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模式分析与机器智能  
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MIT Key Laboratory of  
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# Invariant Information Clustering for Unsupervised Image Classification and Segmentation

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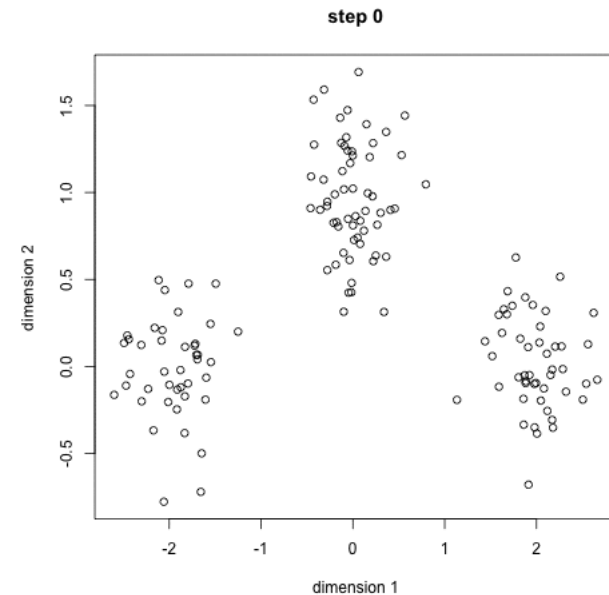
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**ICCV 2019**

- **K-mean**

1. Randomly initialize k center points
2. Each data point is classified by computing the distance between that point and each group center
3. Recompute the group center
4. Repeat 2-3



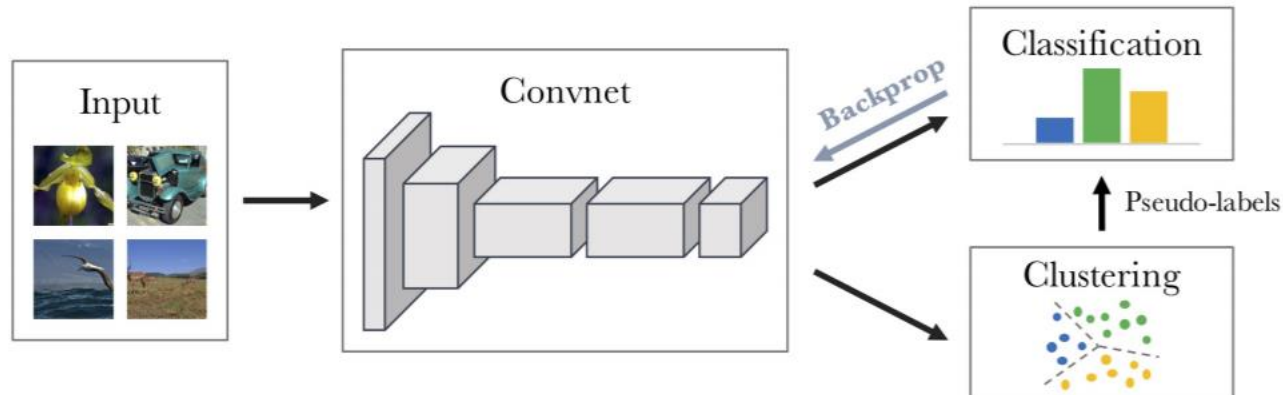
- **Potential Limitations**

- How to decide k center points (k-mean++)
- The curse of dimensionality

# Deep Clustering



- Representation + K-means



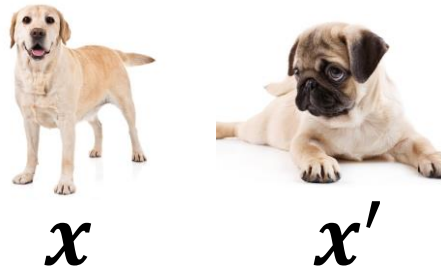
- Representation learning:  $\min_{\theta, W} \frac{1}{N} \sum_{n=1}^N \ell(g_W(f_{\theta}(x_n)), y_n)$
- Clustering:  $\min_{C \in \mathbb{R}^{d \times k}} \frac{1}{N} \sum_{n=1}^N \min_{y_n \in \{0,1\}^k} \|f_{\theta}(x_n) - Cy_n\|_2^2 \quad \text{such that} \quad y_n^T \mathbf{1}_k = 1.$

- Issue of **trivial solutions**

- Empty clusters: An optimal decision boundary is to **assign all of the inputs to a single cluster**.
- Trivial parametrization: If the **vast majority of images is assigned to a few clusters**, the parameters  $\theta$  will exclusively discriminate between them.

# Revisiting Deep Clustering

- How to learn the representation  $\Phi$  ?



For a paired data  $(x, x')$ , we would like to learn a representation  $\phi$  that

- emphasizes their **common information** (the class)
- neglects the **instance-specific information** (pose, ...)

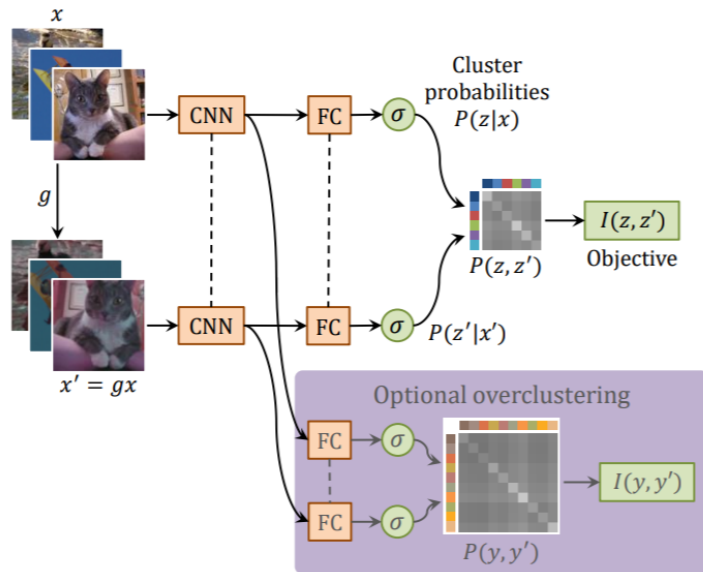
- **Solution:**  $\max_{\Phi} I(\Phi(x), \Phi(x'))$  (mutual information)

$$I(z, z') = H(z) - \boxed{H(z|z')} \quad z = \Phi(x)$$

Instance-specific  
information

# Invariant Information Clustering

- Compute the mutual information  $I(\Phi(\mathbf{x}), \Phi(\mathbf{x}'))$ 
  - The neural network  $\Phi$  is terminated by a softmax layer.



$$P(z = c | \mathbf{x}) = \Phi_c(\mathbf{x})$$

$$\mathbf{P} = \frac{1}{n} \sum_{i=1}^n \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}'_i)^\top \quad (\text{a batch})$$

$$\mathbf{P}_{cc'} = P(z = c, z' = c')$$

$$I(z, z') = I(\mathbf{P}) = \sum_{c=1}^C \sum_{c'=1}^C \mathbf{P}_{cc'} \cdot \ln \frac{\mathbf{P}_{cc'}}{\mathbf{P}_c \cdot \mathbf{P}_{c'}}.$$

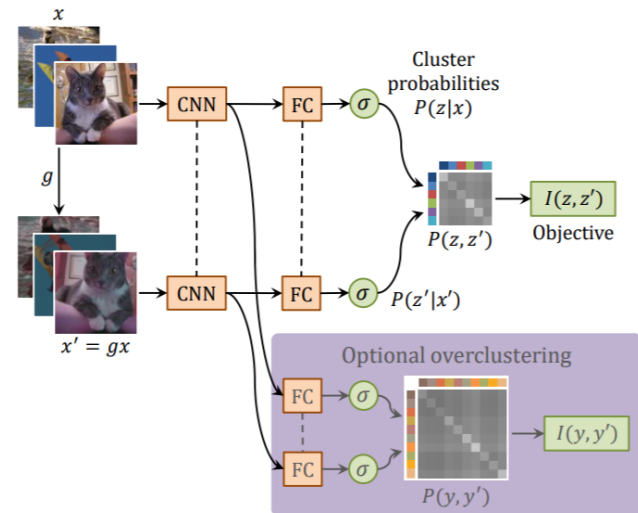
$$I(X; Y) = \sum_{u \in \mathcal{Y}} \sum_{x \in \mathcal{X}} p(x, y) \log \left( \frac{p(x, y)}{p(x) p(y)} \right).$$

- Why degenerate solutions are avoided.
  - If all samples are assigned to a single cluster,  $H(z)$  is not maximized.

# Implementation

- Use generated image pairs, consisting of image  $x$  and its randomly perturbed version.

$$\max_{\Phi} I(\Phi(\mathbf{x}), \Phi(g\mathbf{x}))$$



- Auxiliary overclustering
  - Add an auxiliary overclustering head to deal with distractor classes
  - STL-10
    - 500 training + 800 testing images per class
    - 100  $k$  unlabeled images (with distractor classes)

# Experiments



- Unsupervised learning analysis

|                              | STL10               | CIFAR10            | CFR100-20           | MNIST               |
|------------------------------|---------------------|--------------------|---------------------|---------------------|
| Random network               | 13.5                | 13.1               | 5.93                | 26.1                |
| K-means [53]†                | 19.2                | 22.9               | 13.0                | 57.2                |
| Spectral clustering [49]     | 15.9                | 24.7               | 13.6                | 69.6                |
| Triples [46]‡                | 24.4                | 20.5               | 9.94                | 52.5                |
| AE [5]‡                      | 30.3                | 31.4               | 16.5                | 81.2                |
| Sparse AE [40]‡              | 32.0                | 29.7               | 15.7                | 82.7                |
| Denoising AE [48]‡           | 30.2                | 29.7               | 15.1                | 83.2                |
| Variational Bayes AE [34]‡   | 28.2                | 29.1               | 15.2                | 83.2                |
| SWWAE 2015 [54]‡             | 27.0                | 28.4               | 14.7                | 82.5                |
| GAN 2015 [45]‡               | 29.8                | 31.5               | 15.1                | 82.8                |
| JULE 2016 [52]               | 27.7                | 27.2               | 13.7                | 96.4                |
| DEC 2016 [51]†               | 35.9                | 30.1               | 18.5                | 84.3                |
| DAC 2017 [8]                 | 47.0                | 52.2               | 23.8                | 97.8                |
| DeepCluster 2018 [7]† ‡      | 33.4★               | 37.4★              | 18.9★               | 65.6 ★              |
| ADC 2018 [24]                | 53.0                | 32.5               | 16.0★               | 99.2                |
| IIC (lowest loss sub-head)   | <b>59.6</b>         | <b>61.7</b>        | <b>25.7</b>         | <b>99.2</b>         |
| IIC (avg sub-head $\pm$ STD) | 59.8<br>$\pm 0.844$ | 57.6<br>$\pm 5.01$ | 25.5<br>$\pm 0.462$ | 98.4<br>$\pm 0.652$ |

|                                 | STL10       |
|---------------------------------|-------------|
| No auxiliary overclustering     | 43.8        |
| Single sub-head ( $h = 1$ )     | 57.6        |
| No sample repeats ( $r = 1$ )   | 47.0        |
| Unlabelled data segment ignored | 49.9        |
| Full setting                    | <b>59.6</b> |

Table 1: **Unsupervised image clustering.** Legend: †Method based on k-means. ‡Method that does not directly learn a clustering function and requires further application of k-means to be used for image clustering. ★Results obtained using our experiments with authors' original code.

# Experiments



- Unsupervised learning analysis

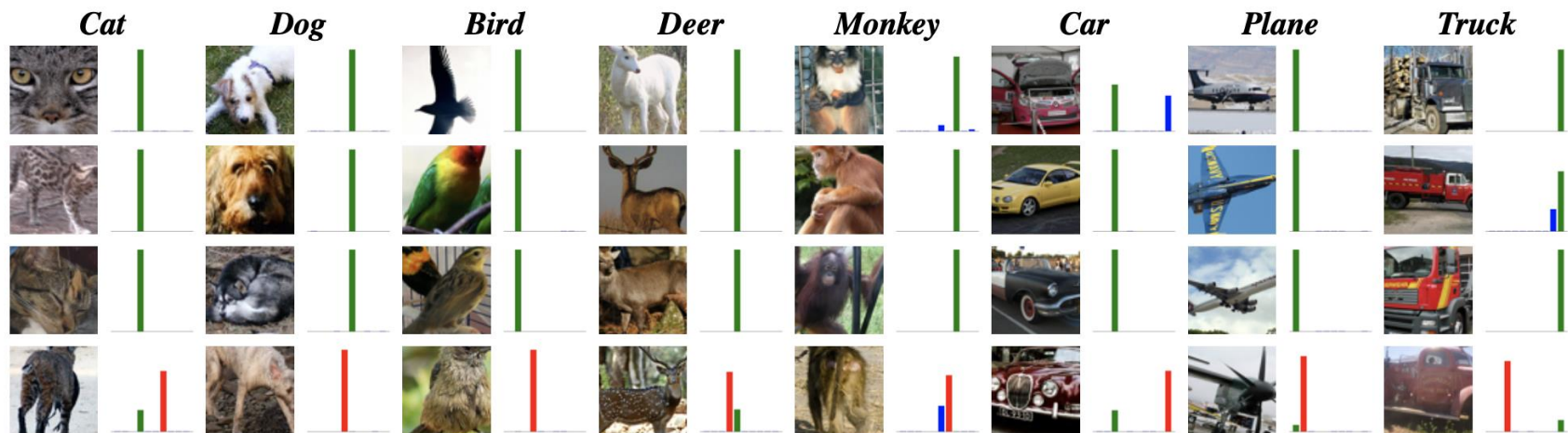


Figure 5: **Unsupervised image clustering (IIC) results on STL10.** Predicted cluster probabilities from the best performing head are shown as bars. Prediction corresponds to tallest, ground truth is green, incorrectly predicted classes are red, and all others are blue. The bottom row shows failure cases.

# Experiments

- Semi-supervised learning analysis

|                        | STL10       |
|------------------------|-------------|
| Dosovitskiy 2015 [18]† | 74.2        |
| SWWAE 2015 [54]†       | 74.3        |
| Dundar 2015 [19]       | 74.1        |
| Cutout* 2017 [15]      | 87.3        |
| Oyallon* 2017 [42]†    | 76.0        |
| Oyallon* 2017 [42]     | 87.6        |
| DeepCluster 2018 [7]   | 73.4★       |
| ADC 2018 [24]          | 56.7★       |
| DeepINFOMAX 2018 [27]  | 77.0        |
| IIC plus finetune†     | <b>79.2</b> |
| IIC plus finetune      | <b>88.8</b> |

Table 3: **Fully and semi-supervised classification.** Legend: \*Fully supervised method. ★Our experiments with authors' code. †Multi-fold evaluation.

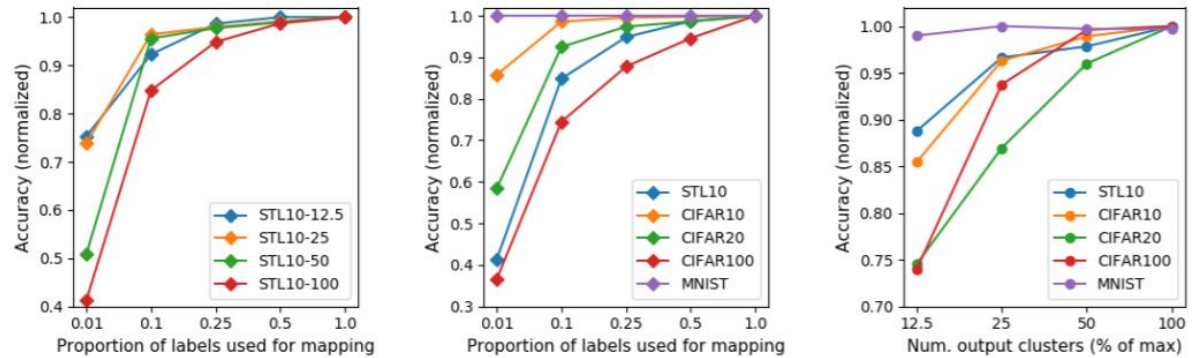


Figure 6: **Semi-supervised overclustering.** Training with IIC loss to overcluster ( $k > k_{gt}$ ) and using labels for evaluation mapping only. Performance is robust even with 90%-75% of labels discarded (left and center). STL10- $r$  denotes networks with output  $k = \lceil 1.4r \rceil$ . Overall accuracy improves with the number of output clusters  $k$  (right). For further details see supplementary material.

$$k = \lceil 1.4r \rceil$$

# Experiments

- Semi-supervised learning analysis

|              | STL10 |             | CIFAR10 |             | CIFAR100-20 |             | CIFAR100 |             | MNIST |             |
|--------------|-------|-------------|---------|-------------|-------------|-------------|----------|-------------|-------|-------------|
| % of max $k$ | $k$   | ACC         | $k$     | ACC         | $k$         | ACC         | $k$      | ACC         | $k$   | ACC         |
| 100          | 140   | <b>63.1</b> | 140     | <b>65.0</b> | 280         | <b>34.7</b> | 1000     | <b>20.3</b> | 100   | 98.6        |
| 50           | 70    | 61.4        | 70      | 62.2        | 140         | 33.1        | 500      | 20.3        | 50    | 98.6        |
| 25           | 35    | 59.7        | 35      | 60.5        | 70          | 30.0        | 250      | 19.1        | 25    | <b>98.7</b> |
| 12.5         | 18    | 54.8        | 18      | 53.7        | 35          | 25.7        | 125      | 15.0        | 13    | 97.9        |

Table 3: Absolute accuracy for semi-supervised overclustering experiments in paper fig. 6-right.

| STL10        | 1.0   |             | 0.5   |             | 0.25  |             | 0.1   |             | 0.01  |             |
|--------------|-------|-------------|-------|-------------|-------|-------------|-------|-------------|-------|-------------|
| % of max $k$ | $n_a$ | ACC         | $n_a$ | ACC         | $n_a$ | ACC         | $n_a$ | ACC         | $n_a$ | ACC         |
| 100          | 5000  | <b>63.1</b> | 2500  | <b>61.0</b> | 1250  | 58.6        | 500   | 52.4        | 50    | 25.5        |
| 50           | 5000  | 61.4        | 2500  | 59.8        | 1250  | <b>59.1</b> | 500   | <b>57.8</b> | 50    | 30.7        |
| 25           | 5000  | 59.7        | 2500  | 59.2        | 1250  | 58.5        | 500   | 57.6        | 50    | <b>44.1</b> |
| 12.5         | 5000  | 54.8        | 2500  | 54.8        | 1250  | 54.1        | 500   | 50.6        | 50    | 41.3        |

|             | 1.0   |             | 0.5   |      | 0.25  |      | 0.1   |      | 0.01  |      |
|-------------|-------|-------------|-------|------|-------|------|-------|------|-------|------|
|             | $n_a$ | ACC         | $n_a$ | ACC  | $n_a$ | ACC  | $n_a$ | ACC  | $n_a$ | ACC  |
| STL10       | 5000  | <b>63.1</b> | 2500  | 61.0 | 1250  | 58.6 | 500   | 52.4 | 50    | 25.5 |
| CIFAR10     | 50000 | <b>62.9</b> | 25000 | 62.7 | 12500 | 62.6 | 5000  | 62.0 | 500   | 53.9 |
| CIFAR100-20 | 50000 | <b>34.5</b> | 25000 | 34.0 | 12500 | 33.6 | 5000  | 31.9 | 500   | 20.1 |
| CIFAR100    | 50000 | <b>20.3</b> | 25000 | 19.2 | 12500 | 17.9 | 5000  | 15.1 | 500   | 7.43 |
| MNIST-25    | 60000 | <b>98.9</b> | 30000 | 98.9 | 15000 | 98.9 | 6000  | 98.9 | 600   | 98.9 |

Table 4: Absolute accuracy for semi-supervised overclustering experiments in paper fig. 6-left (top) and fig. 6-center (bottom).  $n_a$  denotes number of labels used to find mapping from output  $k$  to  $k_{gt}$  for evaluation.

# Experiments



- Unsupervised and semi-supervised segmentation

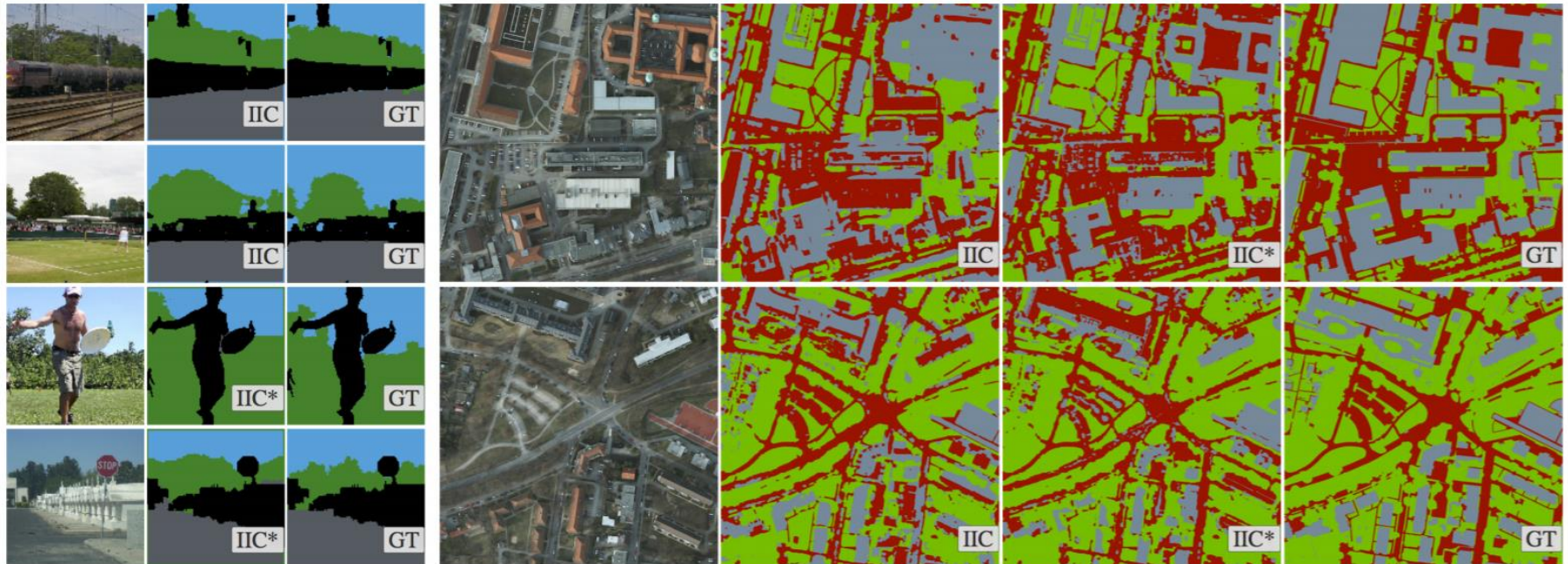


Figure 7: **Example segmentation results (un- and semi-supervised).** Left: COCO-Stuff-3 (non-stuff pixels in black), right: Potsdam-3. Input images, IIC (fully unsupervised segmentation) and IIC\* (semi-supervised overclustering) results are shown, together with the ground truth segmentation (GT).

# Experiments



- Unsupervised and semi-supervised segmentation

|                                     | COCO-Stuff-3 | COCO-Stuff  | Potsdam-3   | Potsdam     |
|-------------------------------------|--------------|-------------|-------------|-------------|
| Random CNN                          | 37.3         | 19.4        | 38.2        | 28.3        |
| K-means [44] <sup>†</sup>           | 52.2         | 14.1        | 45.7        | 35.3        |
| SIFT [39] <sup>‡</sup>              | 38.1         | 20.2        | 38.2        | 28.5        |
| Doersch 2015 [17] <sup>‡</sup>      | 47.5         | 23.1        | 49.6        | 37.2        |
| Isola 2016 [30] <sup>‡</sup>        | 54.0         | 24.3        | 63.9        | 44.9        |
| DeepCluster 2018 [7] <sup>† ‡</sup> | 41.6         | 19.9        | 41.7        | 29.2        |
| IIC                                 | <b>72.3</b>  | <b>27.7</b> | <b>65.1</b> | <b>45.4</b> |

Table 4: **Unsupervised segmentation.** IIC experiments use a single sub-head. Legend: <sup>†</sup>Method based on k-means. <sup>‡</sup>Method that does not directly learn a clustering function and requires further application of k-means to be used for image clustering.



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