CSC 311: Introduction to Machine Learning

Lecture 11 - K-Means and EM Algorithm

Michael Zhang Chandra Gummaluru

University of Toronto, Winter 2023

Outline

Final Exam

- 3 hours.
- One double-sided aid sheet, created by yourself.
- Cumulative up to k-means, with emphasis on post-midterm topics.
- Past exams posted and two review sessions next week. Upvote conceptual questions others have asked.
- Slides, recordings, office hours.

Tuesday 4-5pm Ba 1170

linear algebra
calculus
probl/stats

discriminative
midterm
- kNN
- decision trees
- linear regression
- classification (logistic regression)
- neural networks

generative
- probabilistic modeling — MLE
  - choose params to maximize likelihood of dataset
  - MAP
    - MLE + prior on parameters
- Gaussians
  - eigenvectors
  - values
  - Gaussian Discriminant Analysis

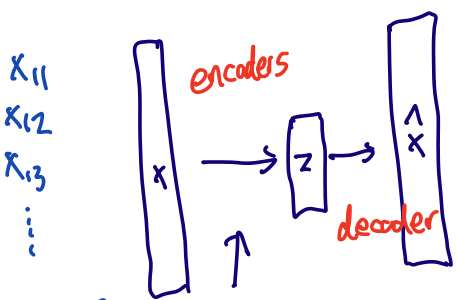
unsupervised
- PCA
- ethics
- k-means + RL

data → model

↘ ↙

optimization problem

autoencoders : NNs for compression



$\min (\hat{x} - x)^2$

reconstruction error

$\sum_i \sum_j (x_{ij} - \hat{x}_{ij})^2$

1 linear layer

many linear/nonlinear layers

If you just use a linear layer $\xrightarrow{\text{optimum}}$ equivalent to PCA

VAE variational — minimizing reconstruction error + similarity term between z and $N(0, I)$

Feedback

generative model

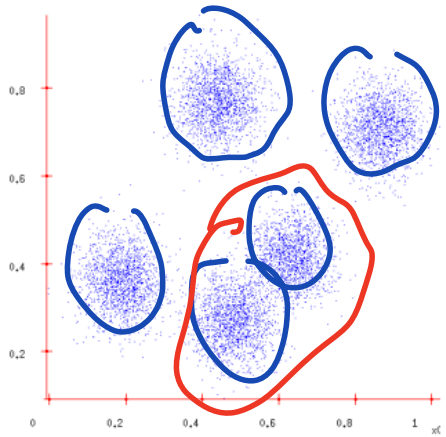
- Please take some time to fill out the course feedback form.
- The main changes we made to the past iteration were adding the Math Diagnostic and an open-ended project option. We also made tutorials more problem-solving oriented.
- Helpful for us to hear what supports your learning.
- Feel free to write to the course email if you have more detailed thoughts.

Overview

- In the previous lecture, we covered PCA, Autoencoders and Matrix Factorization—all unsupervised learning algorithms.
  - Each algorithm can be used to approximate high dimensional data using some lower dimensional form.
- Those methods made an interesting assumption that data depends on some latent variables that are never observed. Such models are called latent variable models.
  - For PCA, these correspond to the code vectors (representation).
- Today:
  - K-means, a simple algorithm for clustering, i.e. grouping data points into clusters
  - Reformulate clustering as a latent variable model and apply the EM algorithm

Clustering

- Sometimes the data form clusters, where samples within a cluster are similar to each other, and samples in different clusters are dissimilar:
- Such a distribution is multimodal, since it has multiple modes, or regions of high probability mass.



ex: embedding documents

- Clustering: grouping data points into clusters, with no observed labels. It is an unsupervised learning technique.
- E.g. clustering machine learning papers based on topic (deep learning, Bayesian models, etc.) But topics are never observed (unsupervised).

K-means Intuition

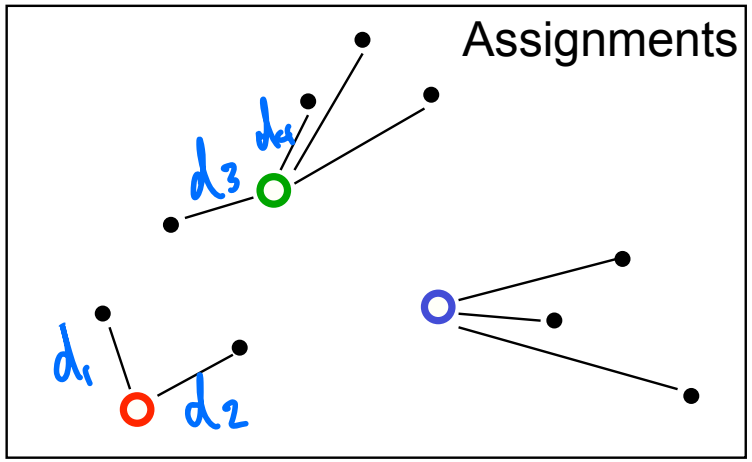
There are k clusters, and each point is close to its cluster center, or mean (the mean of points in the cluster).

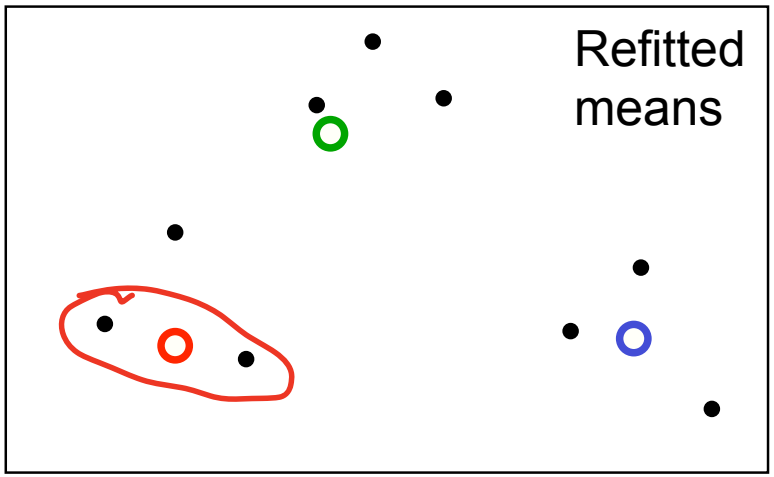
How do we compute the cluster assignments?

- Given the cluster assignments, we could easily compute the cluster centers.
- Given the cluster centers, we could easily compute the cluster assignments.
- Chicken and egg problem!
- Simple heuristic - start randomly and alternate between the two!

K-Means

- Randomly initialize cluster centers
- Alternate between two steps:
  - Assignment step: Assign each data point to the closest cluster
  - Refitting step: Move each cluster center to the mean of its members.





$d_1^2 + d_2^2 + \ldots$

K-Means Example

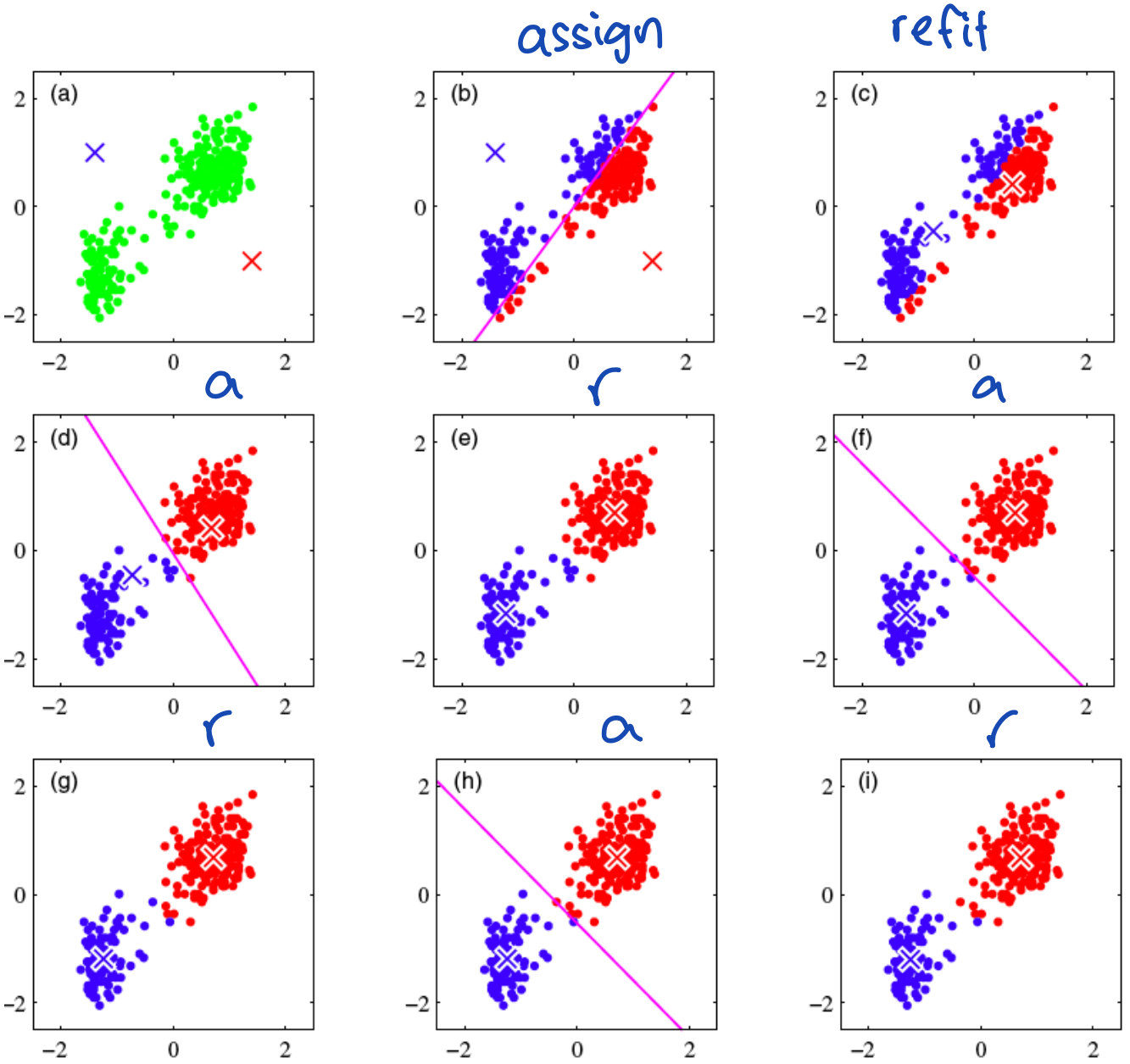


Figure from Bishop

Simple demo: http://syskall.com/kmeans.js/

What is K-means Optimizing?

$x \in \mathbb{R}^d$ $m \in \mathbb{R}^d$ n different r vectors $r^{(n)} \in \mathbb{R}^K$

K-means Objective:
Find cluster centers $\mathbf{m}$ and assignments $\mathbf{r}$ to minimize the sum of squared distances of data points $\{\mathbf{x}^{(n)}\}$ to their assigned cluster centers

$$\min_{\{\mathbf{m}\},\{\mathbf{r}\}} J(\{\mathbf{m}\},\{\mathbf{r}\}) = \min_{\{\mathbf{m}\},\{\mathbf{r}\}} \sum_{n=1}^{N}\sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

$$\text{s.t.} \sum_k r_k^{(n)} = 1, \forall n, \quad \text{where } r_k^{(n)} \in \{0,1\}, \forall k, n$$

datapoints

where $r_k^{(n)} = 1$ means that $\mathbf{x}^{(n)}$ is assigned to cluster k (with center $\mathbf{m}_k$)

- Finding the exact optimum can be shown to be NP-hard.
- K-means can be seen as block coordinate descent on this objective (analogous to ALS for matrix completion)
  - Assignment step = minimize w.r.t. $\{r_k^{(n)}\}$
  - Refitting step = minimize w.r.t. $\{\mathbf{m}_k\}$

Alternating Minimization

Optimization problem:

fixed the centers
=> easy to minimize the loss for each point

$$\min_{\{\mathbf{m}_k\},\{\mathbf{r}^{(n)}\}} \sum_{n=1}^{N}\sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

If we fix the centers $\{\mathbf{m}_k\}$ then we can easily find the optimal assignments $\{\mathbf{r}^{(n)}\}$ for each sample n

$$\min_{\mathbf{r}^{(n)}} \sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

np.argmin

Assign each point to the cluster with the nearest center

$$r_k^{(n)} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{m}_j - \mathbf{x}^{(n)}\|^2 \\ 0 & \text{otherwise} \end{cases}$$

E.g. if $\mathbf{x}^{(n)}$ is assigned to cluster $\hat{k}$,

$$\mathbf{r}^{(n)} = \underbrace{[0, 0, ..., 1, ..., 0]^\top}_{\text{Only } \hat{k}\text{-th entry is 1}}$$

Alternating Minimization

fix the points (and their associated centers)

Likewise, if we fix the assignments $\{\mathbf{r}^{(n)}\}$ then can easily find optimal centers $\{\mathbf{m}_k\}$

np.mean

update m_k => pick the average of all points assigned to center

$$0 = \frac{\partial}{\partial \mathbf{m}_l} \sum_{n=1}^{N} \sum_{k=1}^{K} r_k^{(n)} ||\mathbf{m}_k - \mathbf{x}^{(n)}||^2$$

$$= 2 \sum_{n=1}^{N} r_l^{(n)} (\mathbf{m}_l - \mathbf{x}^{(n)}) \implies \mathbf{m}_l = \frac{\sum_n r_l^{(n)} \mathbf{x}^{(n)}}{\sum_n r_l^{(n)}}$$

look at the points assigned to m_l

K-Means simply alternates between minimizing w.r.t. assignments and centers. This is an instance of alternating minimization, or block coordinate descent.

monotonically decreasing sequence that is bounded below => converges

sequence: k-means loss

The K-means Algorithm

① bounded ≥ 0

② monotonic sequence

→ both update steps do not increase the loss

- Initialization: Set K cluster means $\mathbf{m}_1, \ldots, \mathbf{m}_K$ to random values
- Repeat until convergence (until assignments do not change):
  - Assignment (Optimize w.r.t $\{\mathbf{r}\}$)
    Each data point $\mathbf{x}^{(n)}$ assigned to nearest center.

$$r_k^{(n)} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{m}_j - \mathbf{x}^{(n)}\|^2 \\ 0 & \text{otherwise} \end{cases}$$

  - Refitting (Optimize w.r.t. $\{\mathbf{m}\}$)
    Each center is set to mean of data assigned to it.

$$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}.$$

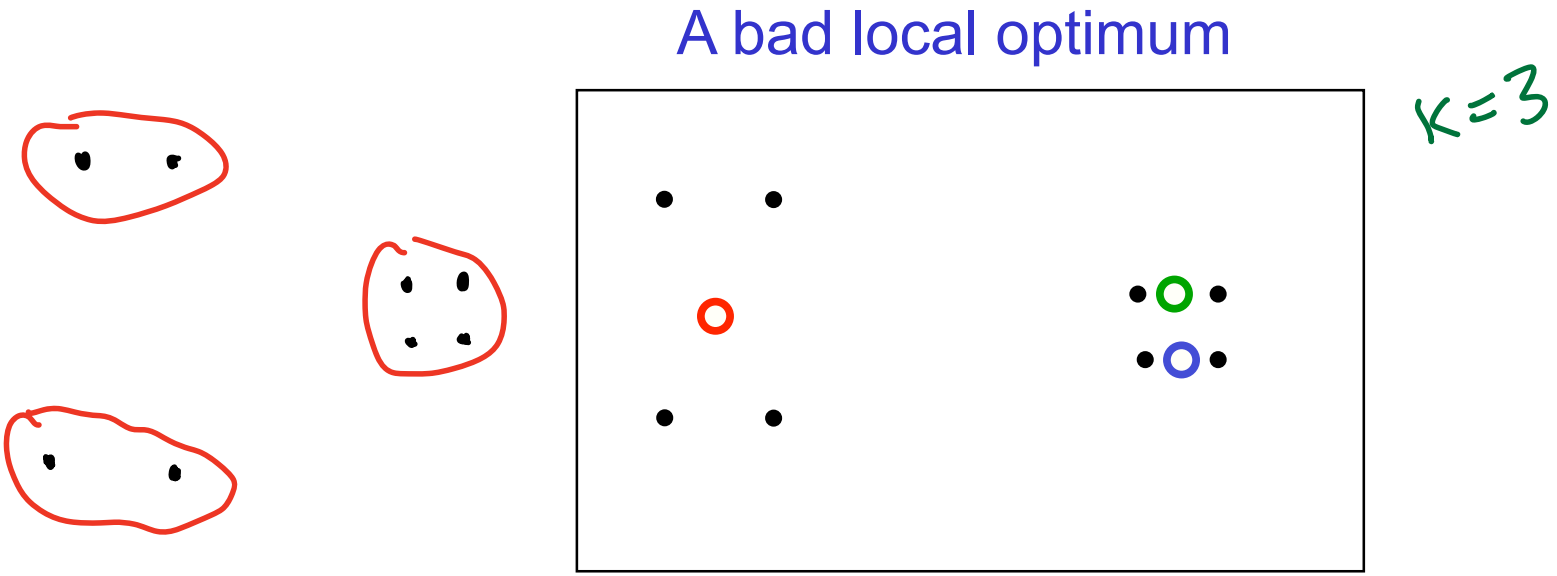
coordinate descent

Why K-means Converges

- K-means algorithm reduces the cost at each iteration.
- If the assignments do not change in the assignment step, we have converged (to at least a local minimum).
- Convergence will happen after a finite number of iterations, since the number of possible cluster assignments is finite

Local Minima

- The objective J is non-convex.
- Coordinate descent on J is not guaranteed to converge to the global minimum.
- Nothing prevents k-means getting stuck at local minima.
- We could try many random starting points



K-means for Vector Quantization

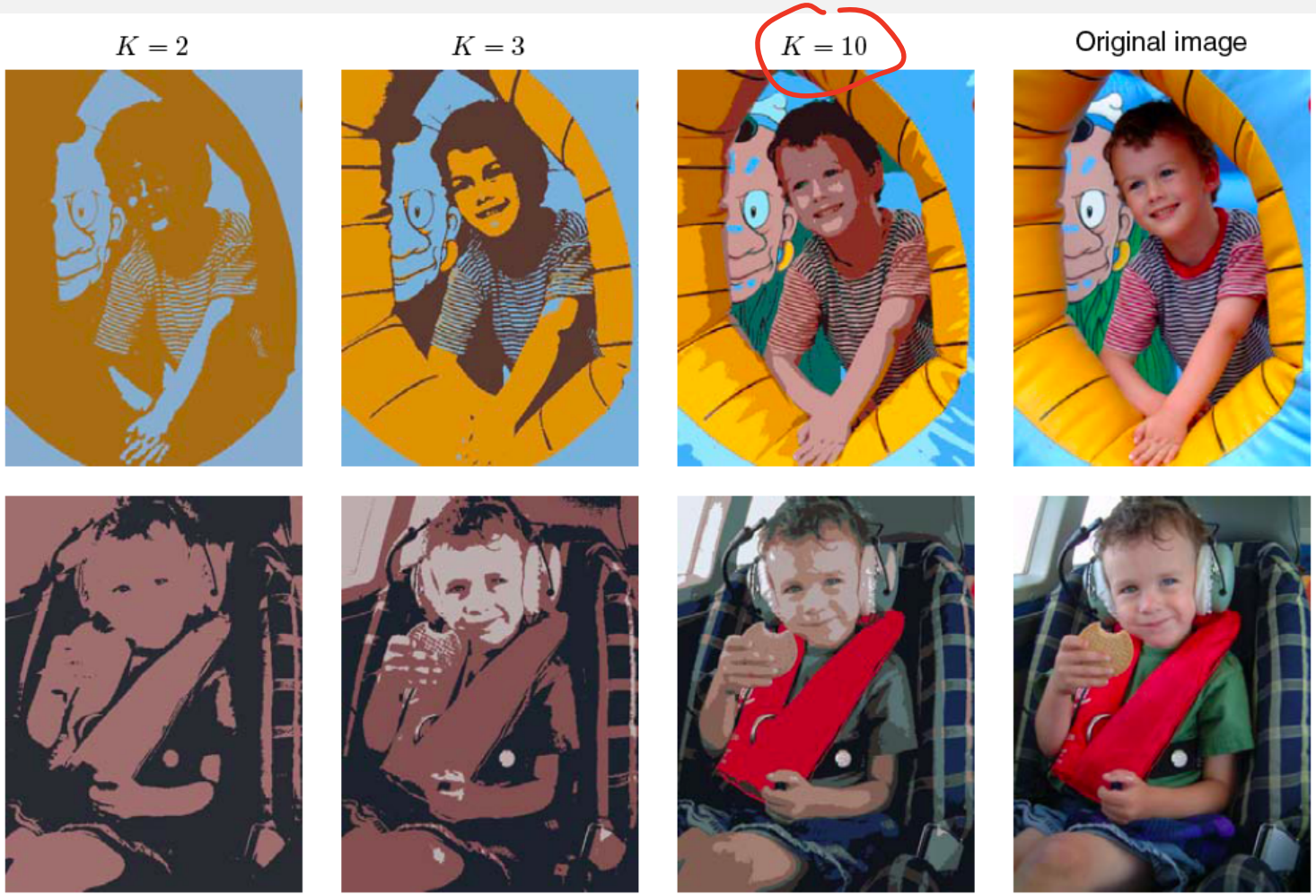
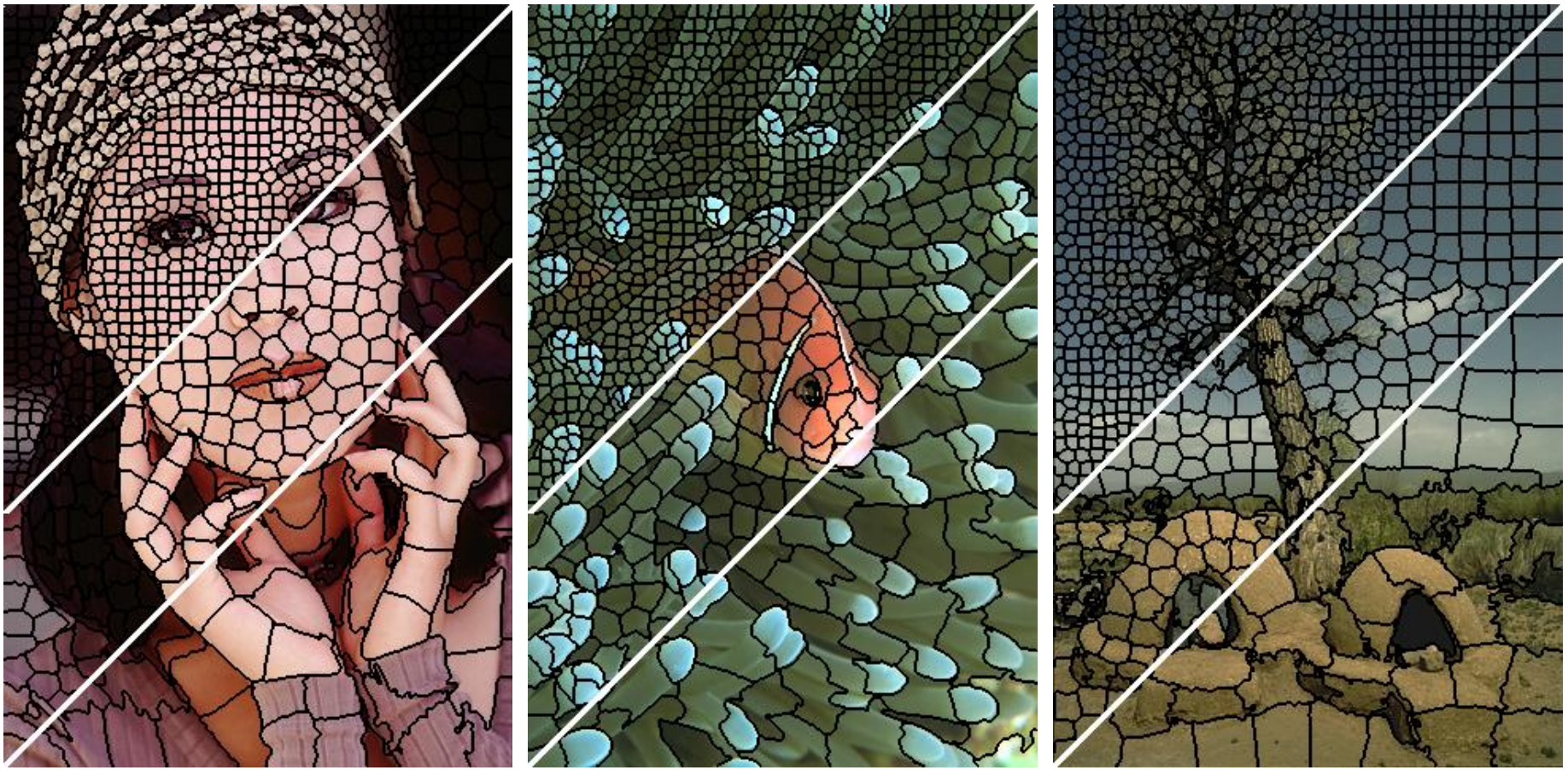


Figure from Bishop

- Given image, construct "dataset" of pixels represented by their RGB pixel intensities
- Run k-means, replace each pixel by its cluster center
-

K-means for Image Segmentation



- Given image, construct "dataset" of pixels, represented by their RGB pixel intensities and grid locations
- Run k-means (with some modifications) to get superpixels

Soft K-means

deep Bayesian learning

is it deep learning or Bayesian learning?

- Instead of making hard assignments of data points to clusters, we can make soft assignments.
- For example, one cluster may have a responsibility of .7 for a datapoint and another may have a responsibility of .3.
- This allows a cluster to use more information about the data in the refitting step.
- How do we decide on the soft assignments?
- We already saw this in multi-class classification: 1-of-K encoding vs softmax assignments.

Soft K-means Algorithm

rather than r be 1-hot,

- Initialization: Set K means $\{\mathbf{m}_k\}$ to random values — softer version of r_s
- Repeat until convergence (measured by how much J changes):
  - Assignment: Each data point n given soft "degree of assignment" to each cluster mean k, based on responsibilities

$\beta \to \infty$ k-means algorithm

$$r_k^{(n)} = \frac{\exp[-\beta \|\mathbf{m}_k - \mathbf{x}^{(n)}\|^2]}{\sum_j \exp[-\beta \|\mathbf{m}_j - \mathbf{x}^{(n)}\|^2]}$$

β: temperature

$\beta \to 0$ uniform dist.

$$\implies \mathbf{r}^{(n)} = \text{softmax}(-\beta\{\|\mathbf{m}_k - \mathbf{x}^{(n)}\|^2\}_{k=1}^K)$$

  - Refitting: Cluster centers are adjusted to match sample means of datapoints they are responsible for:

$$\mathbf{m}_k = \frac{\sum_n r_k^{(n)} \mathbf{x}^{(n)}}{\sum_n r_k^{(n)}}$$

weighted average

Questions about Soft K-means

Some remaining issues

- How to set β?
- Clusters with unequal weight and width?

GMM fixes some of the issues

These aren't straightforward to address with K-means.
Instead, we'll reformulate clustering using a generative model.
As $\beta \to \infty$, soft k-Means becomes k-Means! (Exercise)