## Background

## Data Clustering

- Partition data points into groups such that points in each group are more similar to each other than to points in the other groups.


## Image Clustering

- Traditional methods (e.g. K-means, GMM, DBSCAN, etc..) do not work well with raw images in pixel-space.
- More meaningful data representation is required for effective clustering.


## Deep Clustering

- Solve image representation learning and clustering jointly in a unified framework.


## Unsupervised Clustering Algorithm

- Given images $\left\{x_{i}\right\}_{i=1}^{n}$, fix $n$ targets randomly sampled from a Gaussian Mixture Model:

$$
Y=\left\{y_{i} \mid y_{i} \in \mathbb{R}^{d},\left\|y_{i}\right\|_{2}=1\right\}, \quad|Y|=n
$$

- Learn model $f_{\theta}: X \rightarrow \mathbb{R}^{d}$ and mapping $P:[n] \rightarrow[n]:$

$$
\min _{P, \theta} \frac{1}{n} \sum_{i} \ell\left(f_{\theta}\left(x_{i}\right), y_{P(i)}\right)
$$

## Optimization:

1. Obtain batch of images $b$ and targets $c$
2. Compute $f_{\theta}\left(X_{b}\right)$
3. Compute $\mathrm{P}^{*}$ by minimizing $L$ w.r.t P
4. Compute $\nabla_{\theta} L(\theta)$ using $\mathrm{P}^{*}$
5. Update $\theta \leftarrow \lambda \nabla_{\theta} L(\theta)$
(3) Is solved with the Hungarian algorithm

- Assign clusters by mixture component association:

$$
c_{i}=\operatorname{argmin}_{j \in[k]} \ell\left(f_{\theta}\left(x_{i}\right), \mu_{j}\right)
$$

where $\left\{\mu_{j}\right\}_{j=1}^{k}$ are GMM mean vectors.

## Full Method



Enhance image features, to facilitate a better clustering, by solving an additional auxiliary self-supervised task of predicting image rotations.

## Refinement Stage



In final stage we relax equally sized mixture component assumption. Discard fixed targets, iteratively apply K-means on $f_{\theta}(X)$ and use cluster assignments as pseudo-targets.

## Experimental Results

Clustering results using a ResNet-18 backbone for natural image datasets and a 4-layer CNN for MNIST.

|  | MNIST |  | CIFAR-10 |  | CIFAR-100 |  | STL-10 |  | ImageNet-10 |  | Tiny-ImageNet |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | NMI | ACC | NMI | ACC | NMI | ACC | NMI | ACC | NMI | ACC | NMI | ACC |
| k-means | 0.499 | 0.572 | 0.087 | 0.228 | 0.083 | 0.129 | 0.124 | 0.192 | 0.119 | 0.241 | 0.065 | 0.025 |
| sc | 0.663 | 0.696 | 0.103 | 0.247 | 0.090 | 0.136 | 0.098 | 0.159 | 0.151 | 0.274 | 0.063 | 0.022 |
| AE | 0.725 | 0.812 | 0.239 | 0.313 | 0.100 | 0.164 | 0.249 | 0.303 | 0.210 | 0.317 | 0.131 | 0.041 |
| dec | 0.772 | 0.843 | 0.257 | 0.301 | 0.136 | 0.185 | 0.276 | 0.359 | 0.282 | 0.381 | 0.115 | 0.037 |
| Jule | 0.913 | 0.964 | 0.192 | 0.272 | 0.103 | 0.137 | 0.182 | 0.277 | 0.175 | 0.300 | 0.102 | 0.033 |
| dAC | 0.935 | 0.978 | 0.396 | 0.522 | 0.185 | 0.238 | 0.249 | 0.303 | 0.394 | 0.527 | 0.190 | 0.066 |
| IIC | 0.978 | 0.992 | 0.512 | 0.617 | 0.224 | 0.257 | 0.431 | 0.499 | - |  | - | - |
| DCCM | - | - | 0.496 | 0.623 | 0.285 | 0.327 | 0.376 | 0.482 | 0.608 | 0.710 | 0.224 | 0.108 |
| Ours (avg.) | 0.971 | 0.990 | 0.703 | 0.820 | 0.418 | 0.446 | 0.593 | 0.694 | 0.719 | 0.811 | 0.274 | 0.119 |
| Ours (ste) | $\pm .000$ | $\pm .000$ | $\pm .011$ | $\pm .019$ | $\pm .003$ | $\pm .006$ | $\pm .005$ | $\pm .013$ | $\pm .008$ | $\pm .012$ | $\pm .001$ | $\pm .001$ |
| Ours (best) | 0.973 | 0.991 | 0.720 | 0.843 | 0.423 | 0.464 | 0.609 | 0.741 | 0.732 | 0.830 | 0.277 | 0.121 |

## Image Features Evaluation

Evaluate image features of trained ConvNet using a linear evaluation protocol and by applying K-means.

|  | CIFAR-10 |  |  | CIFAR-100 |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
|  | K-means |  | Linear | K-means |  | Linear |
|  | NMI | ACC | ACC | NMI | ACC | ACC |
| ImNet Labels | 0.321 | 0.407 | 0.782 | 0.247 | 0.281 | 0.646 |
| NAT | 0.044 | 0.162 | 0.315 | 0.037 | 0.095 | 0.177 |
| RotNet | 0.329 | 0.349 | 0.740 | 0.261 | 0.284 | 0.543 |
| NAT+RotNet | 0.413 | $\mathbf{0 . 5 1 1}$ | 0.764 | 0.190 | 0.232 | 0.499 |
| Ours | $\mathbf{0 . 4 2 8}$ | 0.397 | $\mathbf{0 . 8 6 9}$ | $\mathbf{0 . 3 9 5}$ | $\mathbf{0 . 3 4 7}$ | $\mathbf{0 . 6 6 2}$ |

## Ablation Study

- Sobel filters are often used as pre-processing to discourage clustering based on trivial cues such as color
- With a rotation loss this is not only unnecessary, it harms clustering quality.

| Sobel | Rotations | ACC | NMI |
| :---: | :---: | :---: | :---: |
|  |  | 0.492 | 0.428 |
| $\boldsymbol{V}$ |  | 0.560 | 0.463 |
|  | $\boldsymbol{V}$ | $\mathbf{0 . 8 2 0}$ | $\mathbf{0 . 7 0 3}$ |
| $\boldsymbol{\gamma}$ | $\boldsymbol{\gamma}$ | 0.725 | 0.610 |

Experiments on CIFAR-10.

## Summary

- For the clustering of images we desire meaningful and effective representations.
- We propose a clustering framework that trains a ConvNet by learning cluster assignments alongside model parameters by solving a linear assignment problem using the Hungarian algorithm.
- Random image transformations insert prior knowledge of invariance within clusters into model.
- Auxiliary rotation loss is very effective in helping model learn better image features that produce a quality clustering

