( k \), and each constraint \( k \) sends a message \( \alpha_{i \to k}(c_i) \) to variable \( i \), about the likelihood of each possible value of \( c_i \).

The max-sum algorithm (and the related max-product algorithm for factor graphs) dictates that \( \rho_{i \to k}(c_i) \) equals the sum of messages over \( c_i \)’s neighbors except \( \delta_k \) (i.e., \( \{\delta_{k'}\}_{k' \neq k} \)):

\[
\rho_{i \to k}(c_i) = S(i, c_i) + \sum_{k' \neq k} \alpha_{i \to k'}(c_i) \tag{3}
\]

Also, for MAP estimation, \( \alpha_{i \to k}(c_i) \) equals the maximum possible sum of the messages from all of \( \delta_k \)'s neighbors except \( i \) (i.e., \( \{c_{i'}\}_{i' \neq i} \)), plus the value of \( \delta_k \) itself:

\[
\alpha_{i \to k}(c_i) = \max_{\{c_{i'}\}_{i' \neq i}} \left[ \delta_k(c_1, \ldots, c_n) + \sum_{i' \neq i} \rho_{i' \to k}(c_{i'}) \right] \tag{4}
\]

B Derivation of Algorithm 1 (CAP) and Proof of Theorem 1
In this appendix we derive Algorithm 1 from the definitions of \( \alpha \) and \( \rho \) in the message passing algorithm to optimize the Compositional Affinity Propagation model described in the main paper. We also prove the time cost in Theorem 1.
Recall the definitions of \( \alpha \), \( \rho \), and \( \delta \):

\[
\rho_{i \to k}(c_i) = S(i, c_i) + \sum_{k' \neq k} \alpha_{i \to k'}(c_i) \tag{5}
\]

\[
\alpha_{i \to k}(c_i) = \max_{\{c_{i'}\}_{i' \neq i}} \left[ \delta_k(c_1, \ldots, c_n) + \sum_{i' \neq i} \rho_{i' \to k}(c_{i'}) \right] \tag{6}
\]

\[
\delta_k(c_1, \ldots, c_n) = \begin{cases} 
-\infty & \text{if } \exists i : (c_i \not\in k) \land (c_k \not\in \{k\}) \\
0 & \text{otherwise}
\end{cases} \tag{7}
\]

Each message \( \alpha_{i \to k}(c_i) \) computes, for a given value of \( c_i \) for variable \( i \), an (unnormalized) log-likelihood of the best possible configuration of the assignments of all the other variables \( \{c_{i'} \neq i\} \), given that constraint \( k \) is satisfied (i.e., \( \delta_k \)
is finite). There are four cases in which this occurs; they mirror those in standard Affinity Propagation but differ slightly. For each case, the \( \delta \) term in the RHS of Eqn. 6 vanishes; the only remaining terms are the sum of the \( \rho \)'s. Also, since each summand in Eqn. 6 depends on just a single unique \( c_i \), the max of the sum becomes the sum of the max. Cases:

1. \( i = k, c_i = \{k\} \): Since in this case example \( i = k \) designates itself as an exemplar, then the constraint \( \delta_k \) is immediately satisfied. Moreover, any of the other examples \( i' \neq i \) is free to choose (or not choose) example \( k \) as an exemplar, and therefore we can take the maximum over any possible value for each \( c_{i'} \). Hence,

\[
\alpha_{i \rightarrow k}(c_i) = \max_{\{c_{i'}, \ i' \neq k\}} \left[ 0 + \sum_{i' \neq k} \rho_{i' \rightarrow k}(c_{i'}) \right]
\]

2. \( i = k, c_i \not\subset k \): Since example \( i = k \) does not designate itself as an exemplar, then none of the other examples \( i' \neq i \) may choose \( k \) as its exemplar. Hence, \( \alpha_{i \rightarrow k}(c_i) = \sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) \).

3. \( i \neq k, c_i \supset k \): Since example \( i \) designates its exemplar either to be or to include example \( k \), then \( \alpha \) is finite only if \( c_k = \{k\} \), and each remaining example \( i' \not\in \{i, k\} \) is free to designate any example as its exemplar. Hence, \( \alpha_{i \rightarrow k}(c_i) = \rho_{k \rightarrow k}(\{k\}) + \sum_{i' \not\in \{i, k\}} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) \).

4. \( i \neq k, c_i \not\subset k \): Since example \( i \) does not designate \( k \) as an exemplar, then example \( k \) is free either to be an exemplar or not, and we must take the max over both possibilities:

\[
\alpha_{i \rightarrow k}(c_i) = \max \left[ \max_{c_k \not\in k} \rho_{k \rightarrow k}(c_k) + \sum_{i' \not\in \{i, k\}} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}), \right.
\]

\[
\left. \rho_{k \rightarrow k}(\{k\}) + \sum_{i' \not\in \{i, k\}} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) \right]
\]

Note that \( \alpha_{i \rightarrow k}(c_i) = -\infty \) if \( i = k, c_i \not\subset i \) and \( c_i \not\subset \{i\} \).

Given the four cases above, we have the following definition of \( \alpha \):

\[
\alpha_{i \rightarrow k}(c_i) = \max_{\{c_{i'}, \ i' \neq k\}} \left[ \delta_k(c_1, \ldots, c_n) + \sum_{i' \neq i} \rho_{i' \rightarrow k}(c_{i'}) \right]
\]

Here, in the most naive implementation, evaluating \( \alpha \) for each tuple \((i, k, c_i)\) would take time \( O(n^2) \) due to the summing over the max; the entire table of \( \alpha \) values would thus take time \( O(n^4 \times |\mathcal{C}|) \). However, there is massive redundancy that can be avoided: First, for each tuple \((i, k)\), only two possible values of \( \alpha_{i \rightarrow k}(c_i) \) exist: one for \( c_i \supseteq k \) (i.e., \( \alpha_{i \rightarrow k}(\phi(k)) \)) and one for \( c_i \not\subset k \) (i.e., \( \alpha_{i \rightarrow k}(\overline{k}(k)) \)). Hence, instead of computing \(|\mathcal{C}|\) values for each tuple \((i, k)\), we need to compute and store only 2 values. Second, the expressions \( \sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) \) and \( \sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) \) depend on \( k \) but not on \( i \); hence, they can be reused for many tuples \((i, k)\). Third:

\[
\sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) = \sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) - \max_{c_i} \rho_{i \rightarrow k}(c_i)
\]

Hence, after computing each of the terms of the LHS above (just once for each \( k \)), we need only to “adjust” them for each \( i \), in \( O(1) \) time, by subtracting the corresponding term on the RHS.

At the end of all the CAP iterations, we set

\[
e^{\text{MAP}} = \arg \max_{c_i} \left[ \sum_k \alpha_{i \rightarrow k}(c_i) + S(i, c_i) \right]
\]

Hence, as long as we can update \( \alpha \) during each iteration of message passing, then we never need to know \( \rho \) explicitly.
For convenience, define the following functions:

\[ b(i, k) = \max_{c_i} \rho_{i \rightarrow k}(c_i) \]
\[ \overline{b}(i, k) = \max_{c_i \not\in k} \rho_{i \rightarrow k}(c_i) \]
\[ e(k) = \sum_{i' \neq k} \max_{c_{i'}} \rho_{i' \rightarrow k}(c_{i'}) = \sum_{i' \neq k} b(i', k) \]
\[ \tau(k) = \sum_{i' \neq k} \rho_{i' \rightarrow k}(c_{i'}) = \sum_{i' \neq k} \overline{b}(i', k) \]
\[ h(k) = \rho_{k \rightarrow k}(k) \]
\[ o(i, k) = \alpha_{i \rightarrow k}(\phi(k)) \]
\[ \pi(i, k) = \begin{cases} \tau(k), & i = k \\ \max(\overline{b}(k, k) + \tau(k) - \overline{b}(i, k), h(k) + e(k) - b(i, k)), & i \neq k \end{cases} \]

Visual inspection of Equation 9 confirms that the \( o(i, k) \) and \( \pi(i, k) \) defined above recover all 2n^2 degrees of freedom of \( \alpha \). Below we show how we can compute \( e, \pi, b, \overline{b}, \) and \( h \) in a total time of \( O(dn^2) \) per iteration. First, however, we need to derive the computation of some intermediate quantities.

### B.1 Computing \( q(i, c_i) = \sum_{k'} \alpha_{i \rightarrow k'}(c_i) \) \( \forall i, c_i \)

Define \( q(i, c_i) = \sum_{k'} \alpha_{i \rightarrow k'}(c_i) \). For each \( i \), we can compute \( q(i, c_i) \) for each \( c_i \) by splitting the sum over \( k' \) into two parts: those \( k' \) such that \( \phi(k') \not\in c_i \), and those \( k' \) such that \( \phi(k') \not\in c_i \). We then substitute \( \alpha_{i \rightarrow k'}(c_i) = \alpha_{i \rightarrow k'}(\phi(k')) \) for \( k' \) s.t. \( \phi(k') \not\in c_i \) (and similarly for \( \overline{\phi}(k') \)) to yield:

\[ q(i, c_i) = \sum_{k' : \phi(k') \not\in c_i} \alpha_{i \rightarrow k'}(\phi(k')) + \sum_{k' : \overline{\phi}(k') \not\in c_i} \alpha_{i \rightarrow k'}(\overline{\phi}(k')) \]

\[ = \sum_{k'} \alpha_{i \rightarrow k'}(\phi(k')) + \sum_{k'} \alpha_{i \rightarrow k'}(\overline{\phi}(k')) \]

\[ = \alpha_{i \rightarrow k'}(\phi(k')) - \alpha_{i \rightarrow k'}(\overline{\phi}(k')) \]

\[ = \sum_{k' \in c_i} (\alpha_{i \rightarrow k'}(\phi(k')) - \alpha_{i \rightarrow k'}(\overline{\phi}(k'))) \]

We can define \( q^*(i) = \sum_{k'} \alpha_{i \rightarrow k'}(\overline{\phi}(k')) \). Then we have:

\[ q(i, c_i) = q^*(i) + \sum_{k' \in c_i} (\alpha(i, k') - \pi(i, k')) \]

The term \( q^*(i) \) takes time \( O(n) \) for each \( i \) but is reused for all \( c_i \). The summation on the RHS contains at most \( d \) terms (for a maximum composition size of \( d \)). Hence, for each \( i \), the total computation (over all \( c_i \)) is \( O(n + |C|d) = O(n + dn^2) = O(dn^3) \).

### B.2 Efficiently Finding Maxima of Many Subsets

The next step we need is an efficient method to compute expressions of the forms (a) \( \max_{c_i \in \phi(k)} q(i, c_i) \) and (b) \( \max_{c_i \in \overline{\phi}(k)} q(i, c_i) \) for all \( k \), in a total time of \( O(n^d) \).

Form (a): Since each such \( c_i \) must contain \( k \), there are only \( d - 1 \) remaining degrees of freedom for each \( \phi(k) \); hence, \( |\phi(k)| \leq n^{d-1} \) for each \( k \), and directly computing the maximum of \( q(i, \cdot) \) over every \( \phi(k) \) takes a total time of \( O(n^d) \) (summed over all \( k \)).

Form (b): Define \( \overline{\phi}(k) = \{ c \in \overline{\phi}(k) : |c| = j \} \). Since \( \max_{c_i \in \overline{\phi}(k)} q(i, c_i) = \max_{j \in [d]} \max_{c_i \in \overline{\phi}(k)} q(i, c_i) \), we can split the task into subtasks by \( j \) and then take the max over all of them. Since each \( \overline{\phi}(k) \) is a subset of \( [n]^j \), we can iterate over all \( n^{j-1} \) tuples \( (t_1, \ldots, t_{j-1}) \in [n]^{j-1} \), and update for each \( k \) the highest maximum observed so far. For each such tuple \( \tau \), let \( \psi_{\tau} = \{ t_1, \ldots, t_{j-1} \} : t_1 < \ldots < t_{j-2} \).

For instance, if \( j = 2, n = 4 \), and \( \tau = (1, 2) \), then \( \psi_{\tau} = \{ \{1, 2, 3\}, \{1, 2, 4\} \} \). In each iteration, let \( c_1, c_2 \in \psi_{\tau} \) be the arguments corresponding to the largest and second-largest elements in \( q(i, \psi_{\tau}) \); if \( |\psi_{\tau}| = 1 \), then define \( c_2 = \emptyset \); if \( |\psi_{\tau}| = 0 \), then define both \( c_1 = c_2 = \emptyset \). (Note that \( \emptyset \not\in \overline{\phi}(k) \) for any \( k \).) For any \( k \), it must be the case that the number of elements in the set \( \psi_{\tau} \cap \overline{\phi}(k) \) is either 0 (if any \( k \in \{ t_1, \ldots, t_{j-1} \} \)), \( |\psi_{\tau}|-1 \) (if \( k > t_{j-1} \)), or \( |\psi_{\tau}| \) (if \( k \not\in \{ t_1, \ldots, t_{j-1} \} \) and \( k < t_{j-1} \)). In the first case (intersection is empty), we make no update to \( \max_{c_i \in \overline{\phi}(k)} q(i, c_i) \) with \( q(i, c_i) \) if \( c_i \not\in k \) and with \( q(i, c_i) \) otherwise. And in the third (intersection is of size \( \psi_{\tau} \)), we always update \( \max_{c_i \in \overline{\phi}(k)} q(i, c_i) \) with \( q(i, c_i) \). Since \( c_1 \), \( c_2 \) can be computed in time \( \psi_{\tau} \leq n \) and then reused for each \( k \) (in constant-time) for the updates, and since there are at most \( n^{j-1} \) such tuples \( \tau \) when scanning the entire \( C \), then this amounts to a total time of \( O(dn^3) \) for each \( j \). Summing over all \( j = 1, \ldots, d \), this yields a running time of \( O(dn^3) \).

### B.3 Computing Maxes of Sums Except Row \( k \)

We can now show how expressions of the form \( b(i', k) = \max_{c_i \in \phi(k)} \rho_{i' \rightarrow k}(c_i) \) and \( \overline{b}(i', k) = \max_{c_i \not\in k} \rho_{i' \rightarrow k}(c_i) \) can be computed efficiently. We first examine the former, which by definition is:

\[ \max_{c_i} \rho_{i' \rightarrow k}(c_i) = \max_{c_i} \left[ S(i', c_i) + \sum_{k' \not\in k} \alpha_{i' \rightarrow k'}(c_i) \right] \]

In other words, we need to find the \( c_i \) that maximizes \( S(i', c_i) + \sum_{k' \not\in k} \alpha_{i' \rightarrow k'}(c_i) \) over all \( c_i \). This Round 5 approach reduces to the \( i', k \)th term (the \( k \)th term) of the \( \alpha_{i' \rightarrow k'}(c_i) \) (see Figure 5). As mentioned above, for each \( i', k \), function \( \alpha_{i' \rightarrow k'}(\cdot) \) has only 2 degrees of freedom: one for \( c_i' \not\in \phi(k) \) (the blue regions in Figure 5) and one for \( c_i' \in \overline{\phi}(k) \) (the clear regions); hence, there exist numbers \( u, v \) such that \( \alpha_{i' \rightarrow k'}(\phi(k)) = u \) and \( \alpha_{i' \rightarrow k'}(\overline{\phi}(k)) = v \). Assume we have already computed \( q(i, c_i') = \sum_{k'} \alpha_{i' \rightarrow k'}(c_i') \forall c_i' \) (this is the sum over all \( k' \)) and also, for each \( k \), the...
We have already defined $u_h$ as the last step, we can compute $c_0$ nested for-loops, and (as explained in Section B.1) a further $O(n^2)$ time $O$ calls FindAllMaxes for each $i$. The function ComputeRhoStats calls FindAllMaxes $n$ times (and also executes $O(n^2)$ further operations) for a cost of $dn^{d+1}$. The function ComputeAlphaStats takes $O(n^2)$ for the nested for-loops, and (as explained in Section B.1) a further $O(dn^d)$ for the computation of each $q(i, \cdot)$, amounting to $O(dn^{d+1})$ in total.

This completes the proof.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{For each $i, k$, to compute the max (over $c_{i'}$) of the sum of all rows $k' \neq k$, we can (1) compute the max of the sum of all rows within region $\phi(k)$ and (separately) within region $\phi(k)$; (2) adjust each maximum by subtracting the value of row $k$ in region $\phi(k)$ and the value of row $k$ in region $\phi(k)$, respectively; (3) take the larger result.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure6.png}
\caption{Some audio examples from LibriSpeech. From upper to bottom are the waveforms from speaker 1, speaker 2 and the overlapped version of them.}
\end{figure}

\section*{C Baseline Method}

We first obtain a set of $l$ primitive clusters with associated exemplar indices $E \subseteq [n]$. Then we iterate over every possible subset $E \subseteq \hat{E}$; these represent the compositional clusters. For each $E$, we conduct an inner-loop to iterate over every possible 1-to-1 mapping from $\hat{E}$ to the set of compositions of $E \setminus \hat{E}$; these represent the primitive clusters. If we consider compositions of at most $d$ exemplars, then we have

$$\sum_{i=0}^{l} C(l, i) P \left( \sum_{d'=2}^{d} C(l - i, d'), i \right)$$

total possible remappings, where $C(l, i)$ and $P(l, i)$ are the numbers of combinations and permutations of $i$ objects from a set of $l$, respectively. The $P$ arises due to iterating over all 1-to-1 mappings. Note that the number of possible remappings grows factorially with $l$, and hence it quickly becomes intractable as $l$ grows (e.g., for $l = 15$ and $d = 2$, the number of possibilities is $107770296705436$).

\section*{D LibriSpeech}

Figure 6 shows how overlapped data is synthesized from LibriSpeech data.

Speaker embeddings were extracted from mel-frequency cepstrum coefficient (MFCC) features (32 coefficients, 0.025s window size, 0.01s step size) using an embedding function $f_{\text{emb}}$ that contains a 2-layer LSTM with 256 hidden units. Composition function $g$ is defined as $g(x_a, x_b) = W_1 x_a + W_2 x_b$, where $W_1, W_2$ are learnable weights and $x_a, x_b$ are speaker embeddings. $f_{\text{emb}}$ and $g$ were optimized jointly using the method proposed by ?. During training, 15 audio samples from 5 unique speakers (5 labeled with 1 speaker and 10 with 2 speakers) are used to extract reference speaker embeddings using $f_{\text{emb}}$. 20 query speaker embeddings were extracted from the same 5 speakers using $f_{\text{emb}} g$, with audio or audio pairs $\{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{1,1\}, \{2,2\}, \{3,3\}, \{4,4\}, \{5,5\}, \{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}, \{2,3\}, \{2,4\}, \{2,5\}, \{3,4\}, \{3,5\}, \{4,5\}$. The distances between reference embeddings and query embeddings are
computed and the model is optimized using triplet loss so that the distance between a reference-query pair share the same label is smaller than that of other pairs. After training, the model achieves overall accuracy of 86.9% on a validation set where each episode contains 20 queries as above.

After function $f_{emb}$ and $g$ are trained, we selected hyperparameters of clustering methods based on validation set and then tested on test set. Both validation set and test set contain 10 groups of data and all clusters have the same number of samples in each group of data (For example, in the setting of $l = 3$, $n = 120$, there are 6 clusters with labels $\{1\}$, $\{2\}$, $\{3\}$, $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$ and each one has 20 samples). For all methods, hyperparameters are selected for setting $l = 3$ and $l = 5$ (both $n=150$ and $n=495$) separately. For CAP/CAP, AP and AP+Heur, there is only one hyperparameter preference (the diagonal value of negative squared distance matrix). For AC, there is one hyperparameter threshold. For AC+Heur, there are two hyperparameters preference and threshold. In the search of hyperparameters, we make sure that the hyperparameter yields the best result is in the middle of our searching range.

E OmniGlot

Figure 7 shows 4 groups of examples used in the experiment. Each group contains images with cluster labels $\{1\}$, $\{2\}$, $\{3\}$, $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$. Image embedding function $f_{emb}$ is ResNet18 (He et al. 2016), and $g$ is defined the same as in section 4.4. The training procedure is the same as section 4.4. After training, the model achieves overall accuracy of 75.0% on validation set.

After function $f_{emb}$ and $g$ are trained, the hyperparameters are selected in the same way as in LibriSpeech experiment.