Lecture 11

K-means and Mean Shift







Administrative

A3 is out

- Due Feb 21st

A4 will be out soon





Administrative

Recitation

- Multiview geometry





Content-aware Retargeting Operators



"Important" content







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So far: Segmentation and clustering

• Goal: identify groups of pixels that go together









So far: Agglomerative clustering



- 1. Say "Every point is its own cluster"
- Find "most similar" pair of clusters
- 3. Merge it into a parent cluster
- 4. Repeat

RR

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Today's agenda

- K-means clustering
- Mean-shift clustering
- Normalized cuts

Reading: Szeliski, 2nd edition, Chapter 7.5

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Today's agenda

- K-means clustering
- Mean-shift clustering
- Normalized cuts

Reading: Szeliski Chapters: 5.2.2, 7.5.2

D. Comaniciu and P. Meer, Mean Shift: A Robust Approach toward Feature Space Analysis, PAMI 2002.

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Image Segmentation: Binary image Example



- These pixel values show that there are three things in the image.
- We could label every pixel in the image according to which of these primary intensities it is.
 - \circ i.e., segment the image based on the intensity feature.
- What if the image isn't quite so simple?

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 How do we determine the three main intensities that define our groups?

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- Each cluster has a cluster center
 - A mean cluster value.

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- Goal: choose three "centers" as the representative intensities and label every pixel according to which of these centers it is nearest to.
- Best cluster centers are those that minimize Sum of Square Distance (SSD) between all points and their nearest cluster center c_i:

$$SSD = \sum_{C} \sum_{v \in C} (v - c_i)^2$$

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Clustering

- With this objective, it is a "chicken and egg" problem:
 - If we knew the *cluster centers*, we could allocate points to groups by assigning each to its closest center.



 If we knew the group memberships, we could get the centers by computing the mean per group.





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Given, a set of points, randomly select k=3 of them to be the cluster centers



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Categorize each point into a cluster defined by its closest center.

Next, move the cluster centers to location amongst its cluster



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Repeat with new cluster center locations



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Categorize into new clusters. Move center to the mean



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Repeat with new cluster centers



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Computational Complexity

At each iteration,

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- Computing distance between each of the n objects and the K cluster centers is O(Kn).
- Computing cluster centers: Each object gets added once to some cluster: O(n).

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Assume these two steps are each done once for I iterations: O(IKn).

Q. Is K-means guaranteed to converge to a global maximum?





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- Some seeds can result in poor convergence rate, or convergence to sub-optimal clustering.
- Select good seeds using a heuristic (e.g., object least similar to any existing mean)

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- Try out multiple starting points (very important!!!)
- Initialize with the results of another method.

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Other issues with k-means

Shape of clusters

Assumes isotopic, convex clusters
Sensitive to Outliers



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How to choose the value of k

- Number of clusters K
 - Objective function

Look for "Knee" in objective function



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Clustering

Goal: cluster to minimize distance of pixels to their cluster centers



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1. Initialize (t = 0): cluster centers $c_1, ..., c_K$







- 1. Initialize (t = 0): cluster centers $c_1, ..., c_K$
- 2. Compute δ^t : assign each point to the closest center
 - δ^t denotes the set of assignment for each v_j to cluster c_i at iteration t

$$\delta^{t} = \arg\min_{\delta} \frac{1}{N} \sum_{j}^{N} \sum_{i}^{N} \delta_{ij}^{t-1} (c_{i}^{t-1} - v_{j})^{2}$$





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3. Computer C^{t} : update cluster centers as the mean of the points

$$c^{t} = \arg\min_{c} \frac{1}{N} \sum_{j}^{N} \sum_{i}^{K} \delta_{ij}^{t} (c_{i}^{t-1} - v_{j})^{2}$$

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4. Update t = t + 1, Repeat Step 2-3 till stopped

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Initial cluster centers are randomly initialized

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- Can lead to bad initializations
- Can cause bad clusters



Another example of how K-means Converges to a local minimum solution

Initialize multiple runs!



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K-Means++

Tries to prevent arbitrarily bad local minima?

- 1. Randomly choose first center.
- 2. Pick new center with prob. proportional to $(c_i v_j)^2$
 - a. Basically we want to find as good of an initialization as possible

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3. Repeat until K centers.

Initial cluster centers are randomly initialized

- Can lead to bad initializations
- Can cause bad clusters

Different distance measures can change K-Means clusters

- Euclidean distance of cosine distance.

Different feature space can lead to different cluster

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Segmentation as Clustering



Original image



2 clusters



3 clusters

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Feature Space: pixel value

- Feature space: what measurements do we include in x_i ?
- Depending on what we choose as the *feature space*, we can group pixels in different ways.
- Grouping pixels based on intensity similarity

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• Feature space: intensity value (1D)

Feature Space: RGB

- Depending on what we choose as the *feature space*, we can group pixels in different ways.
- Grouping pixels based on color similarity

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• Feature space: color value (3-dim)



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Feature Space: edges and blobs

- Depending on what we choose as the *feature space*, we can group pixels in different ways.
- Grouping pixels based on oriented gradient similarity







• Feature space: filter bank responses (e.g., 24D)

24 edge & blog filters

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Smoothing Out Cluster Assignments

• Assigning a cluster label per pixel may yield outliers:



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Feature Space: RGB + XY location

- Depending on what we choose as the *feature space*, we can group pixels in different ways.
- Grouping pixels based on *intensity+position* similarity





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 \Rightarrow Way to encode both *similarity* and *proximity*.

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K-Means Clustering Results

• Clusters don't have to be spatially coherent



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K-Means Clustering Results

 Clustering based on (r,g,b,x,y) values enforces more spatial coherence



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How to evaluate clusters?

• Generative

How well are points reconstructed from the clusters?

• Discriminative

- How well do the clusters correspond to labels?
 - Can we correctly classify which pixels belong to the panda?
- Note: unsupervised clustering does not aim to be discriminative as we don't have the labels.

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How to choose the number of clusters?

Try different numbers of clusters in a validation set and look at performance.

Plot of SSD versus values of k

abrupt change at k=2 is suggestive of two clusters in the data



Slide: **Feelphblarry 11**, 2025

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K-Means pros and cons

• Pros

- Good representation of data
- Simple and fast, Easy to implement

• Cons

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- Need to choose K
- Sensitive to outliers
- Prone to local minima
- All clusters have the same parameters (e.g., distance measure is non-adaptive)
- Can still be slow: each iteration is O(KNd) for N d-dimensional pixels







(A): Two natural clusters

(B): k-means clusters

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What will we learn today?

- K-means clustering
- Mean-shift clustering
- Normalized cuts





Mean-Shift Segmentation

An advanced and versatile technique for clustering-based segmentation



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http://www.caip.rutgers.edu/~comanici/MSPAMI/msPamiResults.html

D. Comaniciu and P. Meer, Mean Shift: A Robust Approach toward Feature Space Analysis, PAMI 2002.

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Mean-Shift



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Mean-Shift



Slide by Y. Ukrainitz & B. Sarel

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Real Modality Analysis



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The blue data points were traversed by the windows towards the mode.

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Mean-Shift Algorithm

- 1. Represent each pixel *i* using some feature vector v_i
- 2. Generate a window **W** as a random pixel feature v_{μ}
- 3. Identify all the pixels within a radius *r* of v_w
- 4. Calculate the mean ("center of gravity") amongst the neighbors of **W**

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- 5. Translate the window **W** to the mean feature location
- 6. Repeat Step 2 until convergence

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Mean-Shift Clustering

- Initialize not just 1 window but a multiple windows at random
- All pixels that end up in the same location belong to the same cluster
- Attraction basin: the feature region for which all windows end up in the same location



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Mean-Shift Segmentation Results









http://www.caip.rutgers.edu/~comanici/MSPAM I/msPamiResults.html

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More Results







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More Results



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Problem: Computational Complexity



- Need to shift one window for every pixel
- Many computations will be redundant.

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Speedups: Basin of Attraction



1. Assign all points within radius r of end point to the mode.

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Speedups

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2. Assign all points within radius r/c of the search path to the mode -> reduce the number of data points to search.

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Example of what running mean shift looks like



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Another example





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Mean-Shift Clustering

- Find features (color, gradients, texture, etc)
- Initialize windows at individual pixel locations
- Perform mean shift for each window until convergence
- At every step, merge windows that have high overlap to reduce computation



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Mean-Shift pros and cons

• Pros

- General, application-independent algorithm
- Model-free, does not assume any prior shape (spherical, elliptical, etc.) of data clusters
- Just a single parameter (window size r)
 - r has a physical meaning (unlike k-means)
- Finds variable number of modes
- Robust to outliers

• Cons

- $\circ\,$ Output depends on window size
- $\circ\,$ Window size (bandwidth) selection is not easy
- Computationally (relatively) expensive (~2s/image)
- $\circ\,$ Does not scale well with dimension of feature space

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Today's agenda

- K-means clustering
- Mean-shift clustering
- Normalized cuts





Images as Graphs



- Node (vertex) for every pixel
- Edge between pairs of pixels, (p,q)
- Affinity weight w_{pq} for each edge
 - w_{pg} measures similarity
 - Similarity is inversely proportional to difference (in color and position...)



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Images as Graphs

Which edges to include?

Fully connected:

- Captures all pairwise similarities
- Infeasible for most images

Neighboring pixels:

- Very fast to compute
- Only captures very local interactions

Local neighborhood:

- Reasonably fast, graph still very sparse
- Good tradeoff

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- Distance: $aff(x, y) = \exp\left(-\frac{1}{2\sigma_d^2} \|f(x) f(y)\|^2\right)$
- Examples:

$$f(x) = location(x)$$

- Distance:
- f(x) = intensity(x)

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- Intensity: f(x) = color(x)
- Color: f(x) = filterbank(x)
- Texture:

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Distance: f(x) = location(x)



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Intensity: f(x) = intensity(x)



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Color: f(x) = color(x)



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Texture: f(x) = filterbank(x)

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Segmentation as Graph Cuts





Break Graph into Segments

- Delete links that cross between segments
- Easiest to break links that have low similarity (low weight)
 - Similar pixels should be in the same segments
 - Dissimilar pixels should be in different segments

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slide credit: Steve Seitz



Graph Cut with Eigenvalues

- Given: Affinity matrix W
- Goal: Extract a single good cluster v
 - v(i): score for point *i* for cluster vmax $v^T W v$

$$\begin{array}{c} \max_{v} v v v v \\ \text{s.t.} v^T v = 1 \end{array}$$





Optimizing



Lagrangian:
$$-\frac{1}{2}v^{T}Wv + \lambda(v^{T}v - 1)$$
$$-Wv + \lambda v = 0$$

 $Wv = \lambda v$

v is an eigenvector of W

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Clustering via Eigenvalues

- 1. Construct affinity matrix *W*
- 2. Compute eigenvalues and vectors of *W*
- 3. Until done
 - 1. Take eigenvector of largest unprocessed eigenvalue
 - 2. Zero all components of elements that have already been clustered
 - 3. Threshold remaining components to determine cluster membership

Note: This is an example of a *spectral clustering* algorithm

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Graph Cuts - Another Look



- Set of edges whose removal makes a graph disconnected
- Cost of a cut cut(A, B) =
 - Sum of weights of cut edges:

$$cut(A,B) = \sum_{p \in A, q \in B} w_{pq}$$

- A graph cut gives us a segmentation
 - What is a "good" graph cut and how do we find one?

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Formulation: Min Cut

We can do segmentation by finding the *minimum cut*

- either smallest number of elements (unweighted) or smallest sum of weights (weighted)
- efficient algorithms exist
- Drawback

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- Weight of cut proportional to number of edges
- Biased towards cutting small, isolated components



Solution: Normalized Cuts

- 1. Construct weighted graph G = (V, E)
- 2. Construct affinity matrix W
- 3. Solve for smallest few eigenvectors. $(D W)y = \lambda Dy$
- 4. Threshold eigenvectors to get a discrete cut
 - This is the approximation
 - As before, several heuristics for doing this
 - 5. Recursively subdivide as desired.

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Formulation: Normalized Cuts

- Key idea: normalize segment size
 - Fixes min cut's bias
- Formulation:

$$Ncut(A, B) = \frac{cut(A, B)}{assoc(A, V)} + \frac{cut(A, B)}{assoc(B, V)}$$
$$= cut(A, B) \left[\frac{1}{\sum_{p \in A} w_{p,q}} + \frac{1}{\sum_{q \in B} w_{p,q}} \right]$$

assoc(A, V =) sum of weights of edges in V that touch A

• NP-hard, but can approximate

J. Shi and J. Malik. Normalized cuts and image segmentation. PAMI 2000

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NCuts as Generalized Eigenvector Problem

Definitions:

$$W: affinity matrix$$

 $D: D(i,i) = \sum_{j} w_{i,j}$
 $z: diagonal matrix {-1,1}^N, z_i = 1 \Leftrightarrow i \in A$
 $: vector in$



In matrix form:

$$NCut(A, B) = \frac{cut(A, B)}{assoc(A, V)} + \frac{cut(A, B)}{assoc(B, V)}$$
$$= \frac{(1+z)^T (D-W)(1+z)}{k1^T D1} + \frac{(1-z)(D-W)(1-z)}{(1-k)1^T D1}; \quad k = \frac{\sum_{z_i > 0} D(i, i)}{\sum_i D(i, i)}$$
$$= \dots$$

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After a lot of math...

• After simplification, we get

$$NCut(A, B) = \frac{y^T(D - W)y}{y^T D y},$$
 $y_i \in \{1, -b\}, y^T D 1 = 0$ This is hard,
y is discrete.

- This is a Rayleigh Quotient
 - Solution given by the "generalized" eigenvalue problem $(D-W)y=\lambda Dy$

Relaxation: continuous y

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- Subtleties
 - __Optimal solution is second smallest eigenvector
 - __Gives continuous result—must convert into discrete values of y

Slide credit: Alyosha Efros Ranjay Krishna

Normalized Cuts example



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Normalized Cuts example







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Normalized Cuts example



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Normalized Cuts summary

- Pro
 - Flexible to choice of affinity matrix
 - Generally works better than other methods we've seen so far



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• Con

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- Can be expensive, especially with many cuts.
- Bias toward balanced partitions
- Constrained by affinity matrix model

Today's agenda

- K-means clustering
- Mean-shift clustering
- Normalized cuts





Next time

Cameras and Calibration





Other Kernels

A kernel is a function that satisfies the following requirements :

1.
$$\int_{R^d} \phi(x) = 1$$

 $\mathbf{2.} \ \phi(x) \ge 0$

Some examples of kernels include :

1. Rectangular
$$\phi(x) = \begin{cases} 1 & a \leq x \leq b \\ 0 & else \end{cases}$$

2. Gaussian $\phi(x)=e^{-rac{x^2}{2\sigma^2}}$

3. Epanechnikov
$$\phi(x) = \begin{cases} rac{3}{4}(1-x^2) & if \ |x| \leq 1 \\ 0 & else \end{cases}$$

<u>source</u>

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Technical Details

Taking the derivative of:
$$\hat{f}_{K} = \frac{1}{nh^{d}} \sum_{i=1}^{n} K\left(\frac{\mathbf{x} - \mathbf{x}_{i}}{h}\right)$$

$$\nabla \hat{f}(\mathbf{x}) = \underbrace{\frac{2c_{k,d}}{nh^{d+2}} \left[\sum_{i=1}^{n} g\left(\left\|\frac{\mathbf{x} - \mathbf{x}_{i}}{h}\right\|^{2}\right)\right]}_{\text{term 1}} \underbrace{\left[\frac{\sum_{i=1}^{n} \mathbf{x}_{i} g\left(\left\|\frac{\mathbf{x} - \mathbf{x}_{i}}{h}\right\|^{2}\right)}{\sum_{i=1}^{n} g\left(\left\|\frac{\mathbf{x} - \mathbf{x}_{i}}{h}\right\|^{2}\right) - \mathbf{x}\right]}_{\text{term 2}}, \quad (3)$$

where g(x) = -k'(x) denotes the derivative of the selected kernel profile.

- Term1: this is proportional to the density estimate at x (similar to equation 1 from two slides ago).
- Term2: this is the mean-shift vector that points towards the direction of maximum density.

Comaniciu & Meer, 2002

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Technical Details

Finally, the mean shift procedure from a given point x_{t} is:

1. Compute the mean shift vector **m**:

$$\left[\frac{\sum\limits_{i=1}^{n}\mathbf{x}_{i}g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_{i}}{h}\right\|^{2}\right)}{\sum\limits_{i=1}^{n}g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_{i}}{h}\right\|^{2}\right)}-\mathbf{x}\right]$$

2. Translate the density window:

$$\mathbf{x}_i^{t+1} = \mathbf{x}_i^t + \mathbf{m}(\mathbf{x}_i^t).$$

3. Iterate steps 1 and 2 until convergence.

$$abla f(\mathbf{x}_i) = 0.$$

Comaniciu & Meer, 2002

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Technical Details

Given n data points $\mathbf{x}_i \in \mathbb{R}^d$, the multivariate kernel density estimate using a radially symmetric kernel¹ (e.g., Epanechnikov and Gaussian kernels), $K(\mathbf{x})$, is given by,

$$\hat{f}_K = \frac{1}{nh^d} \sum_{i=1}^n K\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right),\tag{1}$$

where h (termed the *bandwidth* parameter) defines the radius of kernel. The radially symmetric kernel is defined as,

$$K(\mathbf{x}) = c_k k(\|\mathbf{x}\|^2),\tag{2}$$

where c_k represents a normalization constant.

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