CS 446/ECE 449: Machine Learning

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K-Means Clustering

Goals of this lecture

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- Understanding clustering concept

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- Getting to know k-Means

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Reading material:

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- Understanding clustering concept
- Getting to know k-Means

Reading material:

- K. Murphy; Machine Learning: A Probabilistic Perspective; Chapter 11

Recap: Semantic Image Segmentation

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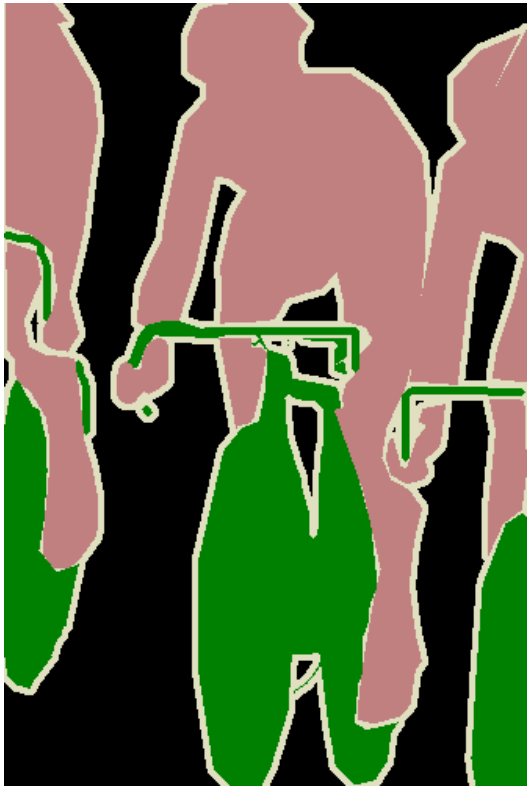

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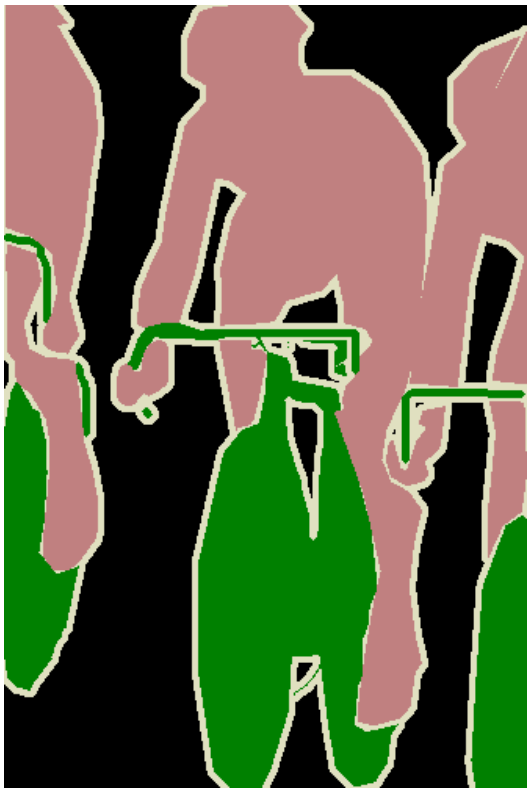

How did we do it?

What if we don't have labels?

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Image

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Image Intensities

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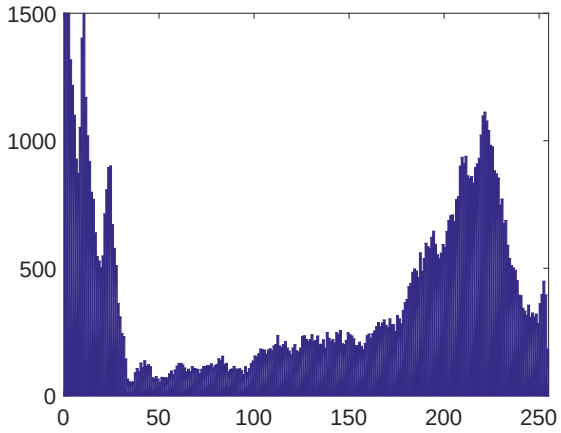

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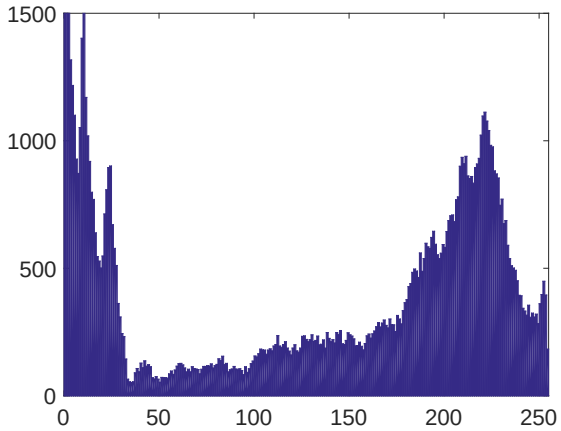

Clustering

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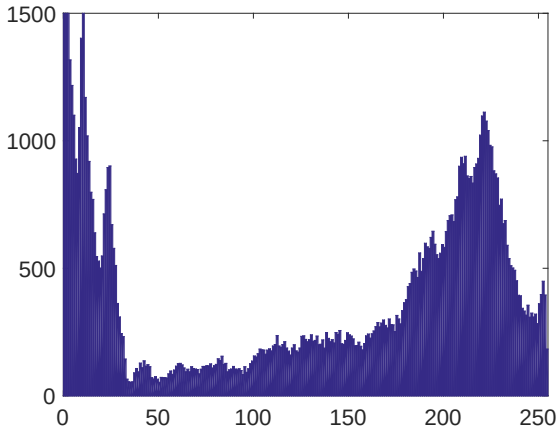

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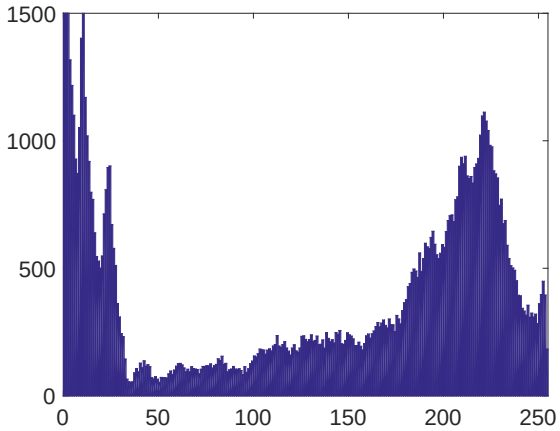

Clustering

Group perceptually or according to another metric similar regions

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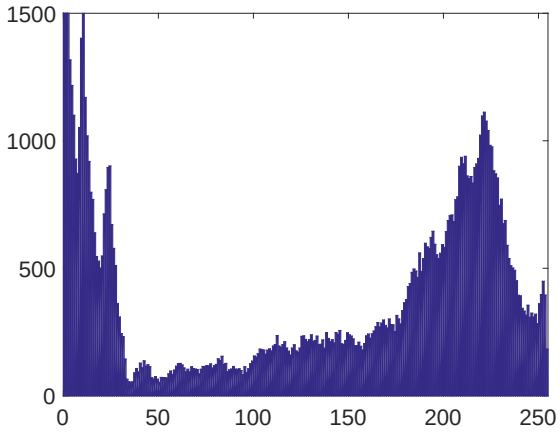

Clustering

Group perceptually or according to another metric similar regions

How can we do it?

kMeans/Lloyd's Algorithm (informal):

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- Initialize: pick K random points as cluster centers μ_k

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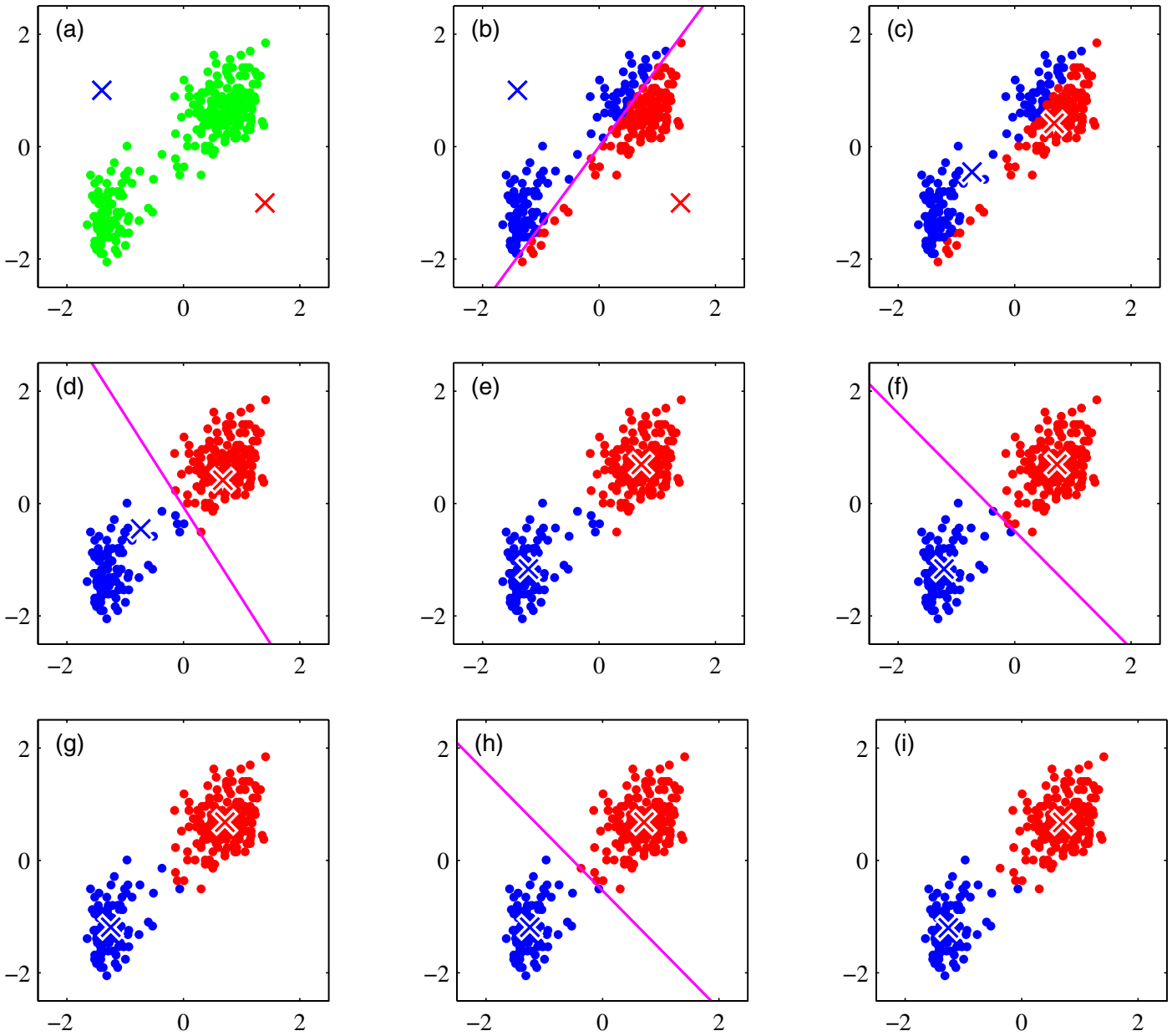
  - Stopping criterion: when no points' assignments change

2D Example:



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What cost function does kMeans optimize?

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$$\min_{\mu} \min_{r} \sum_{i \in \mathcal{D}} \sum_{k=1}^{K} \frac{1}{2} r_{ik} \|x^{(i)} - \mu_k\|_2^2 \quad \text{s.t.} \quad \begin{cases} r_{ik} \in \{0, 1\} & \forall i, k \\ \sum_{k=1}^{K} r_{ik} = 1 & \forall i \end{cases}$$

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What does the constraint remind us of?

How to optimize this cost function?

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$$\nabla_{\mu_k}: \qquad \sum_{i \in \mathcal{D}} r_{ik}(x^{(i)} - \mu_k) = 0$$

$$\mu_k = \frac{\sum_{i \in \mathcal{D}} r_{ik} x^{(i)}}{\sum_{i \in \mathcal{D}} r_{ik}}$$

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- Evaluation

kMeans++: How to initialize kMeans

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kMeans++: How to initialize kMeans

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Try multiple initializations and choose the best

Distance measure:

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- Euclidean (most commonly used)

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- Non-linear (via Kernels): $\phi(x^{(i)})$

How to evaluate clusters?

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- Generative: How well are points reconstructed from the clusters

Distortion

How to evaluate clusters?

- Generative: How well are points reconstructed from the clusters

  Distortion
- Discriminative: How well do the clusters correspond to labels

  Purity

Applications

Applications

- Clustering

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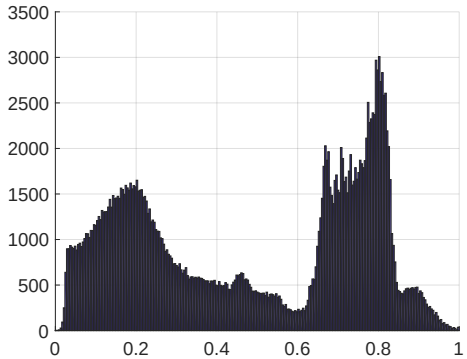
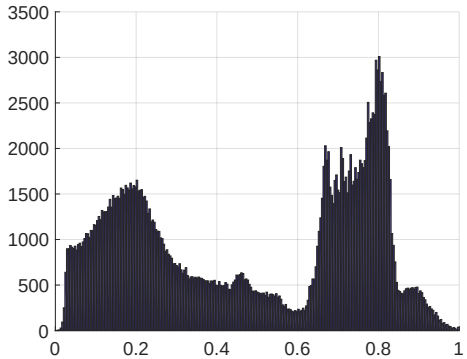
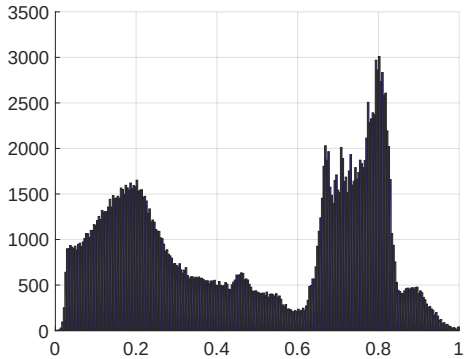
- Clustering
- Super-pixel segmentation


3500
3000
2500
2000
1500
1000
500
0
0
0.2
0.4
0.6
0.8
1



- Grayscale $x^{(i)} \in \mathbb{R}$



2 clusters 3 clusters

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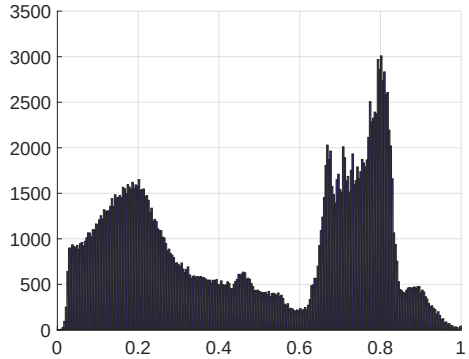

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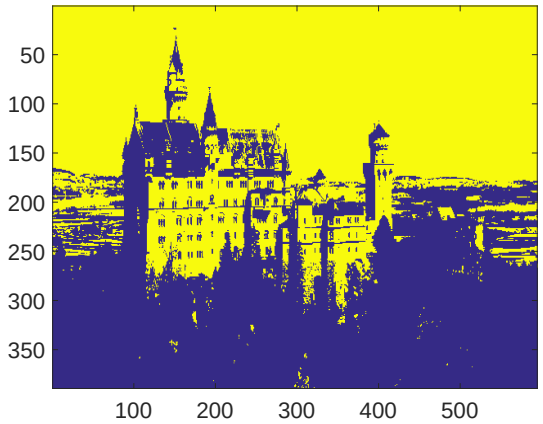

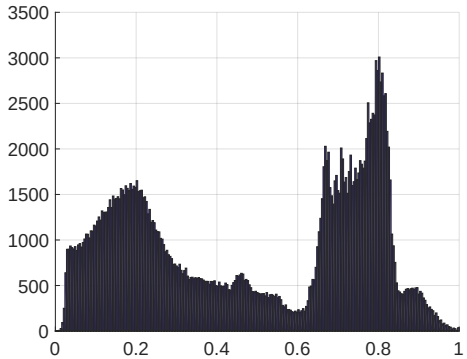

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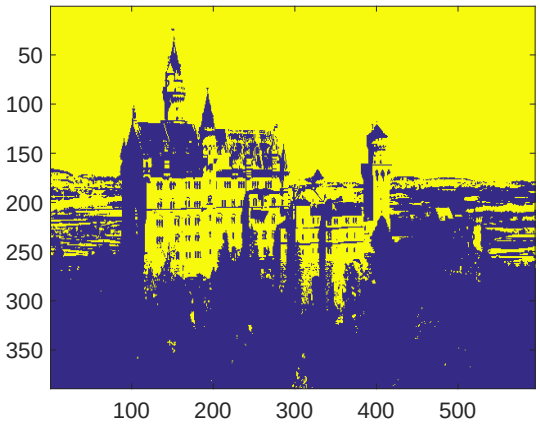

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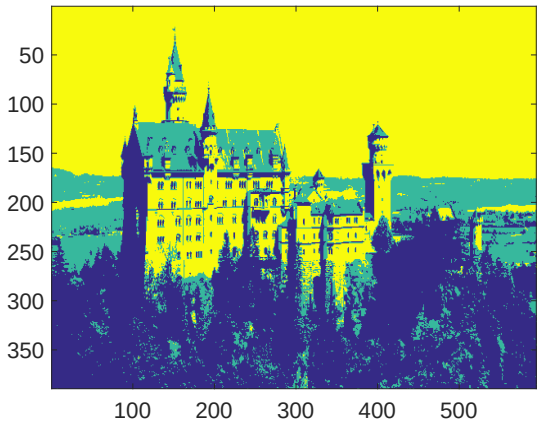

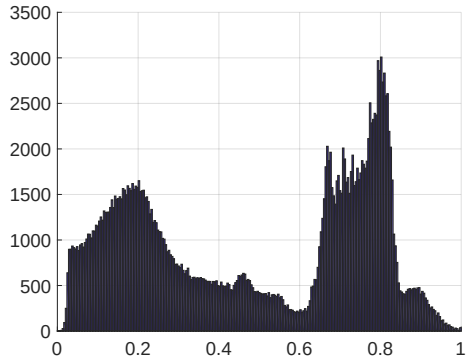

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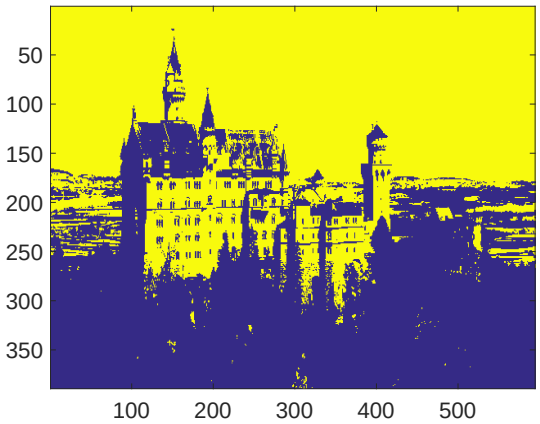

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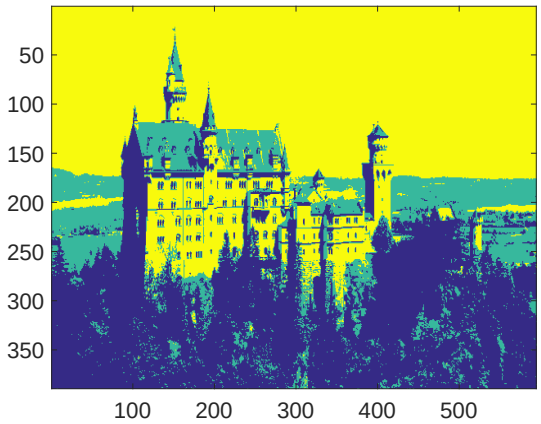
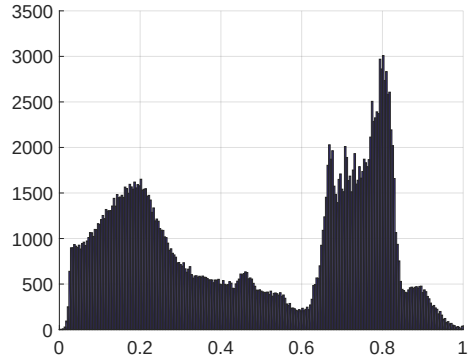
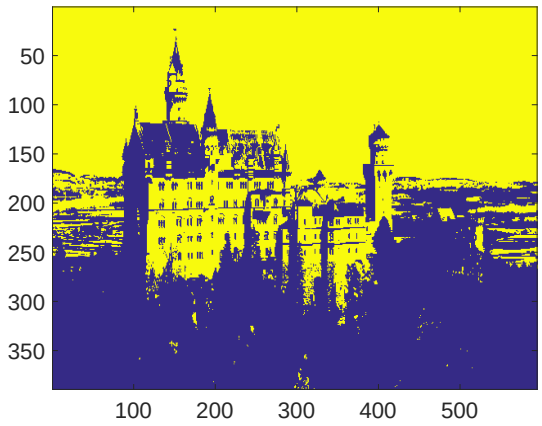
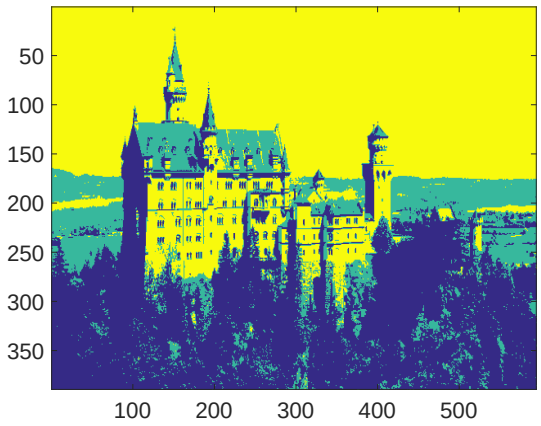


- Color space $x^{(i)} \in \mathbb{R}^3$



- Grayscale $x^{(i)} \in \mathbb{R}$ 2 clusters 3 clusters





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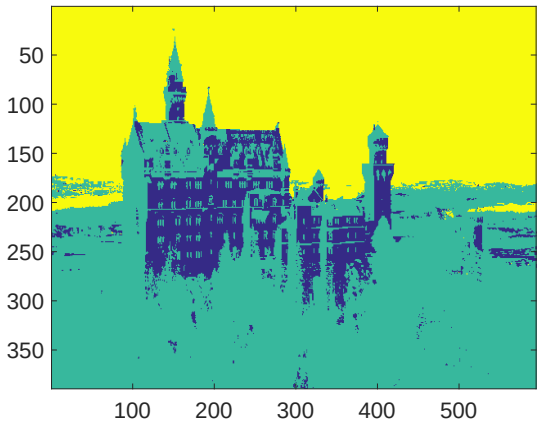

How to obtain spatial smoothness?

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Augment the feature space $\phi(x^{(i)})$ to contain spatial coordinates in addition to intensities

Superpixel segmentation

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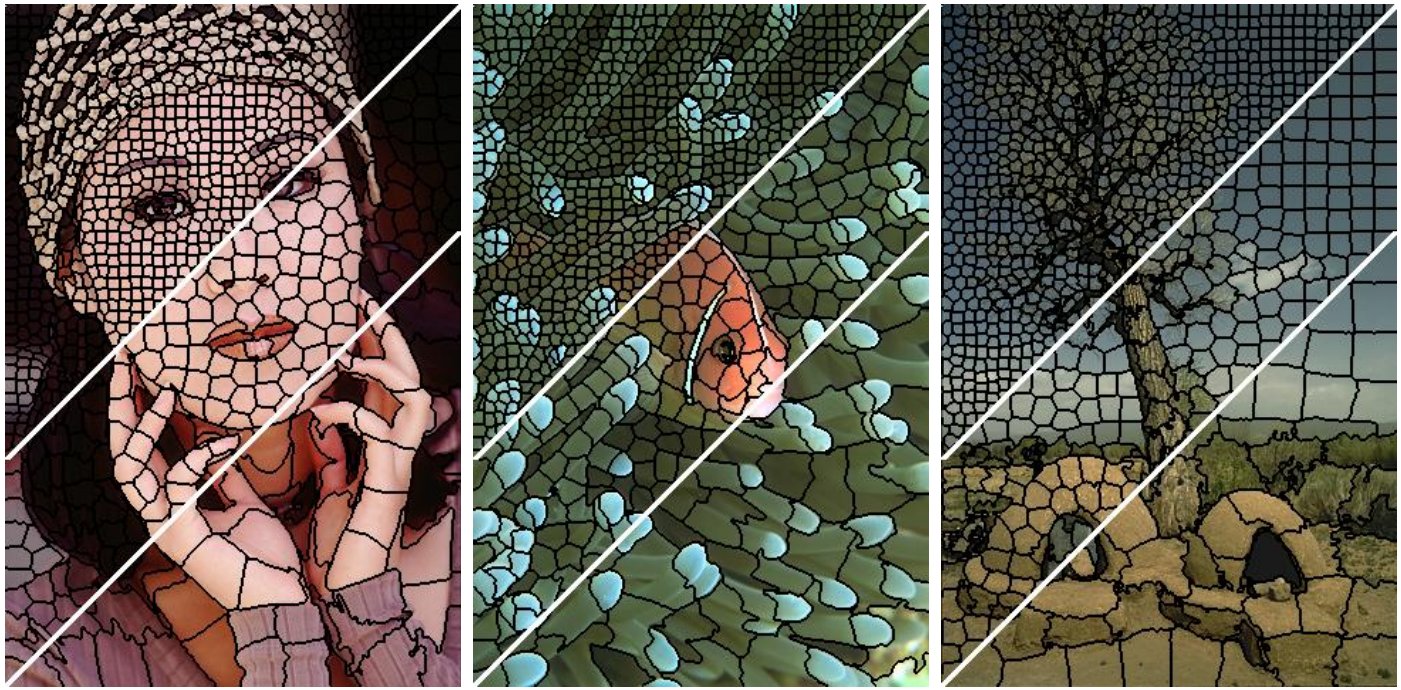

Superpixel segmentation

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- 5D feature space (lab color space, 2d spatial coordinates)

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- Distance metric treats color dimensions and spatial dimensions differently

Superpixel segmentation

- 5D feature space (lab color space, 2d spatial coordinates)
- Distance metric treats color dimensions and spatial dimensions differently
- Initial cluster centers are spaced regularly on the image and slightly perturbed to avoid edges

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- Easy to implement

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Cons:

- Need to choose K
- Sensitive to outliers
- Can get stuck in local minima
- All cluster centers have same parameters (non-adaptive)
- Can be slow $O(KNd)$

Quiz:

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- What are the steps of the kMeans algorithm?
- What are the guarantees of the kMeans algorithm?

Important topics of this lecture

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- Understanding kMeans

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- Getting to know different mechanisms to adjust kMeans