Introduction to Computer Vision

Unsupervised image segmentation
with low-level features

Low-level Segmentation

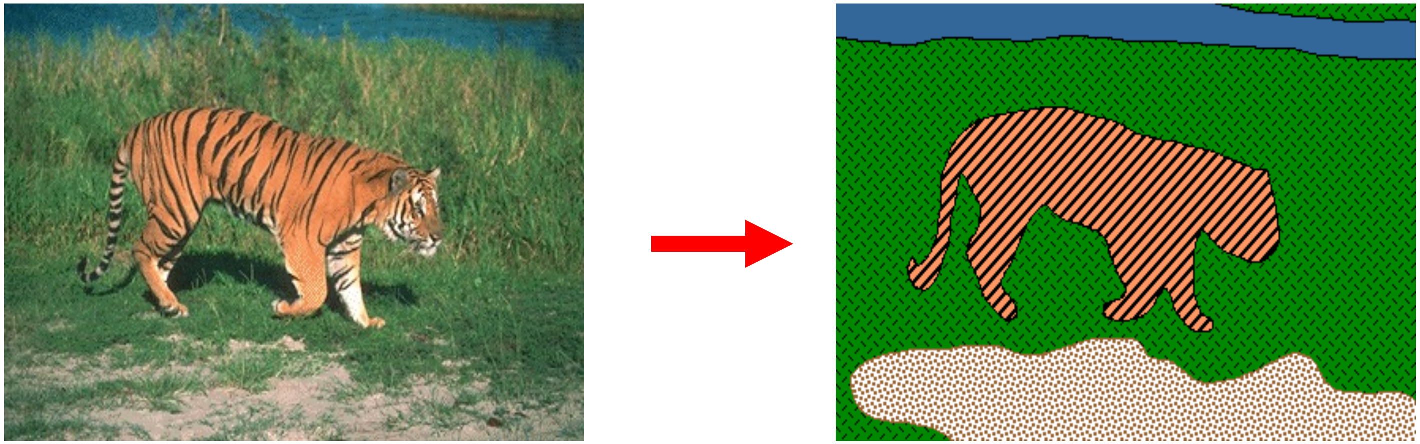
or grouping, partitioning, etc...

MAIN GOAL: in a simpler context of basic low-dimensional image features (e.g. colors, edges)
understand **standard general techniques for grouping data points** (e.g. pixels)

LATER: understand how to automatically build/learn "complex" features
representing high-level (e.g. semantic class) information.
We will also discuss how to group them with or without supervision.

informal overview of

Image Segmentation



Goal:

find coherent "**blobs**" or specific "**objects**"

low-level segmentation
(e.g. color-consistent region, smooth edge-aligned boundaries, coherent motion,...)

high-level / **semantic** segmentation
(e.g. humans, trees, cars, …)

computed from one image only or based on a large training dataset?

unsupervised, semi-supervised, fully supervised ?

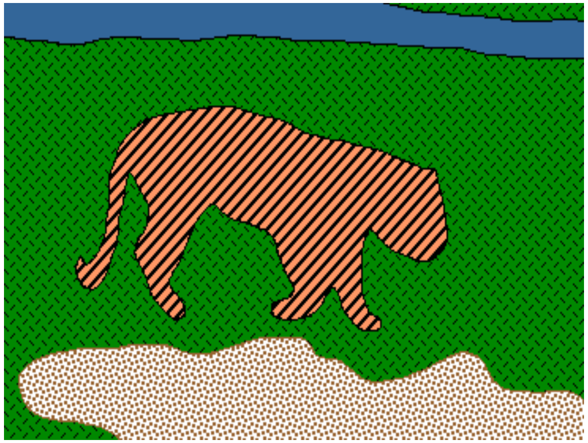
this topic

later topics

Low-level Image Segmentation

- Examples
  - *unsupervised* (background subtraction, color quantization, superpixels)
- "Naïve" low-level segmentation
  - thresholding, region growing, etc
- Low-level segmentation criteria (loss functions)
  - region-based, boundary-based (geometric or shape)
  - **Clustering** criteria for general data points (basics from ML)
    - *K*-means, *K*-medians, *K*-modes, mean-shift
    - variance and distortion clustering, robust metrics
    - hard vs. soft clustering, probabilistic formulations, entropy, likelihoods, EM, GMM
    - parametric & non-parametric methods, kernel/spectral clustering, data embeddings

Two basic types of properties for low-level segmentation



- A: coherent **segment's appearance (region)**
  - e.g. consistent distinct colors, texture, etc
  - or agreement with known expected color distribution
- B: coherent **segment's shape (boundary)**
  - e.g. alignment to contrast edges
  - or boundary regularity / smoothness (low-level "shape prior")
  - or agrees with expected shape (e.g. square, star, convex - higher-level priors)

Low-level Image Segmentation

first

"Naïve" segmentation techniques

A [based on appearance/color]: thresholding, likelihood ratio test

B [based on boundaries/contrast-edges]: region growing

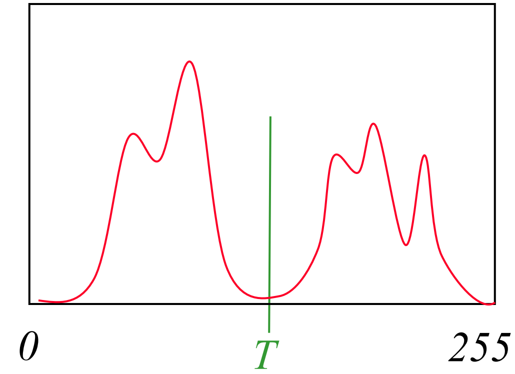
Szeliski, Sec 5.2

Other readings: Sonka et al. Ch. 5
Gonzalez and Woods, Ch. 10

Naive Approach to *Appearance* (A)

SEGMENT'S APPEARANCE

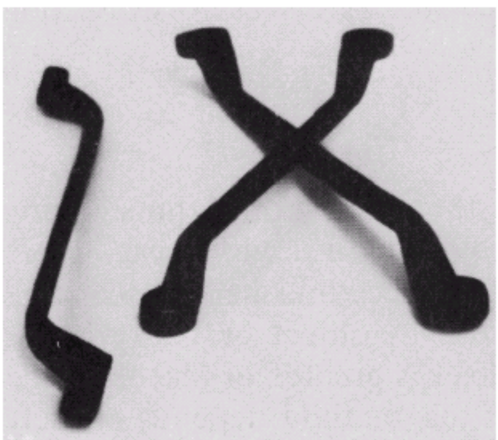
The most basic approach is to partition intensity histogram (**thresholding**)



- point processing, location is ignored

Coherent color "blobs"

- Simplest way to define blob coherence is as similarity in brightness or color:



The tools become blobs

The house, grass, and sky make different blobs

Why is this useful?

AIBO
RoboSoccer
(VelosoLab)

Ideal Segmentation

can recognize objects with known ? simple ? color ? models

Result of a segmentation method

(first learn how to get this, then how to get better results)

even
if

known
simple
color

Basic ideas

segment's region features		basic (naïve) methods
intensities, colors	←	thresholding, likelihood ratio test

(segmentation ← intensities/colors)

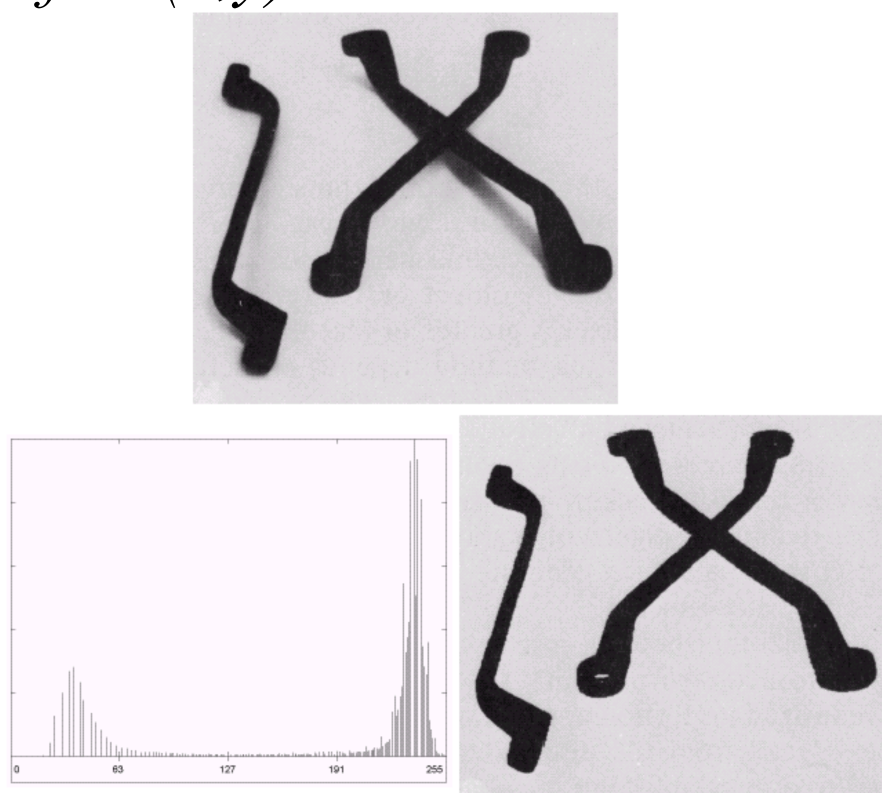
Thresholding

- Basic segmentation operation:

  $$mask(x,y) = 1 \text{ if } im(x,y) > T$$

  $$mask(x,y) = 0 \text{ if } im(x,y) < T$$

- T is threshold
  - user-defined
  - or automatic



a
b c

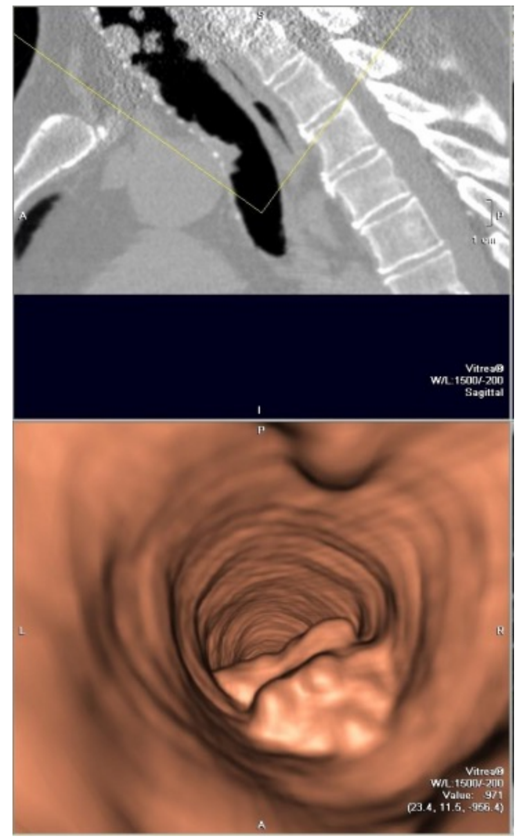
FIGURE 10.28 (a) Original image. (b) Image histogram. (c) Result of global thresholding with T midway between the maximum and minimum gray levels.

- Same as histogram partitioning:

Sometimes works well…

Virtual colonoscopy, bronchoscopy, etc.

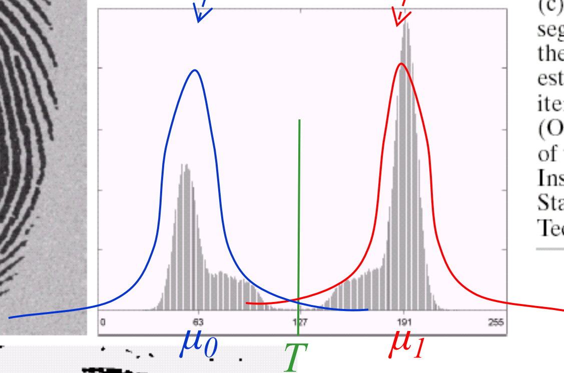
a) threshold CT volume -> binary mask



from real device to non-invasive virtual test

b) extract surface mash from binary mask
(*fast marching cubes* method)

Sometimes works well…



a b
c

FIGURE 10.29 (a) Original image. (b) Image histogram. (c) Result of segmentation with the threshold estimated by iteration. (Original courtesy of the National Institute of Standards and Technology.)

Example: assume known probability distributions

$$P_1 = N(\mu_1, \sigma)$$

$$P_0 = N(\mu_0, \sigma)$$

$$r \geq 0 \quad \Leftrightarrow \quad I \geq T$$

$$T = \frac{\mu_1 + \mu_0}{2}$$

Thresholding could be derived as
a statistical decision: **likelihood ratio test**

$$r_p \quad := \quad \log \frac{P_1(I_p)}{P_0(I_p)}$$

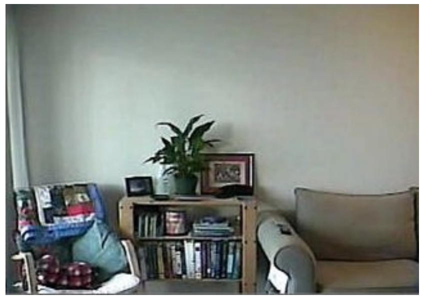
P_1 and P_0 are known color models for object and background

$r_p \geq 0 \quad \Rightarrow$ pixel p is object

$r_p < 0 \quad \Rightarrow$ pixel p is background

Sometimes works well…

-



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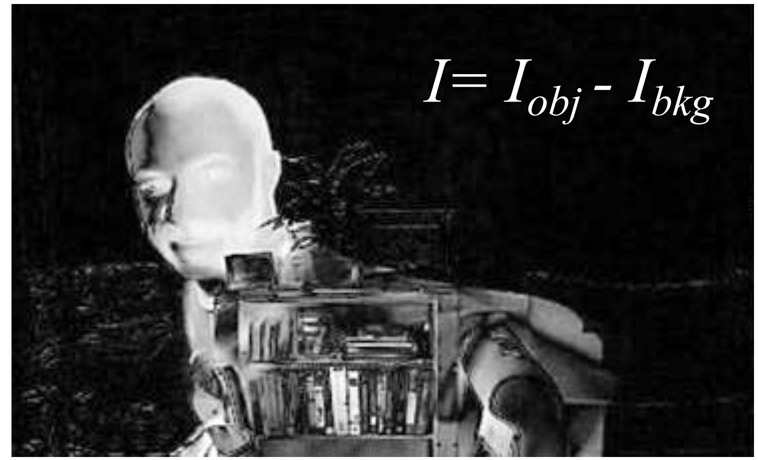
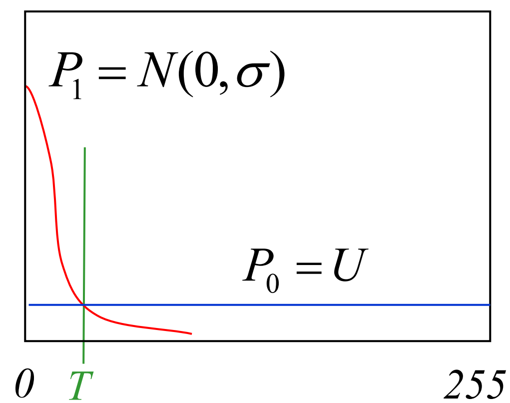
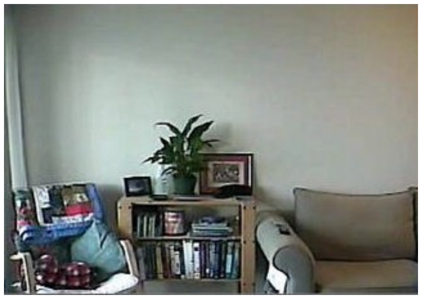


background subtraction



Sometimes works well… more often not

-



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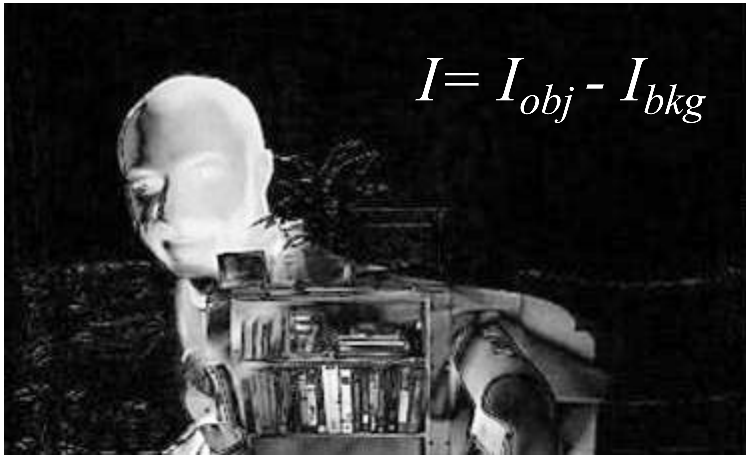
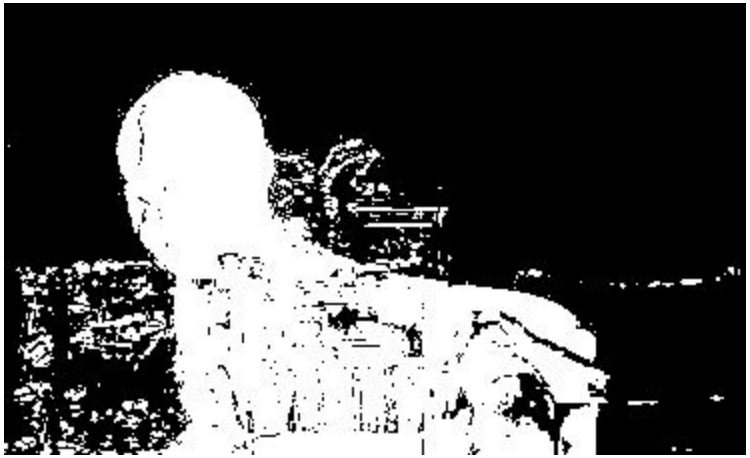
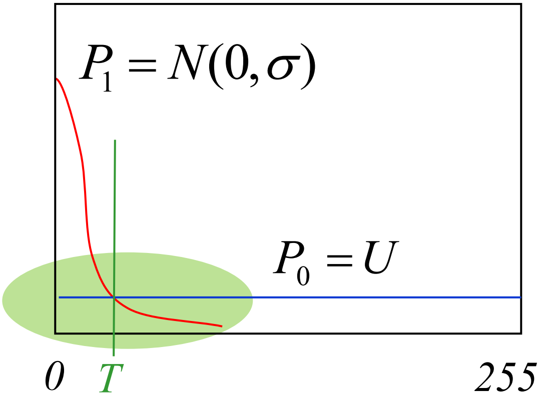


background subtraction



Threshold intensities below T

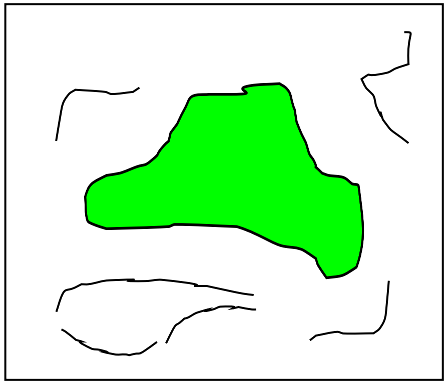


problems when color models have **overlapping support**

Naive Approach to *Boundary* (B)

SEGMENT'S BOUNDARY

Canny edges

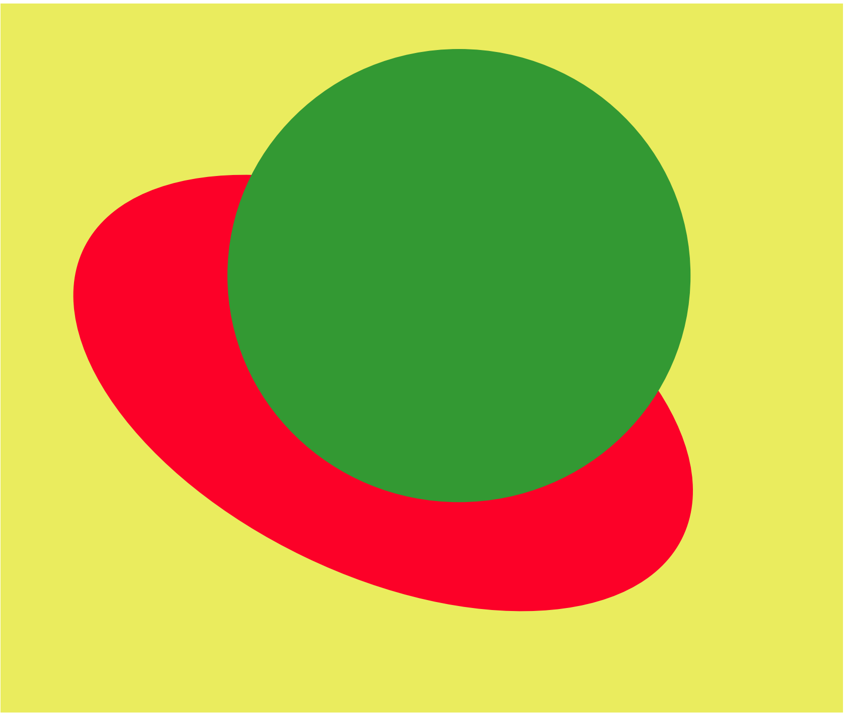


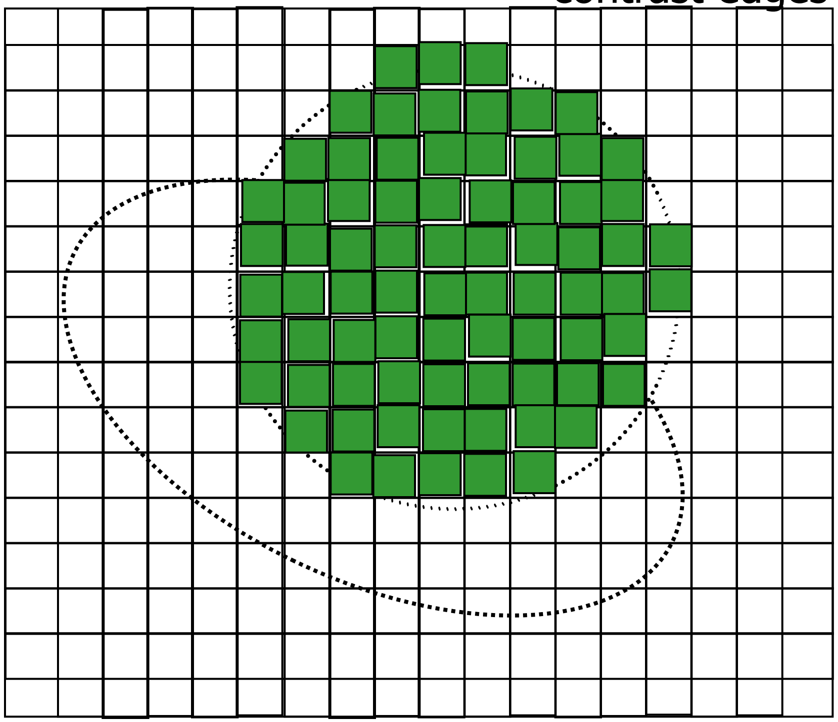
The most basic approaches attempt to find subsets of pixels completely surrounded by strong intensity edges

- **region growing**
- **watersheds**

(segmentation ← contrast edges)

Region growing



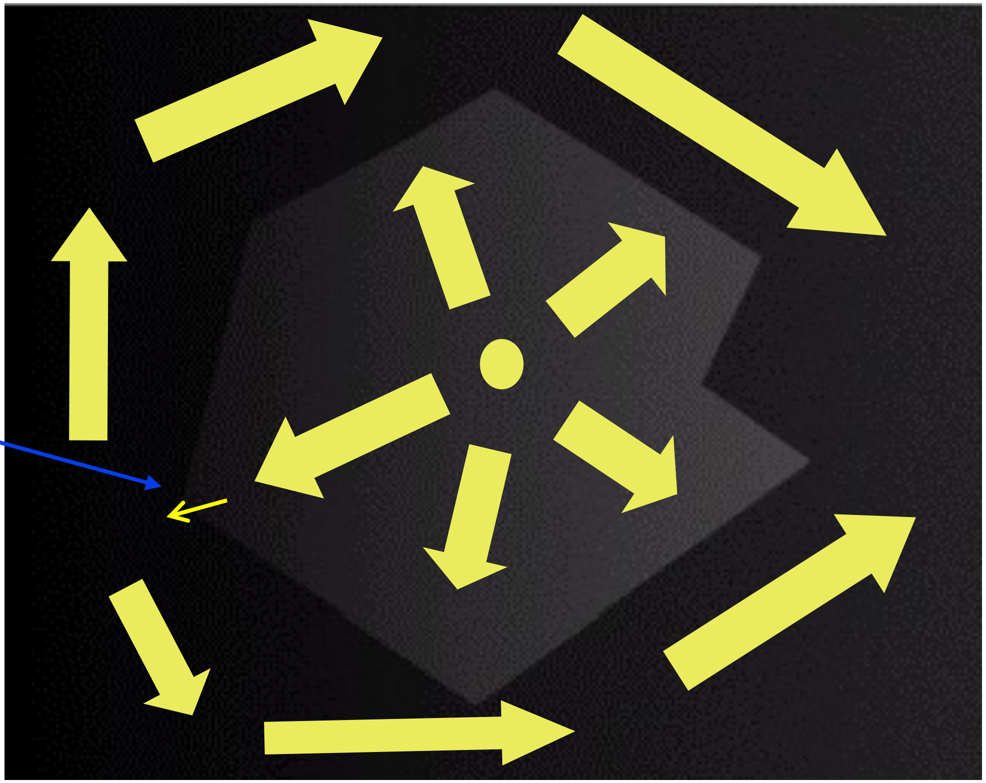


- Interactive initialization: assumes some initial set of pixel(s) K (seeds)
- For any pixel p in K add all its neighbors q such that $|Ip-Iq| < T$
- Iterate the step above until no neighbors of points in K satisfy $|Ip-Iq| < T$

- **Breadth-First Search** (BFS) over grid neighbors (p,q) s.t. $|Ip-Iq|<T$
- Method stops at high-contrast edges (p,q) such that $|Ip-Iq|>T$

What can go wrong with region growing ?

Region growth may "leak" through **a single** **week spot** in the boundary



Region growing

-

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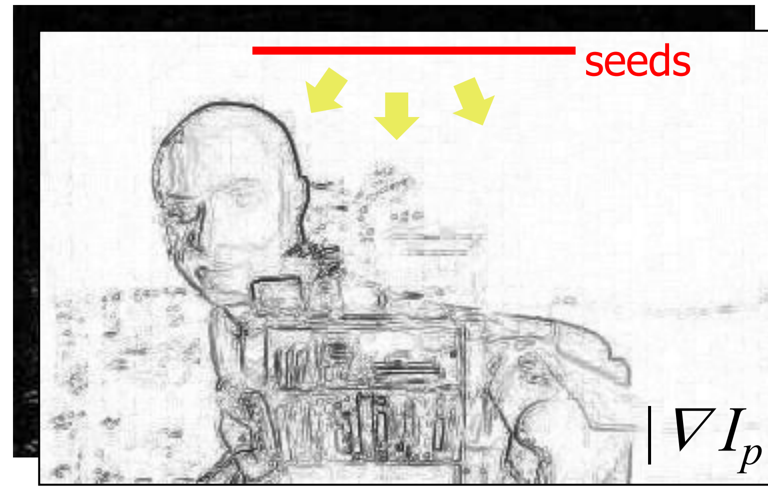
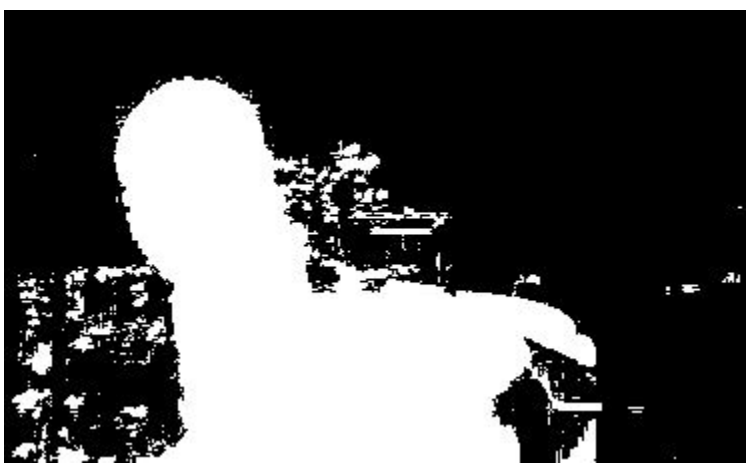




Breadth First Search (seeds) :

$$|\nabla I_p| < T$$

Region growing

See region *leaks* into sky due to a weak boundary between them

From procedurally-defined towards "objective" segmentation

Should learn about **loss functions** (objectives) representing:

- Color/feature appearance consistency
  - replacing (manually-selected) thresholding by automatic partitioning of features
- Boundary/shape regularity
  - contrast edge continuation (fixing " leaks")
  - shape priors/regularization
- Combining multiple objectives (losses)

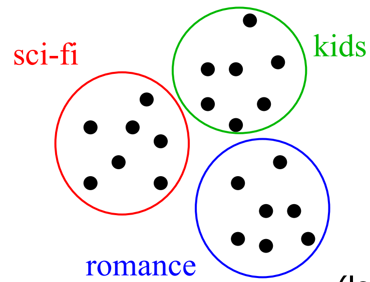
From procedurally-defined towards "objective" segmentation

Should learn about **objectives** (loss functions)

- Part I: **Clustering criteria**
  - general ML methods for unsupervised or weakly-supervised data partitioning
  - can be adapted to image segmentation
- Part II: **Regularization models**
  - designed specifically for image segmentation
  - appearance consistency
  - boundary regularity (graphical/discrete formulations)

Highly informal
comments on terminology

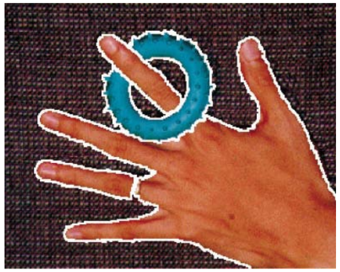
Clustering – general techniques (from ML) for partitioning arbitrary data/features $\{f_i\} \subset R^N$ (of any dimensions) where i is data point index



e.g. movies in some feature space (length, director, tags,…)

Image Segmentation – methods specifically designed for partitioning image features $\{f_p\} \subset R^N$ where p are <u>image grid pixels</u> $p = (x, y)$

- informally, instead of an arbitrary collection $\{f_p\}$ of data points features are viewed as a sample from function $f(x,y) : R^2 \to R^N$



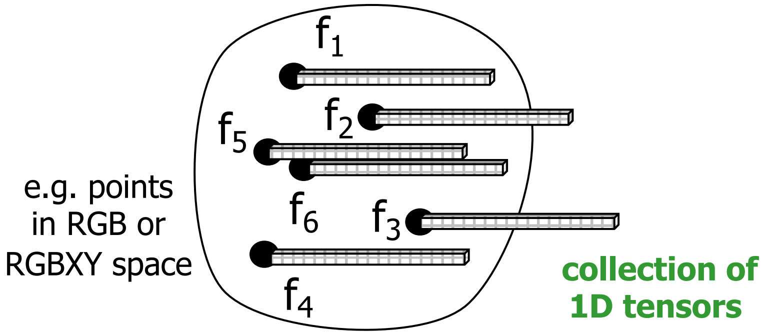
NOTE: general clustering techniques can be adapted to image segmentation problems. Thus, the boundary between the terms **clustering** and image **segmentation** is fuzzy.

f_p - *e.g. intensity I_p or color RGB_p at pixel $p = (x,y)$*

Alternative Views on Data Representation

Part I vs Part II

collection of feature vectors in R^n

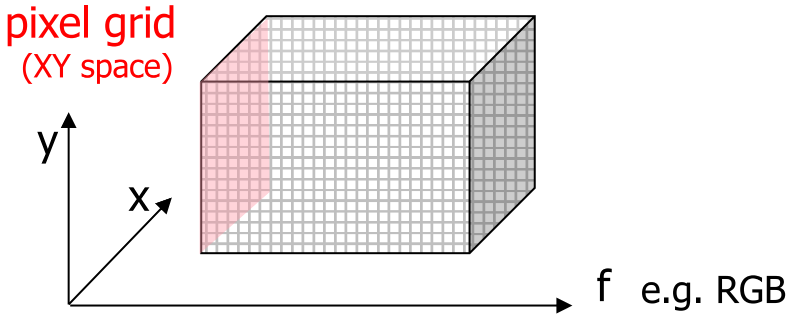


general features

common in ML

K-means, GMM, general graph clustering, ...

3D tensor



features embedded in a regular 2D grid

common in computer vision

convolution, geometry, shape, spatial regularity, ...

We will learn: - clustering criteria and spatial regularization models
- how to combine different approaches

Clustering Methods for General Data

(basics from ML with applications in Computer Vision)

Clustering Methods for General Data

(basics from ML with applications in Computer Vision)

general criteria for unsupervised data clustering

- *K*-means, distortion clustering, probabilistic clustering, EM, GMM
- parametric vs non-parametric formulations
- kernel and spectral methods, graph clustering criteria
- mean-shift

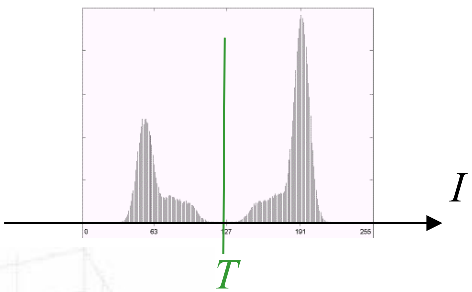
Szeliski, Sec 5.3

examples in image analysis

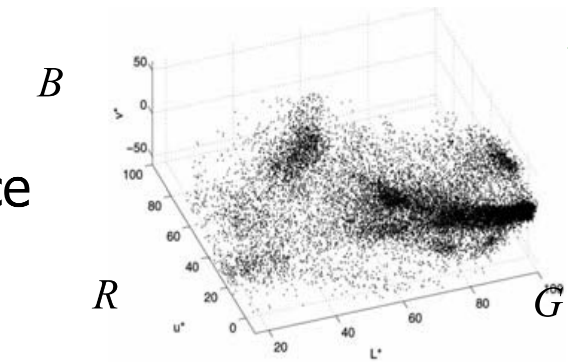
- color quantization, super-pixels, unsupervised segmentation

Motivation

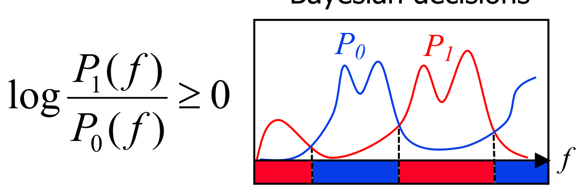
- In 1D feature spaces (gray-scale intensities) it may be possible to set decision boundaries manually.



But, not easy in 3D feature space



- It is possible to use log-likelihood ratio test if (color) distributions for segments, *e.g.* P_1 and P_0, are known.

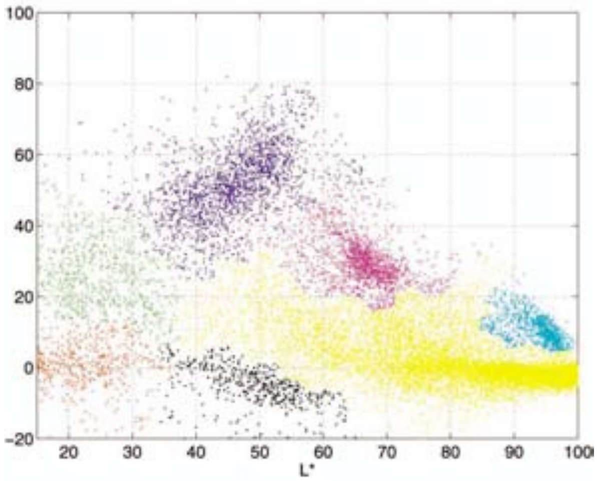


can yield complex decision boundaries in space of any features f

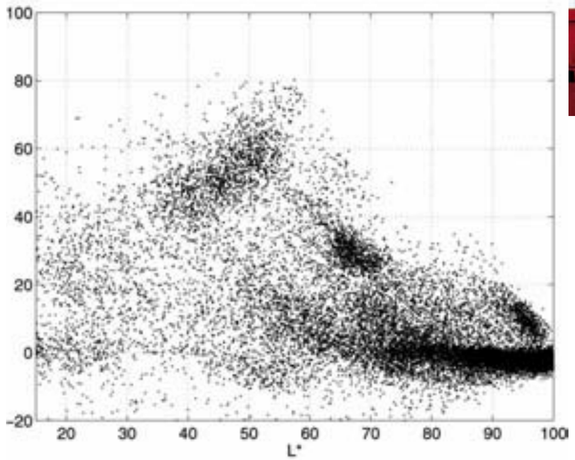
Does not work if distributions are not known.

Motivation

decision boundaries for ND features
could be arbitrarily complex (surfaces)



?

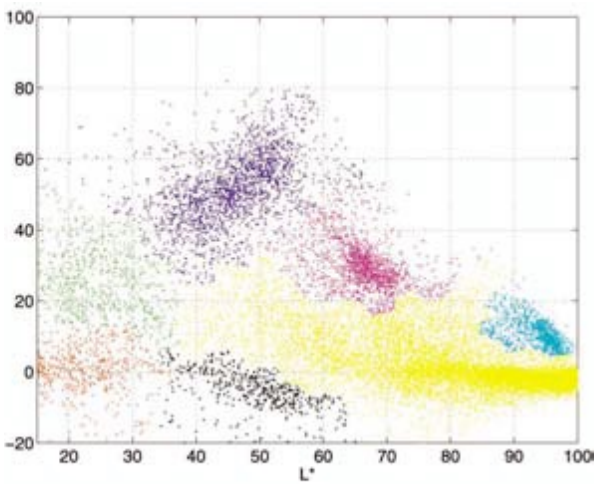


Example: break data points (e.g. RGB or RGBXY space) into a few clusters

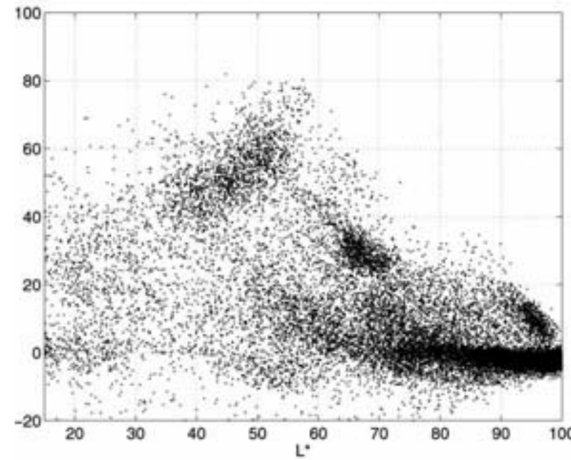
- color quantization
- superpixels
- semantic segmentation (later topic)

Motivation

decision boundaries for ND features
could be arbitrarily complex (surfaces)



?



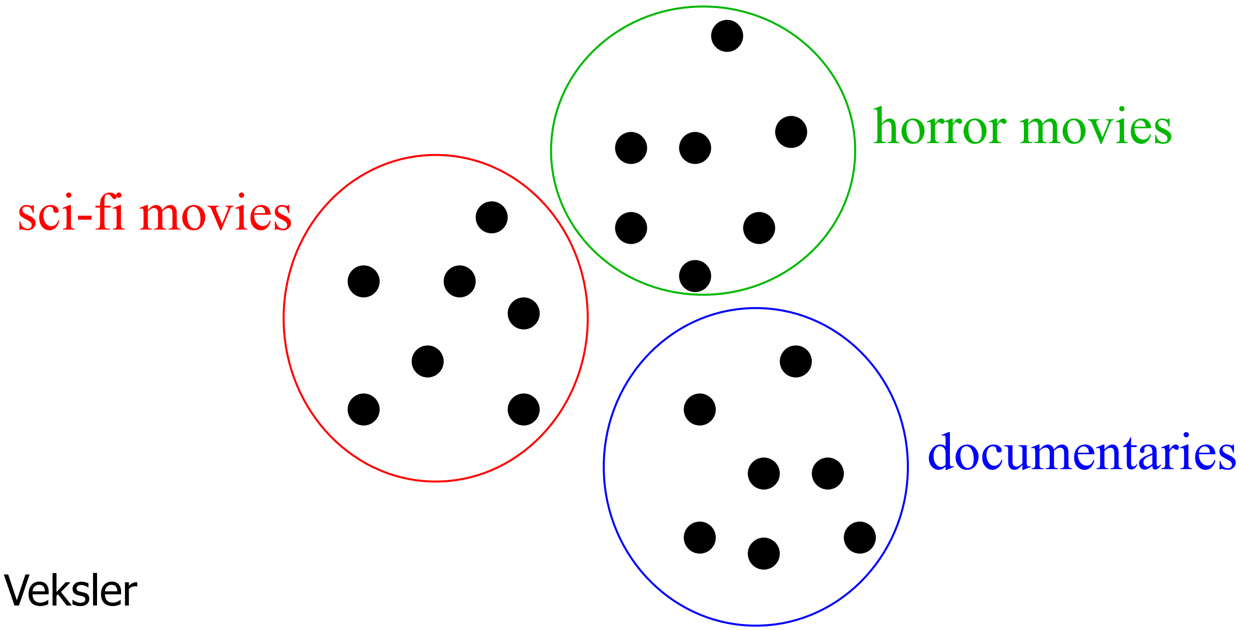
Need automatic data *clustering* methods

Szeliski, Sec 5.3

- parametric methods: *e.g.* K-means, soft K-means, GMM …
  - Note: many such methods are *generative* (implicitly or explicitly estimate distribution parameters)
- non-parametric: *e.g.* kernel K-means, graph partitioning, mean-shift …
  - Note: many of these methods are *discriminative* (only optimize clustering quality)

General Grouping or Clustering
(a.k.a. *unsupervised learning*)

- Have data points (samples, a.k.a. feature vectors, examples, etc.) $\boldsymbol{f}_1, \ldots, \boldsymbol{f}_p, \ldots$
- Cluster similar points into groups
  - points are **not** pre-labeled
  - think of clustering as 'discovering' labels



slides from Olga Veksler

How does this Relate to Image Segmentation?

- Represent image pixels as feature vectors $\boldsymbol{f}_1,\ldots,\boldsymbol{f}_p,\ldots$ or $\{f_p \mid p \in \Omega\}$
  - For example, each pixel can be represented as
    - intensity, gives one dimensional (1D) feature vectors
    - color, gives three-dimensional (3D) feature vectors, e.g. RGB
    - color + coordinates, gives five-dimensional (5D) feature vectors, e.g. RGBXY
- Cluster them into ***K*** clusters, i.e. ***K*** segments

set of all pixels or indices

input image

9 4 2	7 3 1	8 6 8
8 2 4	5 8 5	3 7 2
9 4 5	2 9 3	1 4 4

feature vectors for clustering based on color

[9 4 2] [7 3 1] [8 6 8]

[8 2 4] [5 8 5] [3 7 2]

[9 4 5] [2 9 3] [1 4 4]

RGB (or LUV) space clustering

How does this Relate to Image Segmentation?

- Represent image pixels as feature vectors $\boldsymbol{f}_1, \ldots, \boldsymbol{f}_p, \ldots$ or $\{f_p \mid p \in \Omega\}$
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- Cluster them into ***K*** clusters, i.e. ***K*** segments

input image

9 4 2	7 3 1	8 6 8
8 2 4	5 8 5	3 7 2
9 4 5	2 9 3	1 4 4

feature vectors for clustering based on color and image coordinates

[9 4 2 0 0] [7 3 1 0 1] [8 6 8 0 2]

[8 2 4 1 0] [5 8 5 1 1] [3 7 2 1 2]

[9 4 5 2 0] [2 9 3 2 1] [1 4 4 2 2]

RGBXY (or LUVXY) space clustering

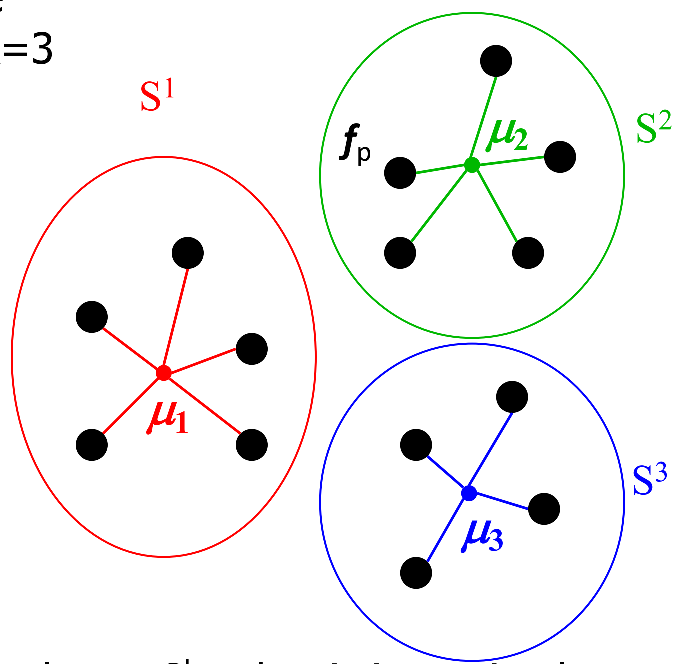
K-means Clustering: Objective Function

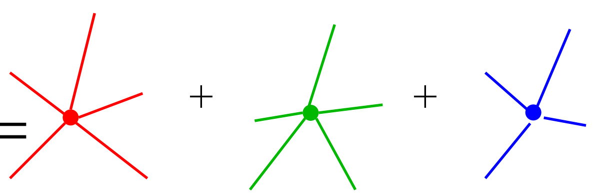
- Probably the most popular clustering algorithm
  - assumes the number of clusters is given - ***K***
- optimizes (approximately) the following **objective function** for variables S^k and μ_k

$$SSE = \sum_{k=1}^{K} \sum_{p \in S^k} \left\| f_p - \mu_k \right\|^2$$

sum of squared errors from cluster center μ_k
(both S^k and μ_k are **unknown**, to be computed)

assume
given K=3



$SSE =$ 

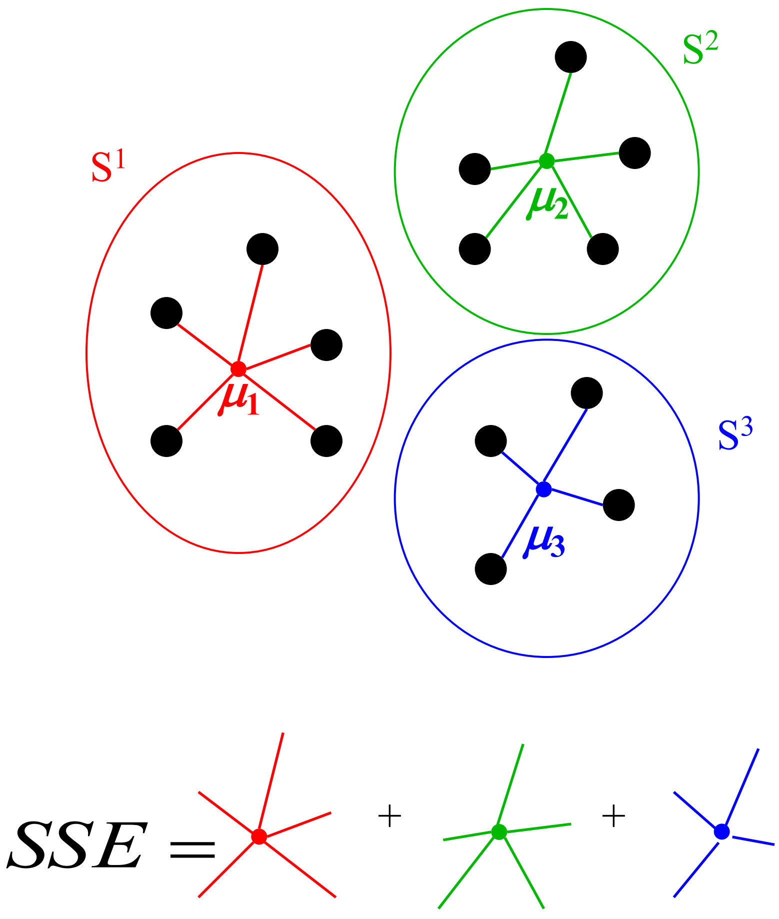
optimization "variables"

subsets $S = (S^1, \ldots, S^K)$

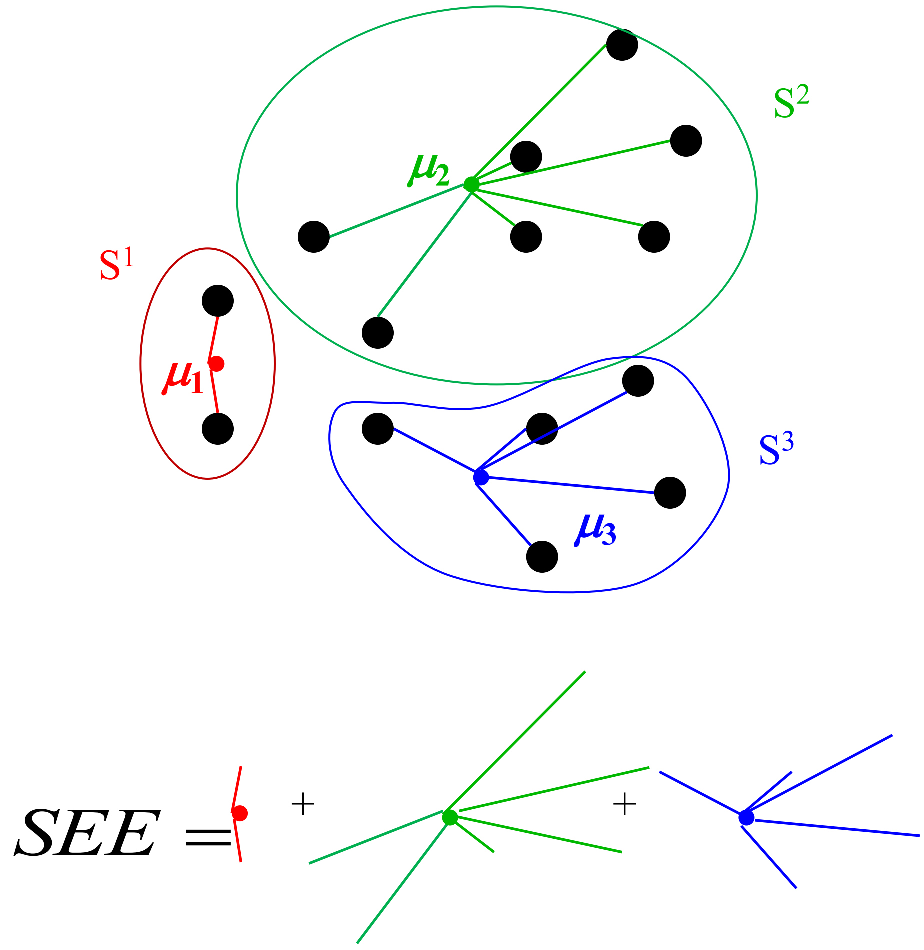
centers $\mu = (\mu_1, \ldots, \mu_K)$

Q: given cluster S^k, what is its optimal center μ_k?
A: least square solver B: average C: median

K-means Clustering: Objective Function



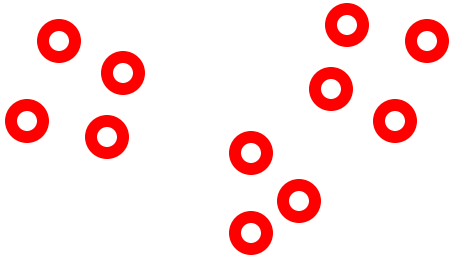
Good (tight) clustering
=> smaller value of SSE



Bad (loose) clustering
=> larger value of *SSE*

K-means Clustering: Algorithm

- Initialization step
  1. pick ***K*** cluster centers randomly (e.g. from data points)



K-means Clustering: Algorithm

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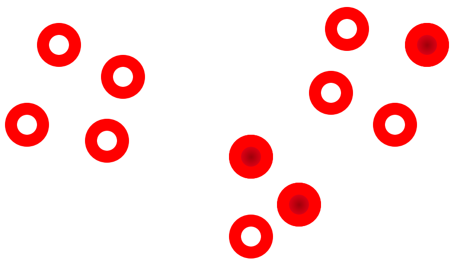
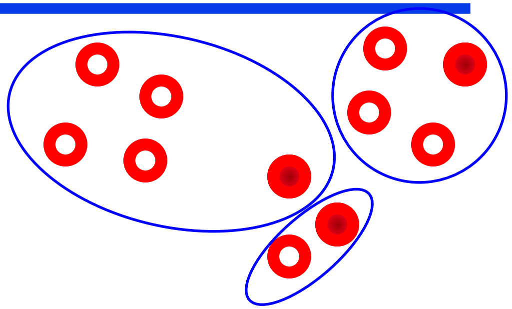


K-means Clustering: Algorithm

- Initialization step
  1. pick ***K*** cluster centers randomly
  2. assign each sample to its closest center



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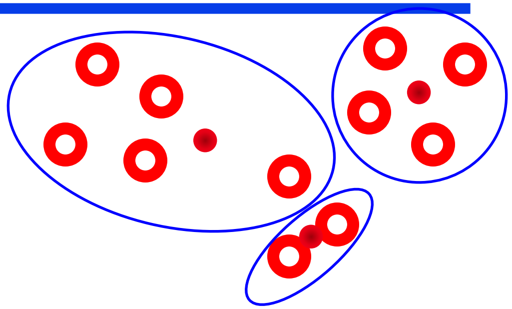
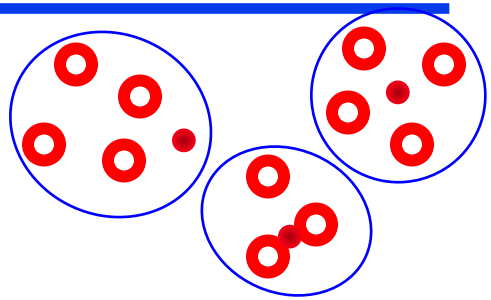


- Iteration steps
  1. compute centers as cluster means $\mu_k = \frac{1}{|S^k|} \sum_{p \in S^k} f_p$

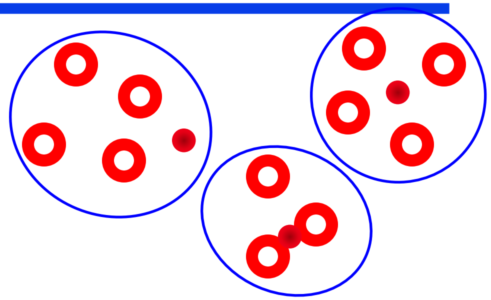
K-means Clustering: Algorithm

- Initialization step
  1. pick ***K*** cluster centers randomly
  2. assign each sample to its closest center



- Iteration steps
  1. compute centers as cluster means $\mu_k = \frac{1}{|S^k|} \sum_{p \in S^k} f_p$
  2. re-assign each sample to the closest mean

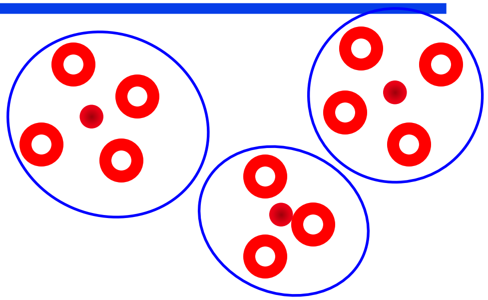
K-means Clustering: Algorithm



- Initialization step
  1. pick ***K*** cluster centers randomly
  2. assign each sample to its closest center

- Iteration steps
  1. compute centers as cluster means $\mu_k = \frac{1}{|S^k|} \sum_{p \in S^k} f_p$
  2. re-assign each sample to the closest mean
- Iterate until clusters stop changing

K-means Clustering: Algorithm



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K-means Clustering: Algorithm

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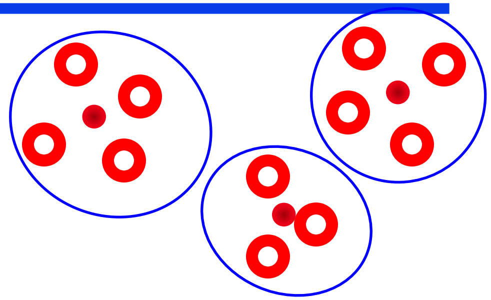

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  1. compute centers as cluster means $\mu_k = \frac{1}{|S^k|} \sum_{p \in S^k} f_p$
  2. re-assign each sample to the closest mean
- Iterate until clusters stop changing

Lloyd's algorithm (1957)

- Each step decreases the value of the objective function

$$E(S,\mu) = \sum_{k=1}^{K} \sum_{p \in S^k} \|f_p - \mu_k\|^2$$

optimization variables

$$S = (S^1, \ldots, S^K)$$
$$\mu = (\mu_1, \ldots, \mu_K)$$

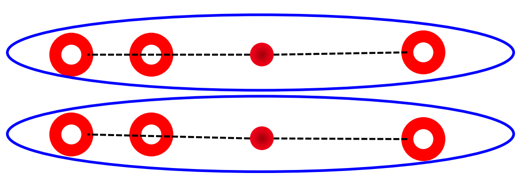
block-coordinate descent: step 1 optimizes $\{\mu_k\}$ for fixed $\{S_k\}$, step 2 optimizes $\{S_k\}$ for fixed $\{\mu_k\}$

K-means: Approximate Optimization

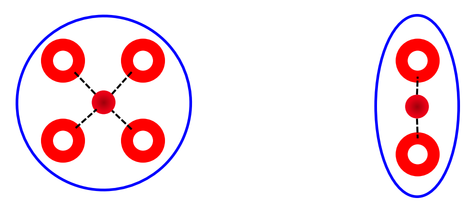
- K-means is fast and (sometimes) works well in practice
- But can get stuck in a local minimum of objective $\boldsymbol{E_K}$
  - not surprising, since the exact optimization of its objective is NP-hard

initialization

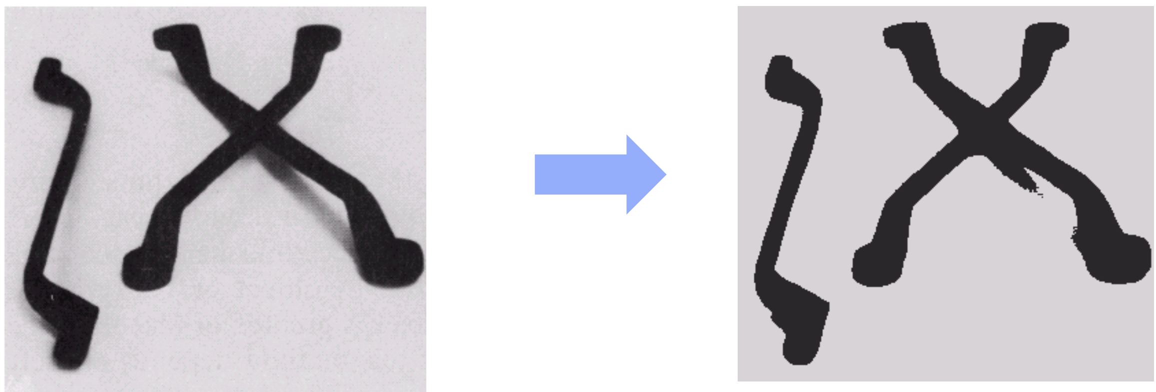
converged to local min



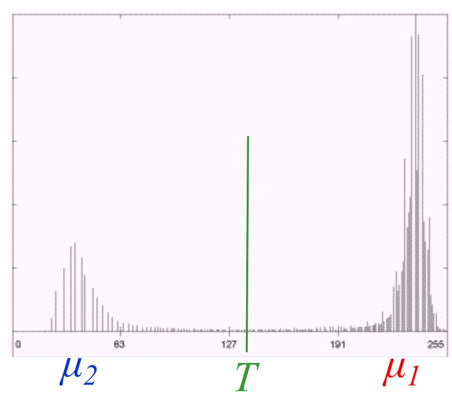
global minimum



K-means clustering examples: Segmentation



$$I_p \in R^1$$



here K-means finds compact clusters of pixels' intensities

In this case K-means (K=2) implicitly finds a good threshold (between 2 clusters)

K-means for colors (RGB features): Segmentation?

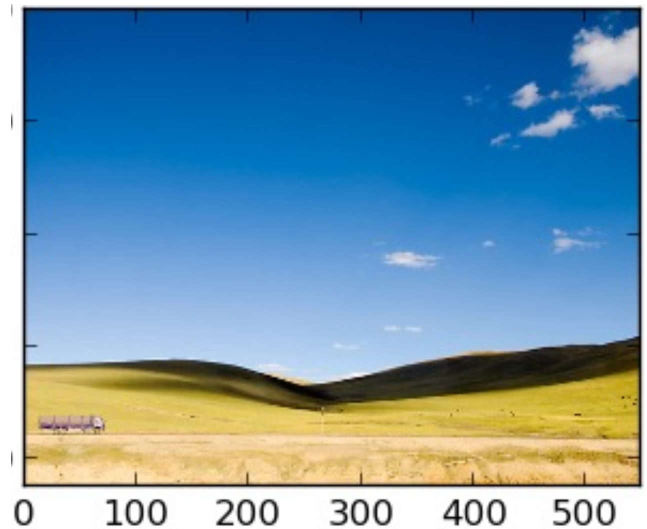
***k* = 3**

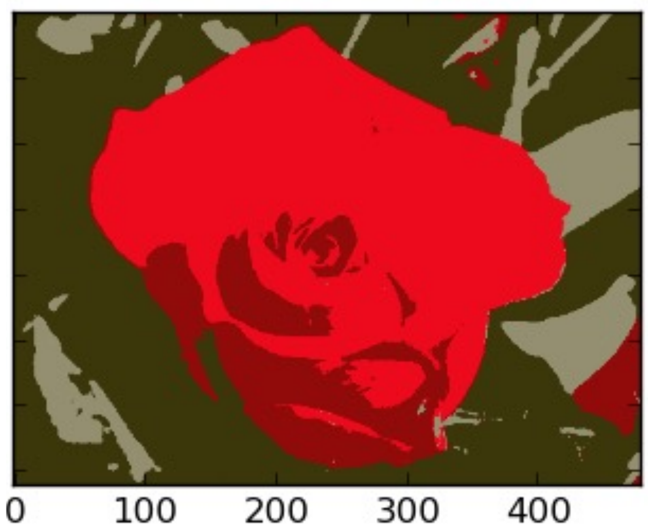
(**mean** color is used to show each segment/cluster)

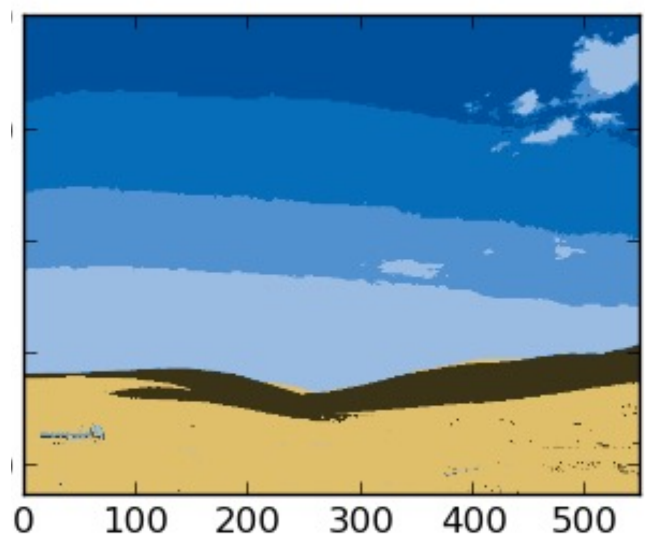
***k* = 5**

***k* = 10**

K-means for colors (RGB features): Color Quantization







NOTE bias to equal-size clusters

Where "size" can mean both clusters' cardinalities and clusters' diameters in the feature space

K-means clustering examples: Adding XY features

color quantization

RGB features

superpixels

RGBXY features

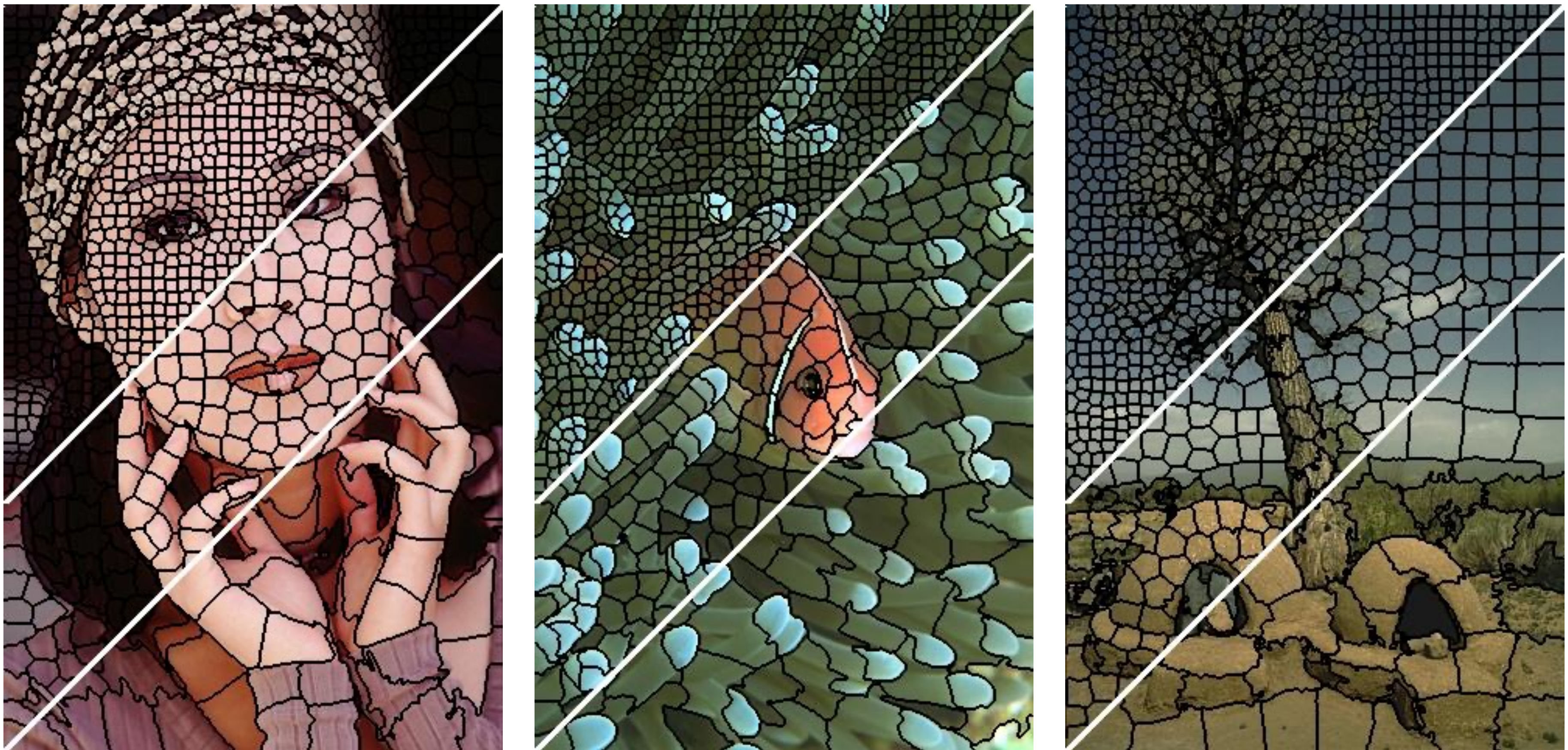
Voronoi cells

XY features only

K-means clustering examples: Superpixels

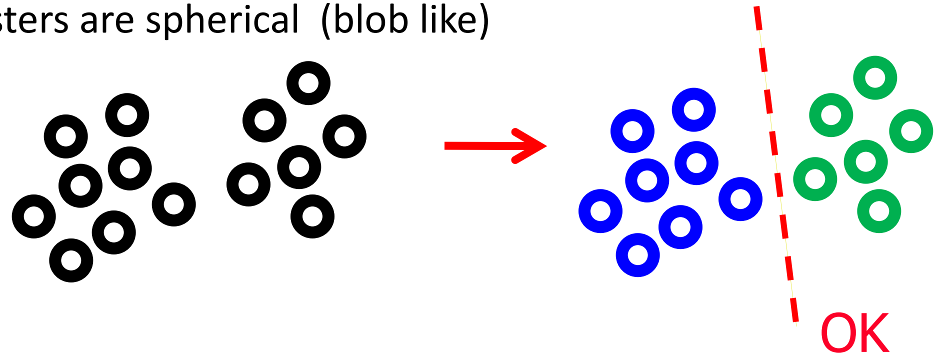
- Apply K-means to RGBXY features

[SLIC superpixels, Achanta et al., PAMI 2011]

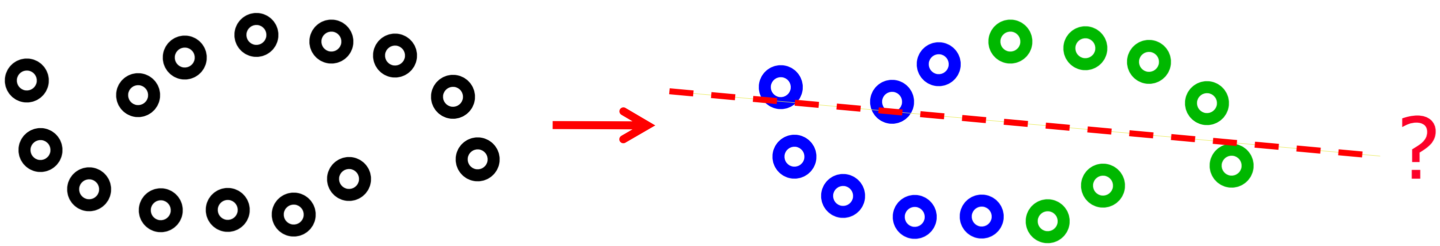


K-means Properties

- Works best when clusters are spherical (blob like)



- Fails for non-compact clusters

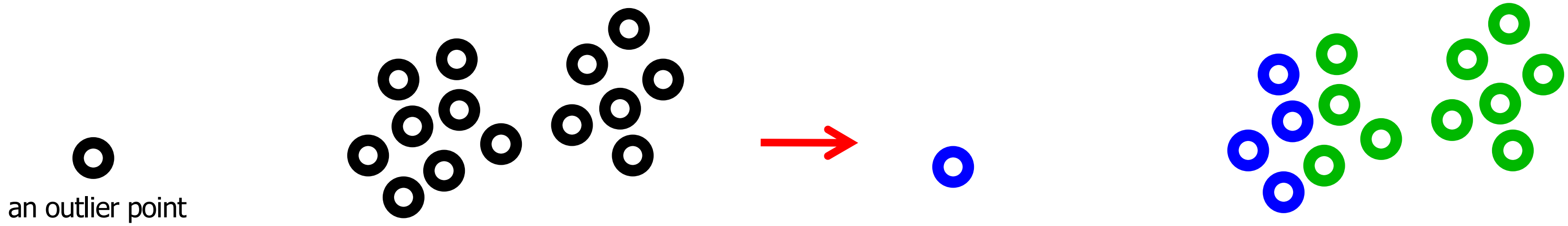


K-means produces <u>linear decision boundaries</u> between features f_p (why?)

Thus, K-means does not work if two clusters can not be separated by a line/plane, *i.e.* if the data is linearly non-separable.

K-means Properties

- Sensitive to outliers

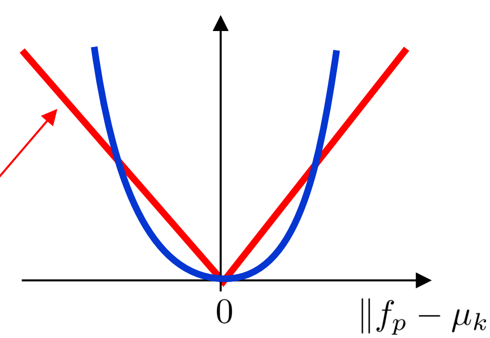


Explanation: squared distance error grows too fast making any outlier extremely costly. This also explains non-robustness of a "sample mean" statistic.

$$SSE = \sum_{k=1}^{K} \sum_{p \in S^k} \left\| f_p - \mu_k \right\|^2$$

Possible solution: replace squared distances by absolute distances that grow at a slower pace.

$$SAE = \sum_{k=1}^{K} \sum_{p \in S^k} \left\| f_p - \mu_k \right\|$$

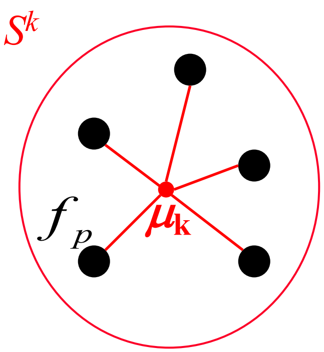


Interestingly, in this case the optimal value of μ_k is the "median" of set S^k instead of its "mean"

K-means as non-parametric clustering

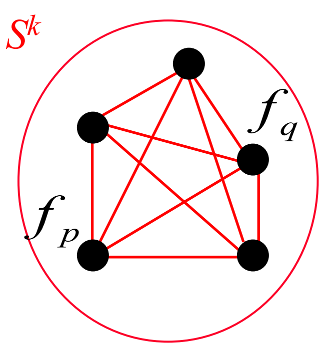
just plug-in expression

$$\mu_k = \frac{1}{|S^k|} \sum_{q \in S^k} f_q$$



$$E(S,\mu) \;=\; \sum_{k=1}^{K} \sum_{p \in S^k} \| f_p - \mu_k \|^2$$

equivalent (easy to check)

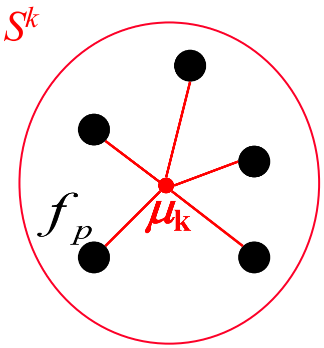


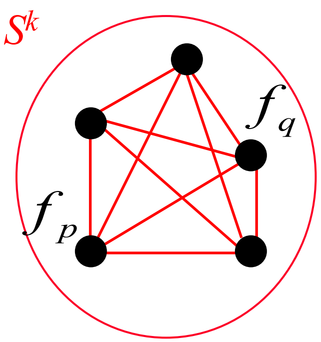
$$E(S) \;=\; \sum_{k=1}^{K} \sum_{pq \in S^k} \frac{\| f_p - f_q \|^2}{2|S^k|}$$

equivalent criterion without parameters μ_k

sample variance: $\mathrm{var}(S^k) = \frac{1}{|S^k|} \sum_{p \in S^k} \| f_p - \mu_k \|^2 = \frac{1}{2|S^k|^2} \sum_{pq \in S^k} \| f_p - f_q \|^2$

K-means as variance clustering criteria





both formulas can be written as

$$E(S) = \sum_{k=1}^{K} |S^k| \, \mathbf{var}(S^k)$$

sample variance: $\mathbf{var}(S^k) = \frac{1}{|S^k|} \sum_{p \in S^k} \| f_p - \mu_k \|^2 = \frac{1}{2|S^k|^2} \sum_{pq \in S^k} \| f_p - f_q \|^2$

K-means Summary

Good

- Principled (objective function) approach to clustering
- Simple to implement (the approximate iterative optimization)
- Fast

Not so good

- Only a local minimum is found   (sensitive to initialization)
- May fail for non-blob like clusters
- Maybe sensitive to outliers
- How to choose ***K*** ?

Can add **sparsity/complexity** term
making K an additional variable

$$E(S,\mu,K) \;=\; \sum_{k=1}^{K}\sum_{p\in S^k}\|f_p-\mu_k\|^2 \;+\; \gamma\,|K|$$

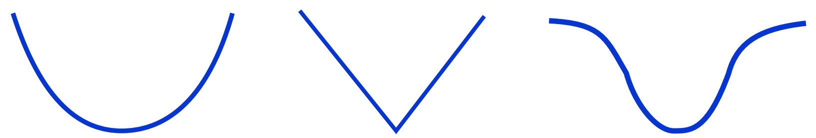
Akaike Information Criterion (AIC) or
Bayesian Information Criterion (BIC)

(summary of)

Standard extensions of K-means:

- **Parametric:** with arbitrary *distortion* measure $\|\cdot\|_d$ (***distortion clustering***)

$$\sum_{k=1}^{K} \sum_{p \in S^k} \left\| f_p - \mu_k \right\|_d$$



Examples of $\|\cdot\|_d$: *quadratic* (*K-means*) *absolute* (*K-medians*) *bounded* (*K-modes*)

- **Non-parametric:** with any *affinity or similarity measure, a.k.a. kernel* $k(x,y)$ (***kernel K-means***, *average association, average distortion, normalized cut*)

$$\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} \left\| f_p - f_q \right\|^2}{2\,|S^k|} = const - \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} \langle f_p, f_q \rangle}{|S^k|} \quad \Rightarrow \quad -\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} k(f_p, f_q)}{|S^k|}$$

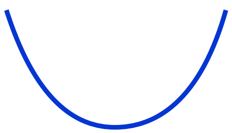
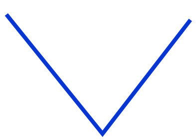
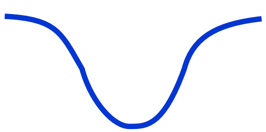
generalize from dot-product to "**inner product**" or arbitrary **affinity measure** or **kernel** k

(generalization)

Distortion Clustering

can use different "distortion" measures

$$E(S,\mu) \;=\; \sum_{k=1}^{K} \sum_{p \in S_k} \|f_p - \mu_k\|_d$$

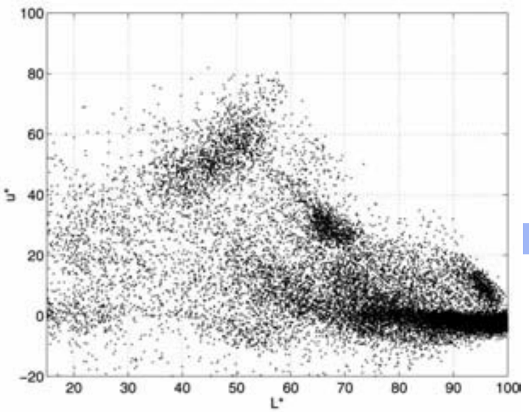
examples of distortion measure $\|\cdot\|_d$			interpretation of parameters μ_k
	$\|\cdot\|_d \;=\; \|\cdot\|^2$	squared L_2 norm	**K-means**
	$\|\cdot\|_d \;=\; \|\cdot\|$	absolute L_2 norm	**K-medians**
	$\|\cdot\|_d \;=\; 1 - \exp(-\|\cdot\|^2)$		**K-modes**

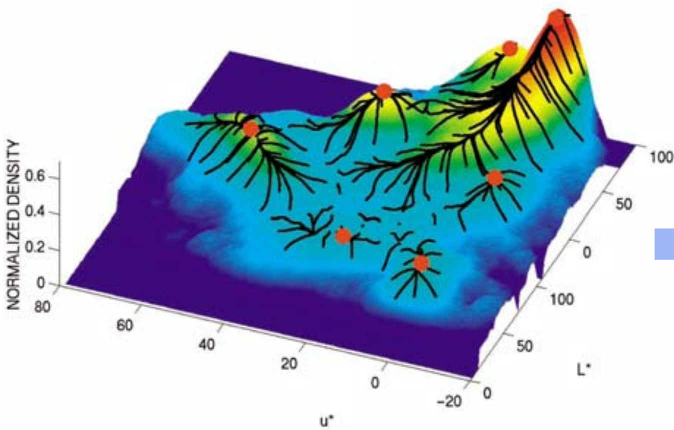
NOTE: besides changing the distortion measure, there are different generalizations of K-means requiring **other interpretations of SSE objective**

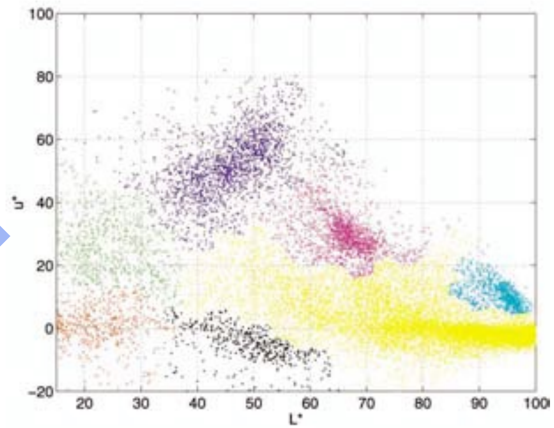
From "**means**" towards "**modes**" clustering:
Kernel-based ***mode clustering***

Optional Material

- Formulate clustering as *histogram partitioning*
  - look for **modes** in data histograms
  - assign points to modes

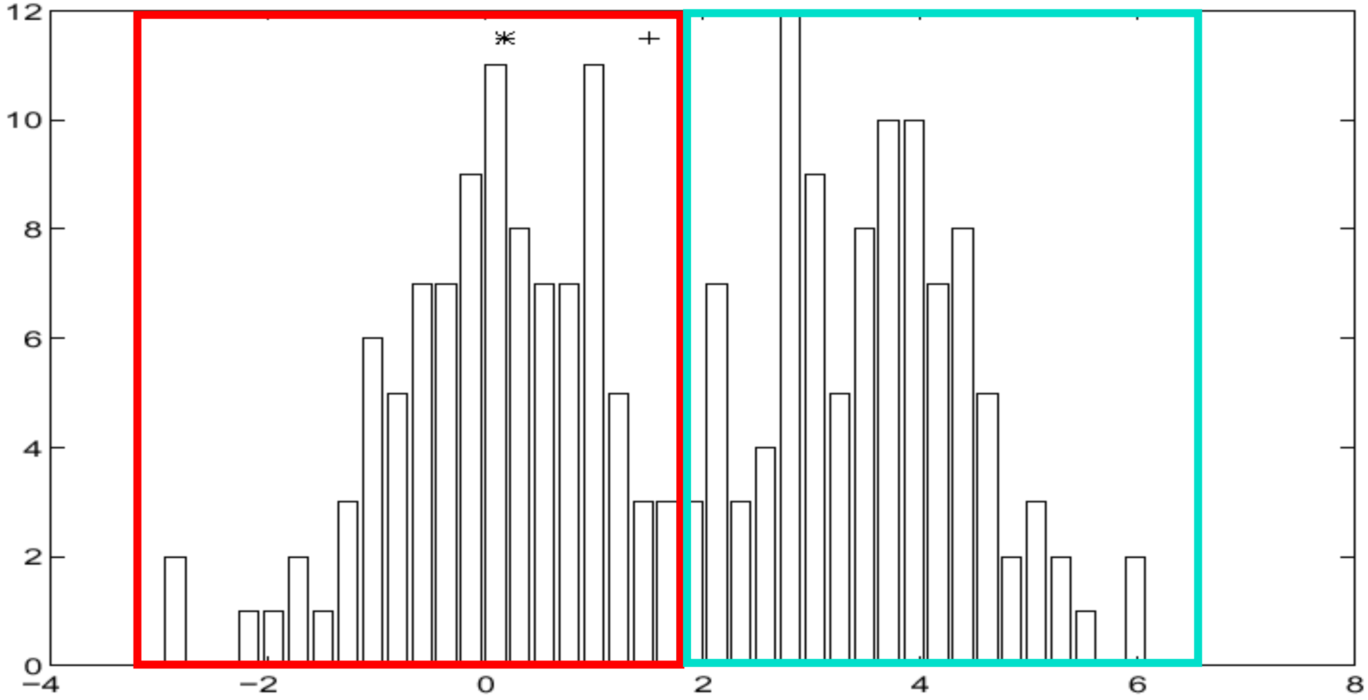






data points | data histogram and its modes | clustering

Finding Modes in a Histogram

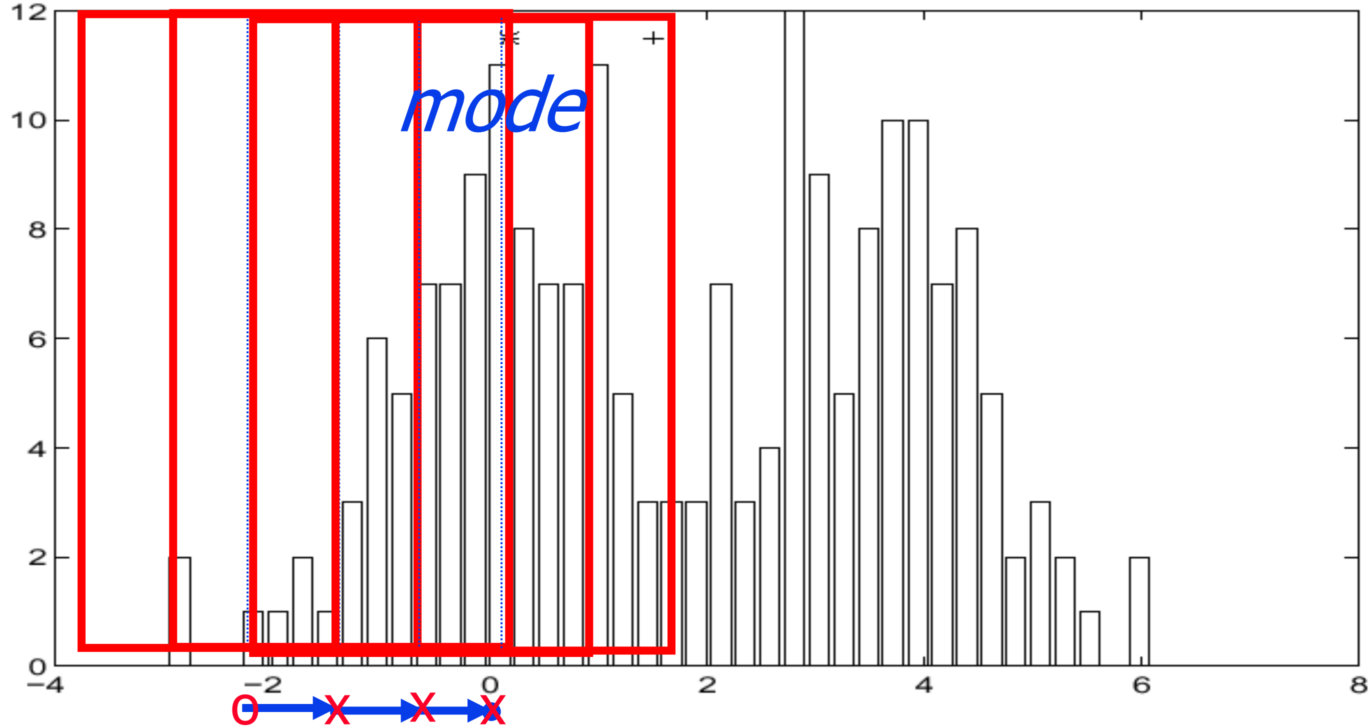


- How Many Modes Are There?
  - Easy to see, not too obvious how to compute

Mean Shift

[Fukunaga and Hostetler 1975, Cheng 1995, Comaniciu & Meer 2002]

Optional Material



Iterative Mode Search

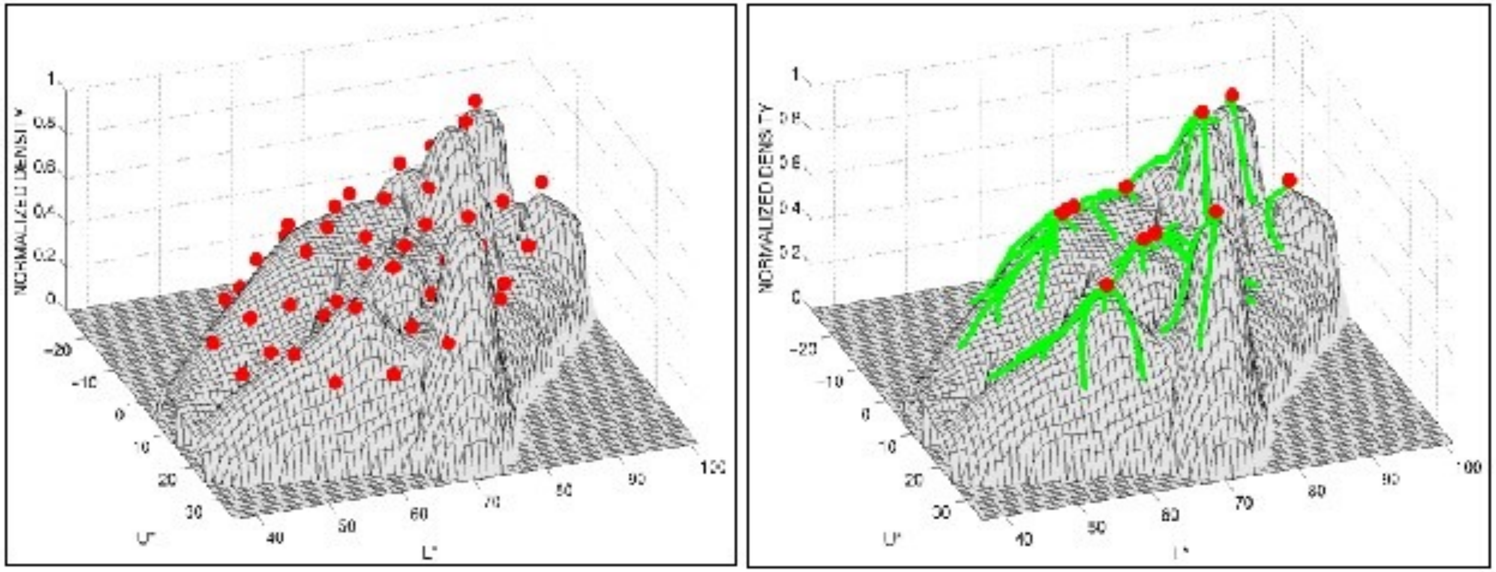
1. Initialize random seed, and fixed window
2. Calculate center of gravity 'x' of the window (the"mean")
3. Translate the search window to the mean
4. Repeat Step 2 until convergence

Mean Shift

[Fukunaga and Hostetler 1975, Cheng 1995, Comaniciu & Meer 2002]

Multimodal Distributions

- Parallel processing of an initial tessellation.
- Pruning of mode candidates.
- Classification based on the basin of attraction.



Mean shift trajectories

Mean Shift as K-modes

[Salah, Mitche, Ben-Ayed 2010]

Optional Material

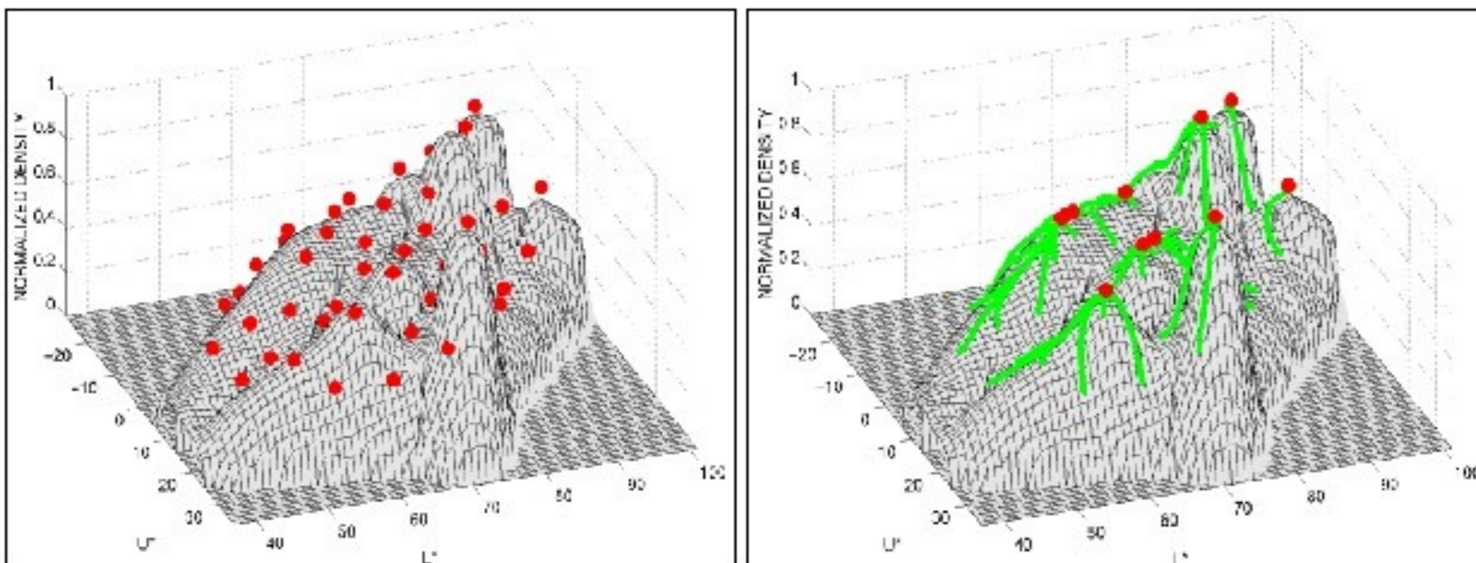
$$\sum_{k=1}^{K}\sum_{p\in S^k}\left\|f_p-\mu_k\right\|_d \qquad \|\cdot\|_d \quad :$$

quadratic (*K-means*)

absolute (*K-medians*)

bounded (*K-modes*)

Mean-shift segmentation relates to distortion clustering with a bounded loss (**K-modes**)



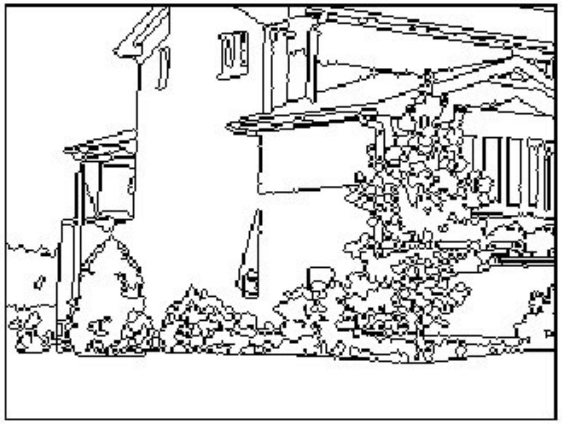
Mean shift trajectories

Mean-shift results for segmentation

Optional Material

RGB+XY clustering
[Comaniciu & Meer 2002]

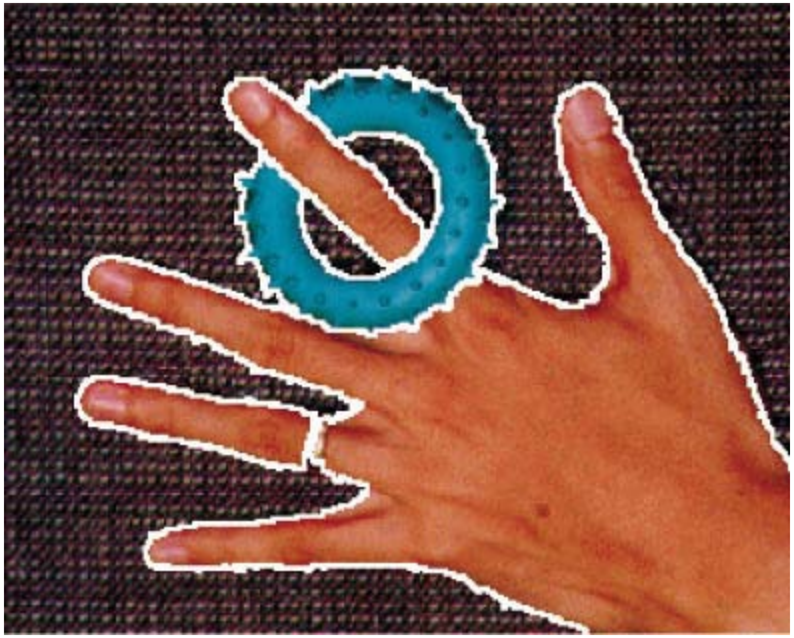
Figure 2: The *house* image, 255×192 pixels, 9603 colors.



Mean-shift results for segmentation

Optional Material

RGB+XY clustering
[Comaniciu & Meer 2002]



Mean-shift results for segmentation

Optional Material

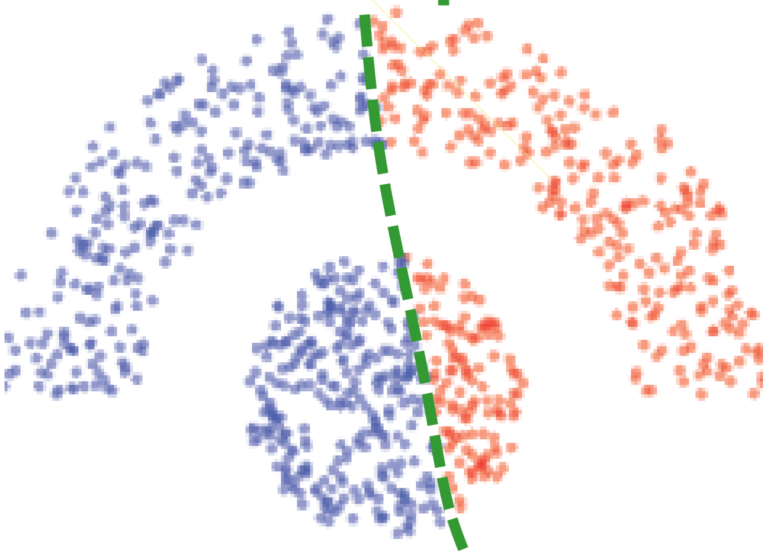
RGB+XY clustering
[Comaniciu & Meer 2002]

works well for segments with near-consistent color

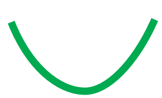
Basic K-means vs kernel K-means

$$\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} ||f_p - f_q||_K^2}{2|S^k|} \quad = \quad const - \sum_{k=1}^{K} \frac{\sum_{pq\in S^k} k(f_p, f_q)}{|S^k|}$$

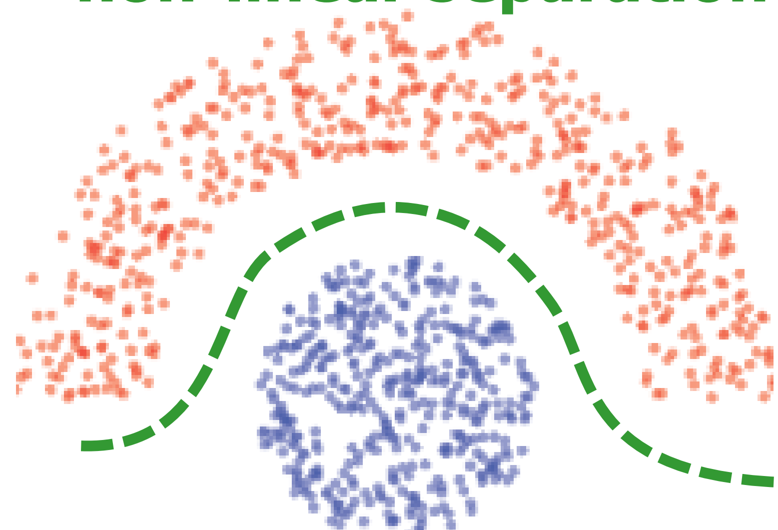
linear separation



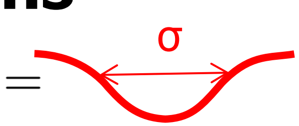
basic K-means

$\|f_p - f_q\|_K =$ 

non-linear separation



kernel K-means

e.g. Gaussian kernel => $\|f_p - f_q\|_K =$ 

From basic K-means to *kernel K-means*

(example: **Gaussian kernel** and its **robust metric** story)

easy to show

minimize distances within clusters — maximize affinities within clusters

$$\boxed{\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} ||f_p - f_q||_K^2}{2|S^k|}} = const - \boxed{\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} k(f_p, f_q)}{|S^k|}}$$

for any kernel-induced metric: $\quad ||f_p - f_q||_K^2 := k(f_p, f_p) + k(f_q, f_q) - 2k(f_p, f_q)$

NOTE: this is proper *metric* for any pos. def. kernels
e.g. works for *inner products*

Examples:

$k(f_p, f_q) = \langle f_p, f_q \rangle$
basic (linear) kernel

$\Longrightarrow$

squared L2 distance in standard K-means

$$||f_p - f_q||^2 = \langle f_p, f_p \rangle + \langle f_q, f_q \rangle - 2\langle f_p, f_q \rangle = \langle f_p - f_q, f_p - f_q \rangle$$

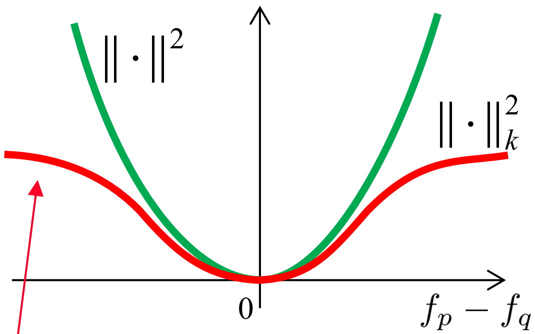
squared Euclidean distance

$k(f_p, f_q) = e^{-\frac{\|f_p - f_q\|^2}{2\sigma^2}}$
Gaussian kernel

$\Longrightarrow$

distance in Gaussian kernel K-means

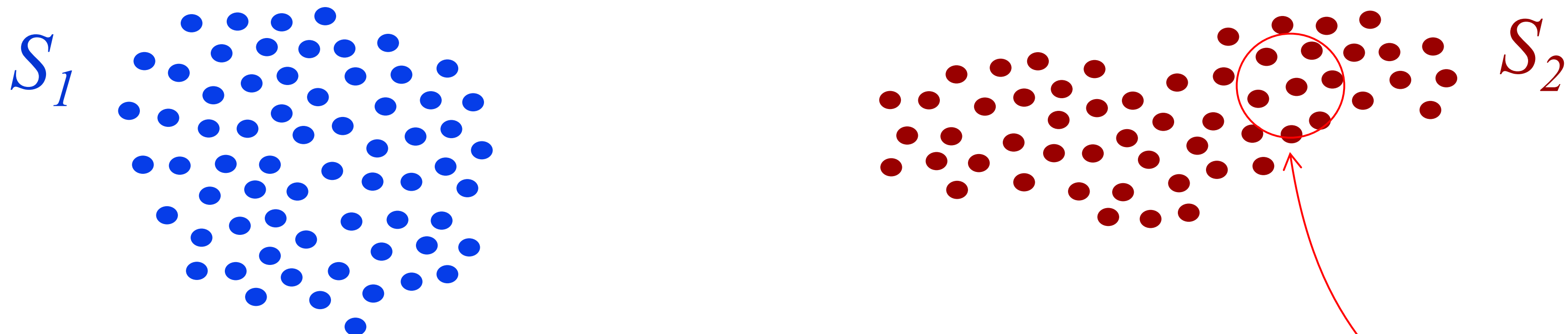
$$||f_p - f_q||_K^2 = 2\left(1 - e^{-\frac{\|f_p - f_q\|^2}{2\sigma^2}}\right)$$



robust metric focuses on **local distortion** (deemphasizes larger distances)

From basic K-means to *kernel K-means*

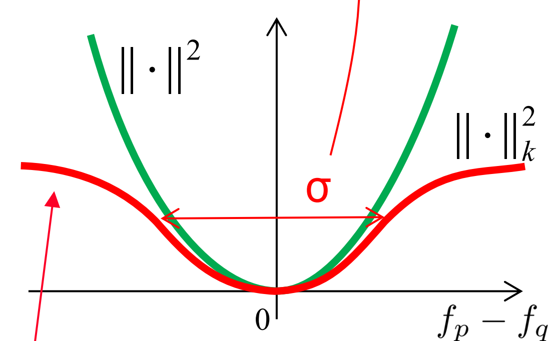
(example: **Gaussian kernel** and its **robust metric** story)



$$\boxed{\sum_{pq\in S_1} ||f_p - f_q||^2 \ll \sum_{pq\in S_2} ||f_p - f_q||^2}$$

$$\boxed{\sum_{pq\in S_1} ||f_p - f_q||_K^2 \approx \sum_{pq\in S_2} ||f_p - f_q||_K^2}$$

For Gaussian kernel both clusters look **equally tight/compact** since it “inspects” only their **neighborhoods of size σ**.



robust metric focuses on **local distortion** (deemphasizes larger distances)

Basic K-means vs kernel K-means

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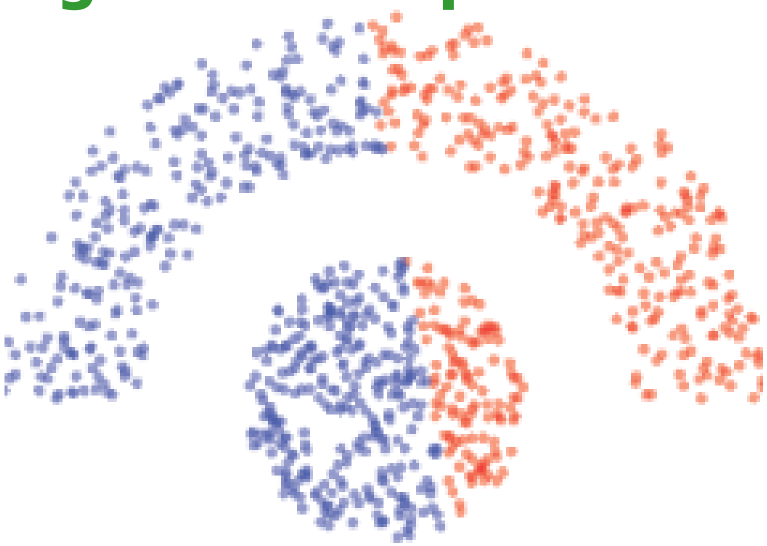
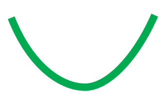
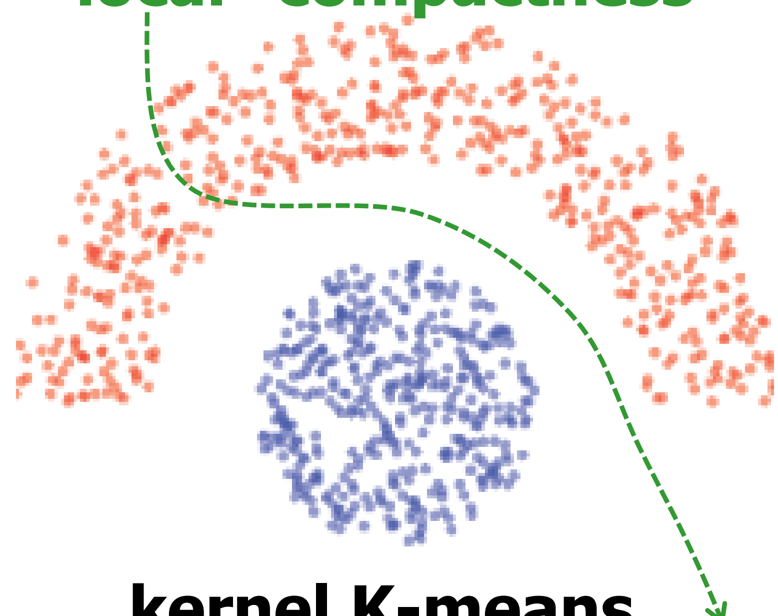
global "compactness"



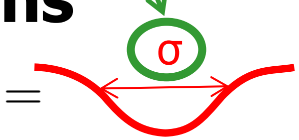
basic K-means

$\|f_p - f_q\|_K =$ 

local "compactness"



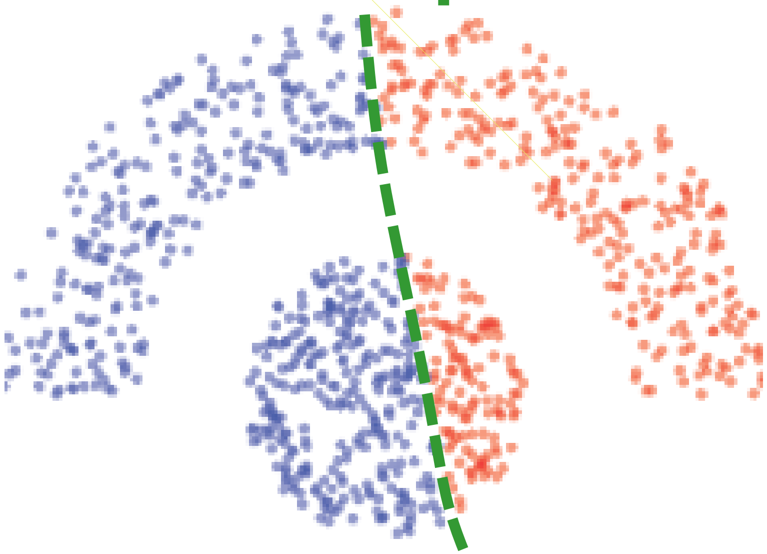
kernel K-means

e.g. Gaussian kernel => $\|f_p - f_q\|_K =$ 

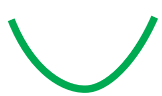
Basic K-means vs kernel K-means

$$\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} ||f_p - f_q||_K^2}{2|S^k|} \quad = \quad const - \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} k(f_p, f_q)}{|S^k|}$$

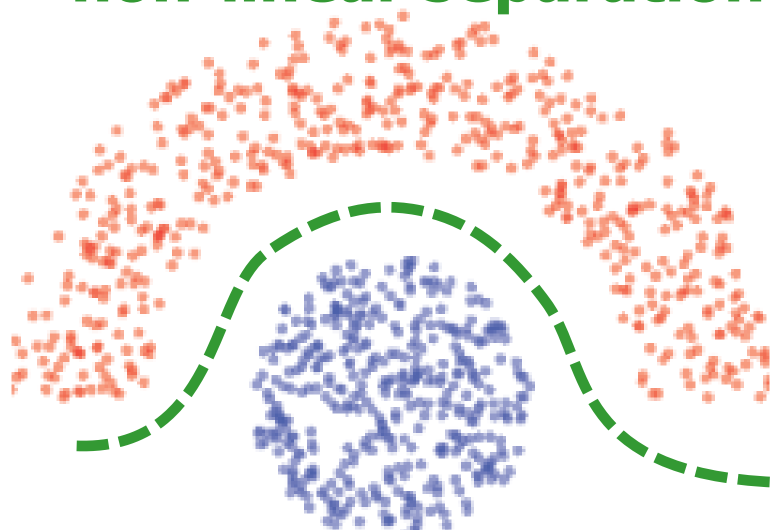
linear separation



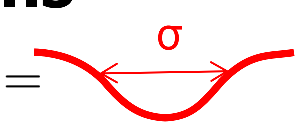
basic K-means

$\|f_p - f_q\|_K =$ 

non-linear separation



kernel K-means

e.g. Gaussian kernel => $\|f_p - f_q\|_K =$ 

kernel K-means

non-parametric (kernel) clustering

$$-\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} k(f_p, f_q)}{|S^k|}$$ - objective

Kernel-based clustering (a.k.a. pairwise clustering):

- robustness to outliers

- non-parametric approach, arbitrary separation boundary, assumes only “local compactness” instead of fitting parameters of distributions (of known class) to clusters

- there are known biases, **many variants** addressing them

- **optimization?** (no block-coordinate descent as we dropped cluster parameters)

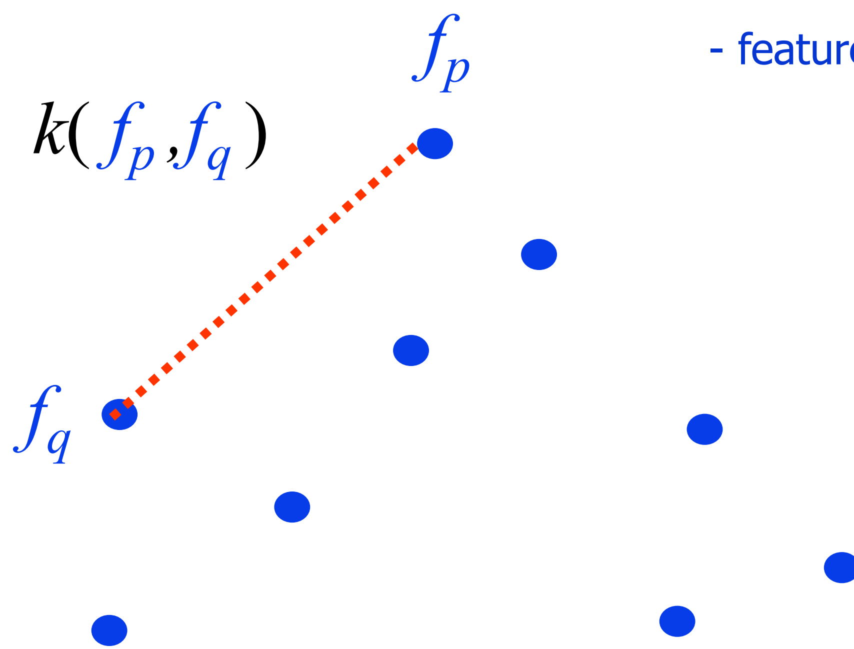
kernel K-means

non-parametric (kernel) clustering

$$-\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} k(f_p, f_q)}{|S^k|}$$

- objective

$$A_{pq} = k(f_p, f_q)$$



- features

kernel K-means

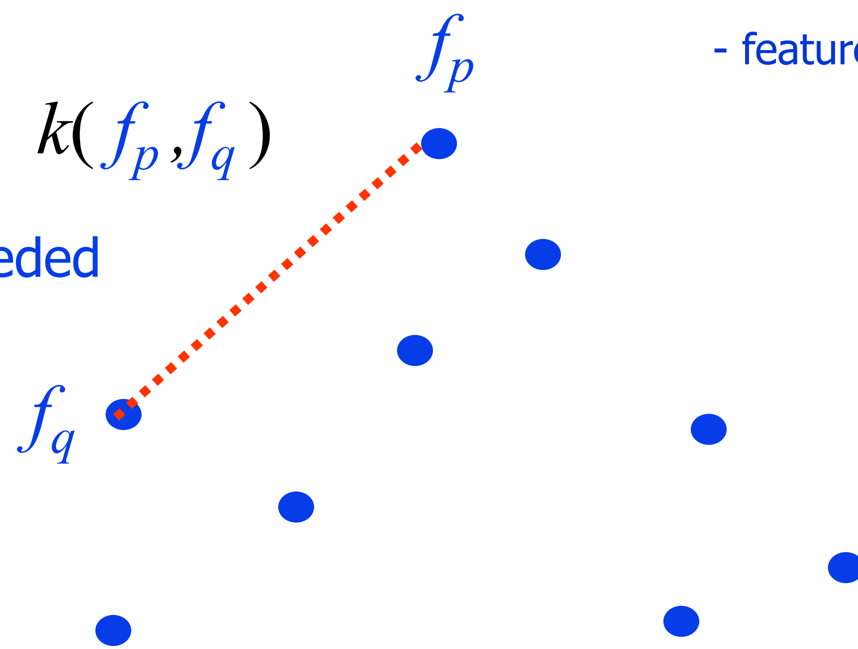
non-parametric (kernel) clustering

$$-\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} A_{pq}}{|S^k|}$$

- objective

- features

$$A_{pq} = k(f_p, f_q)$$



explicit features f_p are no longer needed

kernel K-means

non-parametric (kernel) clustering

$$-\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} A_{pq}}{|S^k|}$$

- objective

only need
affinity (or kernel) matrix

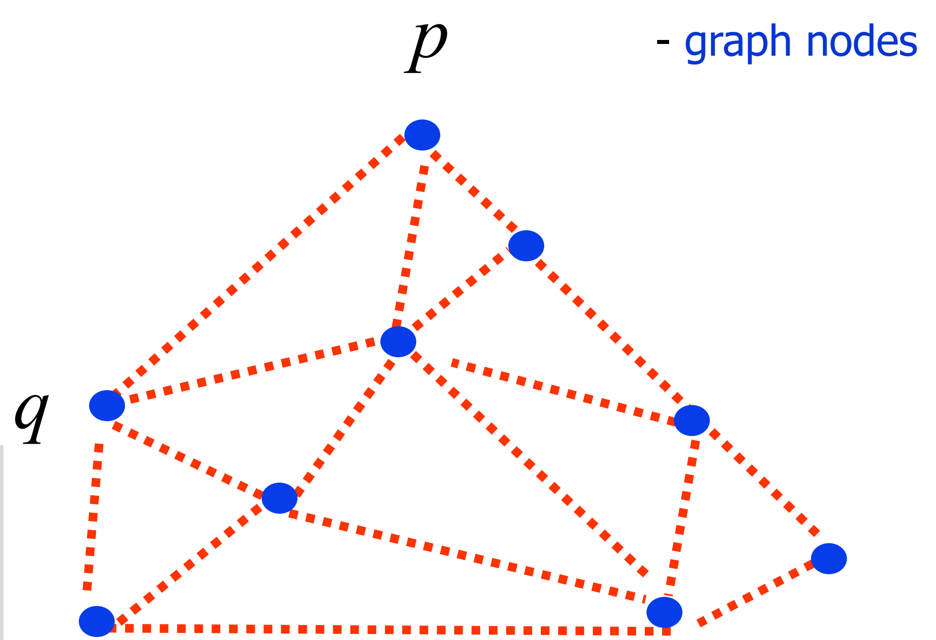
$A = [A_{pq}]$

(finite dimensional version of) MERCER THEOREM

if needed, can find "embedding" $\{\phi_p\}$

s.t. $A_{pq} = \langle \phi_p, \phi_q \rangle$

using eigen decomposition for p.s.d. A



Essentially, we formulated a **graph clustering problem**

kernel K-means

non-parametric (kernel) clustering

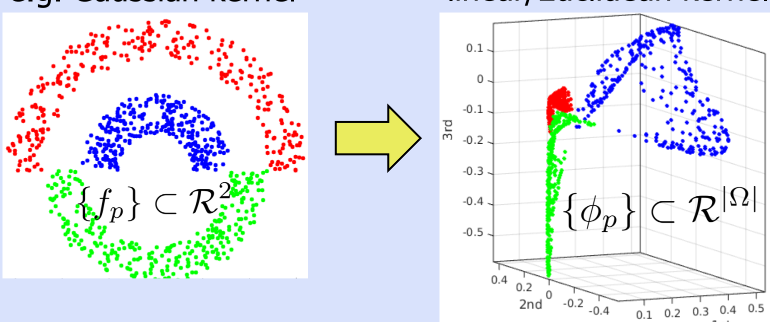
$$-\sum_{k=1}^{K} \frac{\sum_{pq\in S^k} A_{pq}}{|S^k|}$$

- objective

<u>high-dimensional isometric *Euclidean* embedding "story"</u>

$k(f_p, f_q) \;=\; A_{pq}$ = $A_{pq} \;=\; \langle \phi_p, \phi_q \rangle$

e.g. Gaussian kernel | linear/Euclidean kernel



if needed, can find "embedding" $\{\phi_p\}$

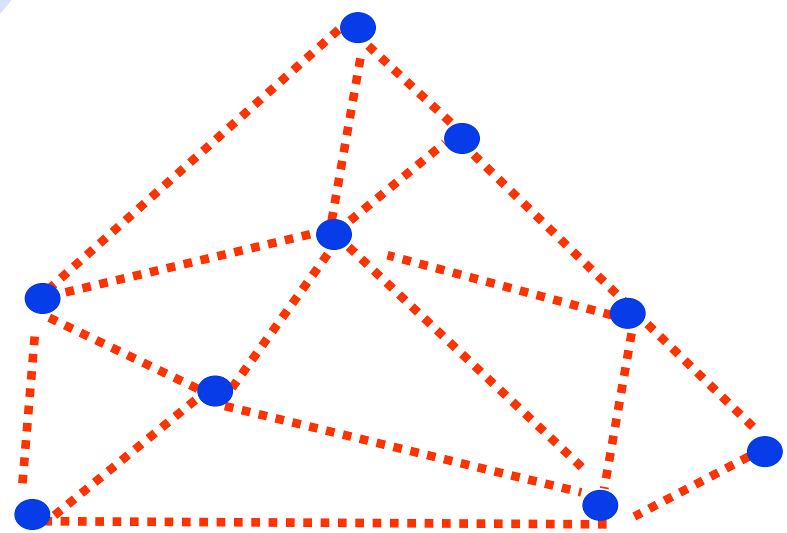
s.t. $A_{pq} \;=\; \langle \phi_p, \phi_q \rangle$

using eigen decomposition for p.s.d. A

(problem from HW4)

p - graph nodes

q



Essentially, we formulated a

graph clustering problem

Optimization for kernel clustering
(brief overview, details are left for homework 4)

- Idea 1: find (Euclidean) embedding $\{\phi_p\}$ s.t.

$$\langle \phi_p, \phi_q \rangle \;=\; A_{pq}$$

eigen decomposition of A *(p.s.d)*
(HW4 problem)

and use basic K-means (Lloyd's algorithm) over points $\{\phi_p\}$.

Problem: in general $\{\phi_p\} \subset \mathcal{R}^{|\Omega|}$ where $|\Omega|$ is the size of the data set

- Idea 2 **[spectral clustering]**: find embedding $\{\tilde{\phi}_p\}$ s.t.

$$\langle \tilde{\phi}_p, \tilde{\phi}_q \rangle \;=\; \tilde{A}_{pq}$$

where $\tilde{A}$ is a *low rank approximation* of A (of any rank m).

[*a la* **Eckart-Young-Mirsky theorem** in Topic 7].

In this case can check $\{\tilde{\phi}_p\} \subset \mathcal{R}^m$ and K-means over $\{\tilde{\phi}_p\}$ is practical (for smaller m).

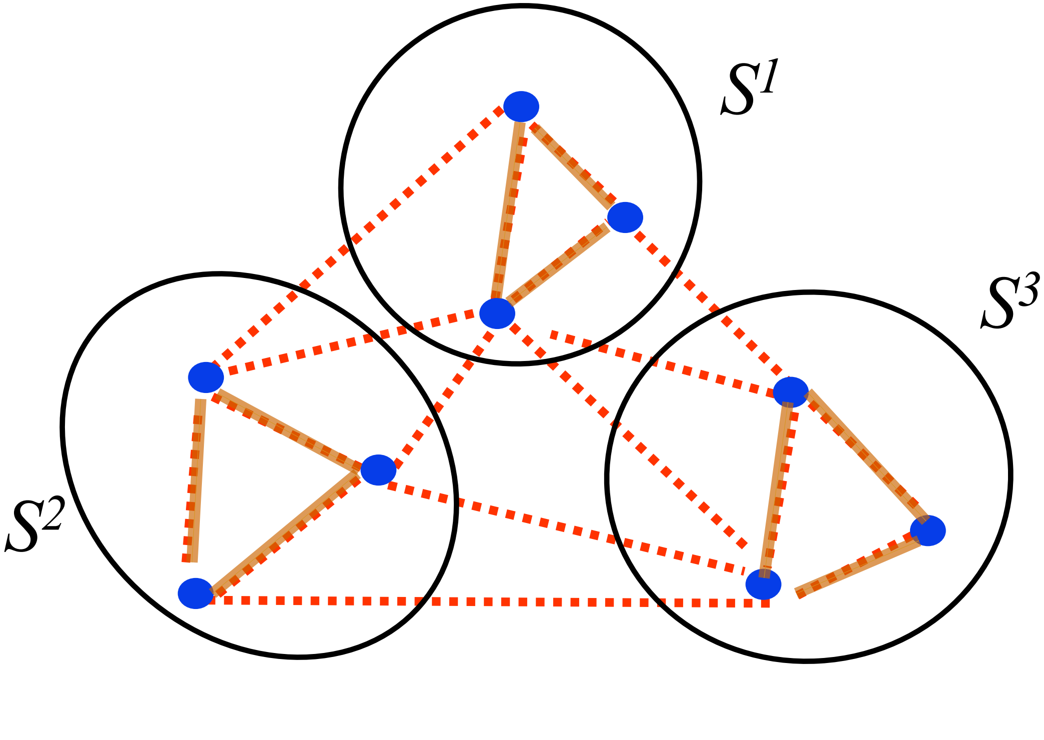
NOTE (relation to PCA): low-rank approximation $\tilde{A}$ keeps the most significant (m largest) eigen values of A.

kernel K-means or ***average association***

non-parametric (kernel) clustering

"self-association" of cluster S^k

$$E(S) = -\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} A_{pq}}{|S^k|}$$



kernel K-means or ***average association***

non-parametric (kernel) clustering

$$E(S) = -\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} A_{pq}}{|S^k|} \qquad \sum_{pq \in S^k} A_{pq} \equiv S^{k\prime} A S^k$$

in matrix notation:

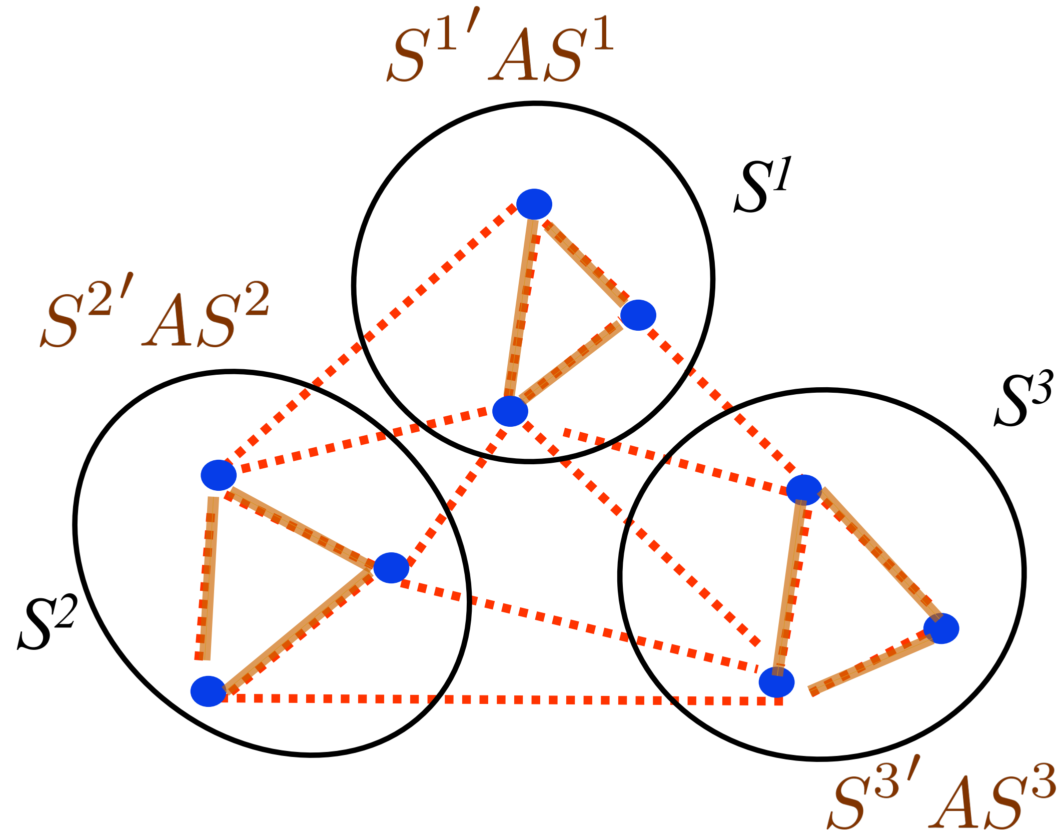
S^k - indicator vector

' means *transpose*

node indices

	1	2	3	4	5	6	7	8	9
$S^1 =$	[1	1	1	0	0	0	0	0	0]
$S^2 =$	[0	0	0	1	1	1	0	0	0]
$S^3 =$	[0	0	0	0	0	0	1	1	1]

assume clusters are represented by *indicator vectors* S^k



kernel K-means or ***average association***

non-parametric (kernel) clustering

$$E(S) = -\sum_{k=1}^{K} \frac{\qquad}{|S^k|}$$

$S^{k\prime} A S^k$

in matrix notation:

S^k - indicator vector

' means *transpose*

node indices

	1	2	3	4	5	6	7	8	9
$S^1 =$	[1	1	1	0	0	0	0	0	0]
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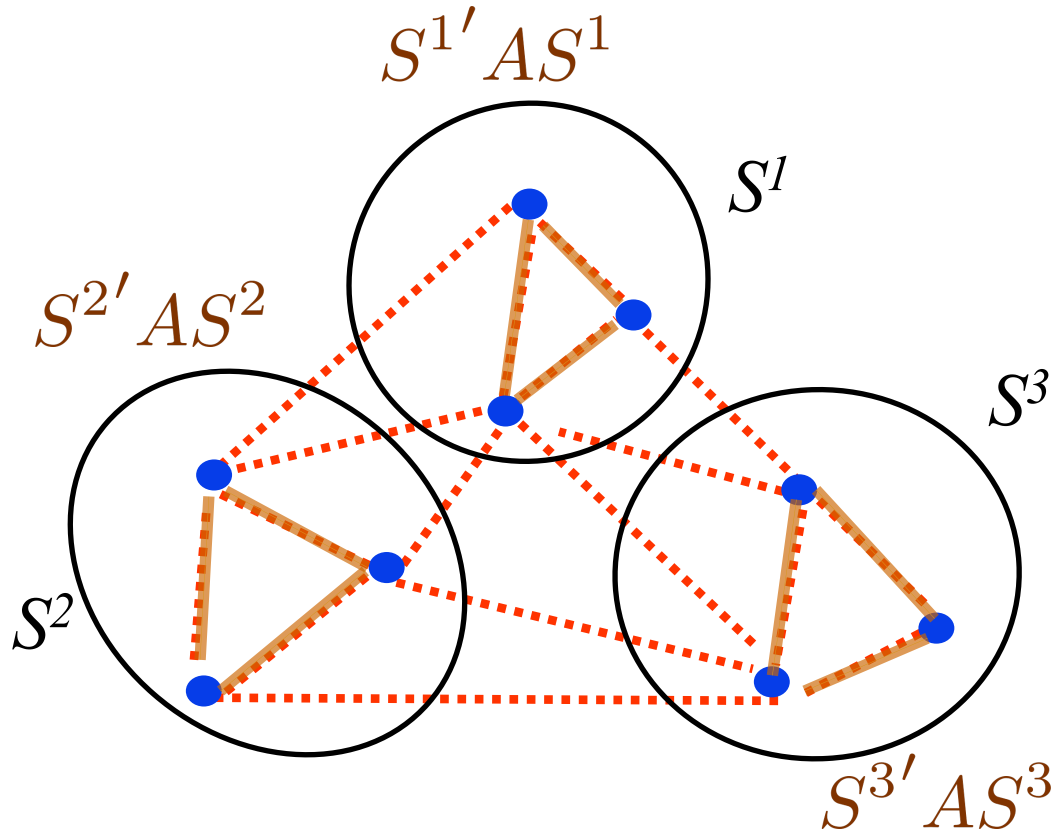
$S^3 =$	[0	0	0	0	0	0	1	1	1]

assume clusters are represented by
indicator vectors S^k



kernel K-means or ***average association***

non-parametric (kernel) clustering

$$E(S) = -\sum_{k=1}^{K} \frac{S^{k\prime} A S^k}{|S^k|}$$

in matrix notation:

S^k - indicator vector

` means *transpose*

node indices

	1	2	3	4	5	6	7	8	9
$S^1 =$	[1	1	1	0	0	0	0	0	0]
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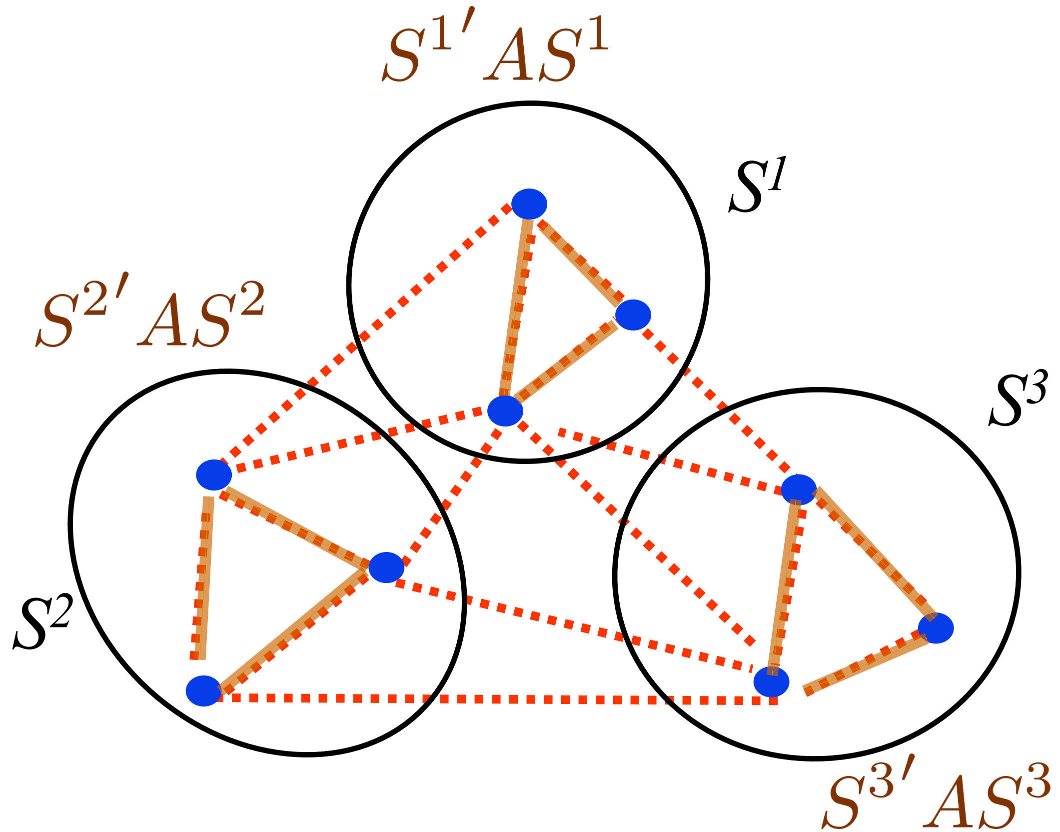
$S^3 =$	[0	0	0	0	0	0	1	1	1]

assume clusters are represented by *indicator vectors* S^k



Convenient general notation

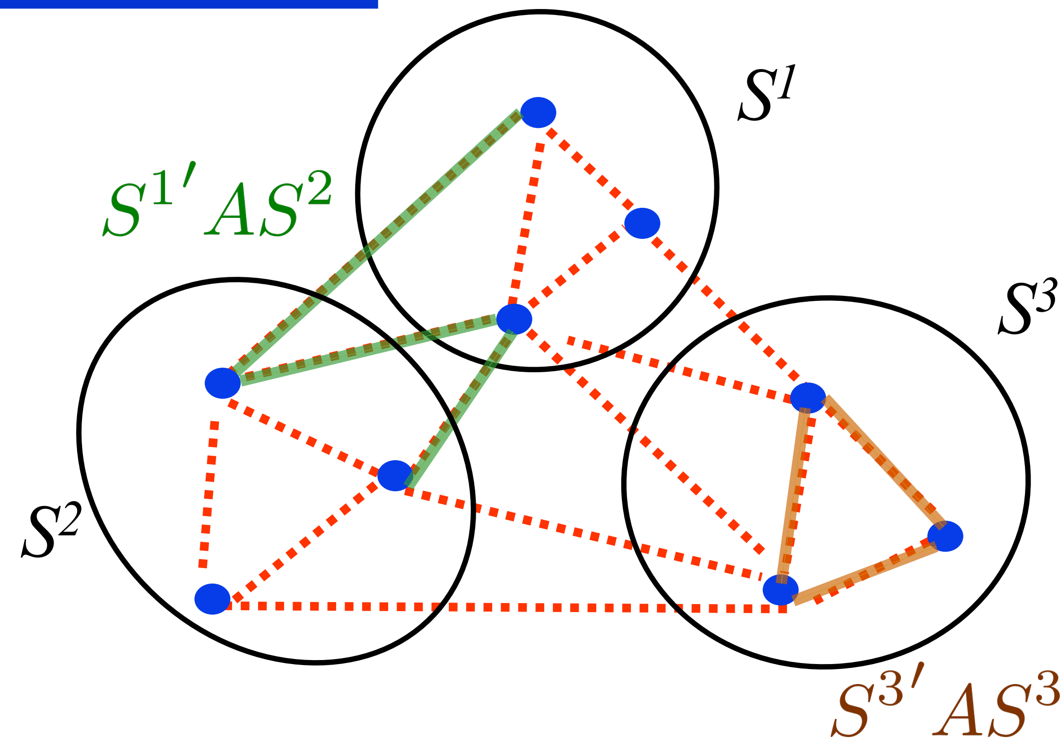
$$S^{i\prime} A S^{j} \equiv \sum_{p \in S^{i}, q \in S^{j}} A_{pq}$$

sum of all graph edge weights A_{pq} from set S^i to set S^j

node indices

	1	2	3	4	5	6	7	8	9
$S^1 =$	[1	1	1	0	0	0	0	0	0]
$S^2 =$	[0	0	0	1	1	1	0	0	0]
$S^3 =$	[0	0	0	0	0	0	1	1	1]

assume clusters are represented by *indicator vectors* S^k



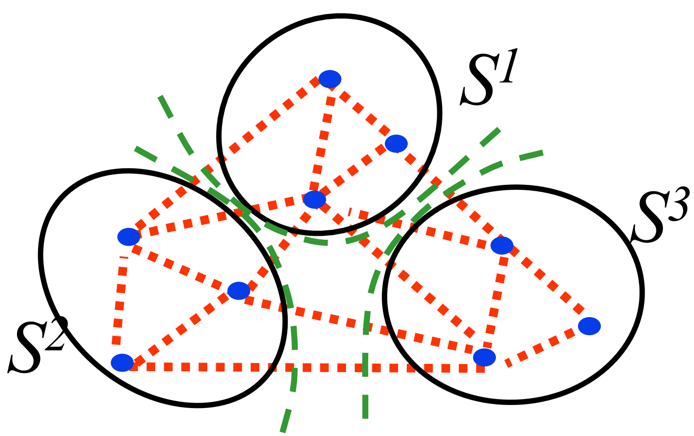
Other graph clustering objectives

related to Cheeger cut,
spectral graph theory,
isoperimetic constant, etc

Average Cut

"cut" for S^k

$$\sum_{k=1}^{K} \frac{S^{k'} A \, (\mathbf{1} - S^k)}{|S^k|}$$

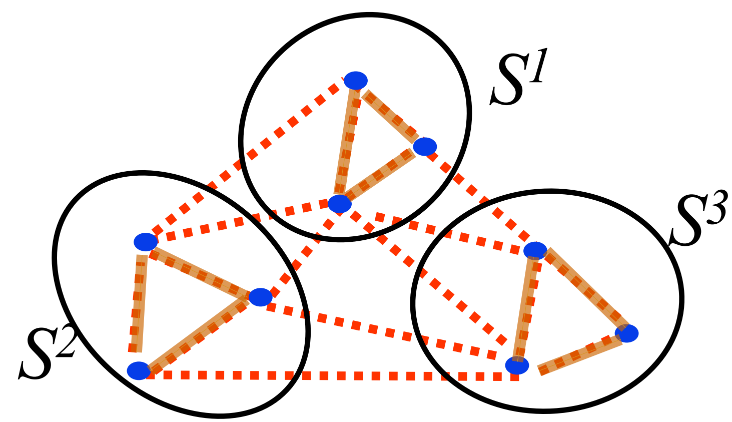


so far only looked at

Average Association

"self-association" for S^k

$$-\sum_{k=1}^{K} \frac{S^{k'} A \, S^k}{|S^k|}$$



Typically, approximately optimized via spectral methods using strongest *eigenvalues / eigenvectors of A*

Other graph clustering objectives

- **Average Association**

$$-\sum_{k=1}^{K} \frac{S^{k'} A\, S^{k}}{|S^k|}$$

- **Average Cut**

$$\sum_{k=1}^{K} \frac{S^{k'} A\,(\mathbf{1} - S^{k})}{|S^k|} \qquad \mathbf{1}' S^k$$

- **Normalized Cut**

[Shi & Malik, 2000]

$$\sum_{k=1}^{K} \frac{S^{k'} A\,(\mathbf{1} - S^{k})}{d' S^k} \equiv K - \sum_{k=1}^{K} \frac{S^{k'} A\, S^{k}}{d' S^k}$$

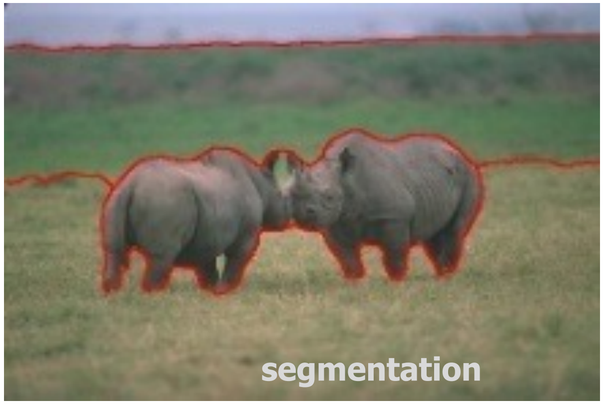
for $d := A\mathbf{1}$

Basic K-means vs Kernel Clustering

$$E(S) = -\sum_{k=1}^{K} \frac{S^{k\prime} A S^k}{|S^k|}$$

compact "blobs" in RGB**XY** space

[Achanta et al., PAMI 2011]



[Shi&Malik 2000]

"segments" in RGB**XY** space

not just super-pixels

basic K-means

for $A_{pq} = \langle f_p, f_q \rangle$

kernel K-means

e.g. for Gaussian kernel $A_{pq} = \exp - \frac{\|f_p - f_q\|^2}{2\sigma^2}$

What have we learned today

- K-means clustering
- K-modes clustering via mean-shift
- Kernel K-means for nonlinear clustering