# **Graph Theoretic Clustering**



## Renyi entropy

- Free parameter:  $\alpha$  or q
- Denoted as  $H_{R\alpha}$  or  $H_{R\alpha}$

$$H_{\alpha}(X) = \frac{1}{1 - \alpha} \log_2 \left( \sum_{i=1}^n p_i^{\alpha} \right)$$

$$H_{R2}$$
 (i.e.  $\alpha = 2$ )

•
$$H_{R2}$$
=-log  $\Sigma_i p_i^2$ 



## Information potential

$$H_{\alpha}(X) = \frac{1}{1-\alpha} \log \left( \sum_{k=1}^{N} p_k^{\alpha} \right) = -\log \left( \sum_{k=1}^{N} p_k^{\alpha} \right)^{\frac{1}{\alpha-1}}$$

Information Potential = 
$$V^{\alpha}(x) = \sum_{k=1}^{n} p_k^{\alpha}$$

Information potential is Sum of powered probabilities



# Information potential is Sum of powered probabilities

- How to get PDF?
- Parzen windowing



## Example

Given a set of five data points x1 = 2, x2 = 2.5, x3 = 3, x4 = 1 and x5 = 6

Find Parzen probability density function (pdf) estimates at x = 3, using the Gaussian function with  $\sigma = 1$  as window function



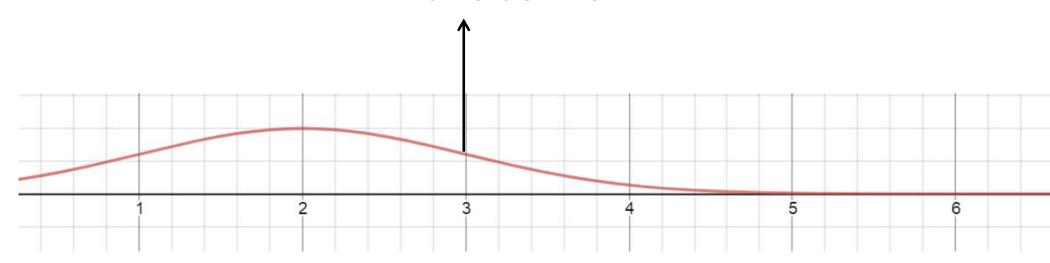
## Algorithm

#### x1 = 2, x2 = 2.5, x3 = 3, x4 = 1 and x5 = 6

- 1. Place a Gaussian at x=2 i.e.  $\mu=2$
- 2. Find its value @ x=3
- 3. Place a Gaussian at x=2.5 i.e.  $\mu=2.5$
- 4. Find its value @ x=3
- 5. ..
- 6. ..
- 7. ..
- 8. ..
- 9. Place a Gaussian at x=6 i.e.  $\mu = 6$
- 10. Find its value @ x=3



Find value x=3

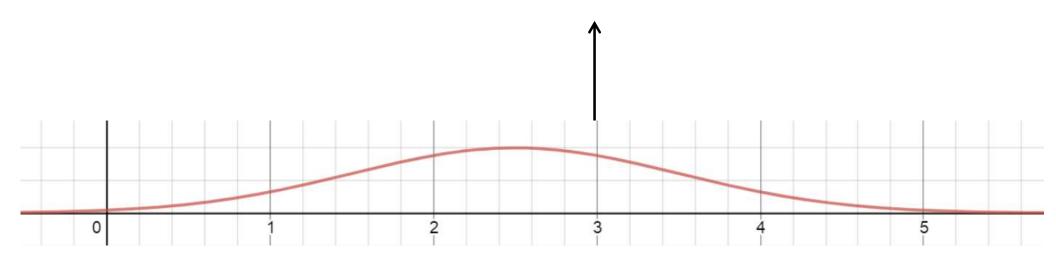


$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_1-x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(2-3)^2}{2}\right) = 0.2420$$



Find value x=3

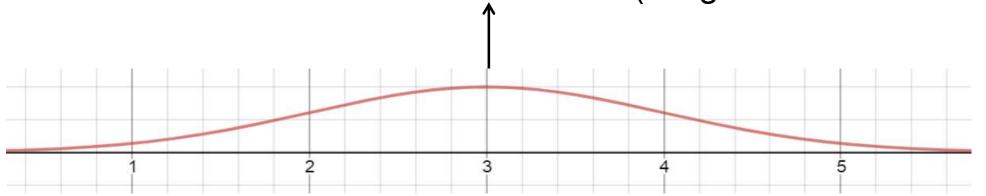


$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_2-x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(2.5-3)^2}{2}\right) = 0.3521$$



Find value x=3 (we get maximum value)

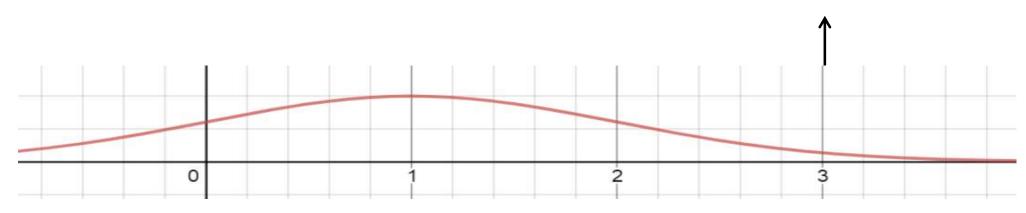


$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_3 - x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(3 - 3)^2}{2}\right) = 0.3989$$



Find value x=3

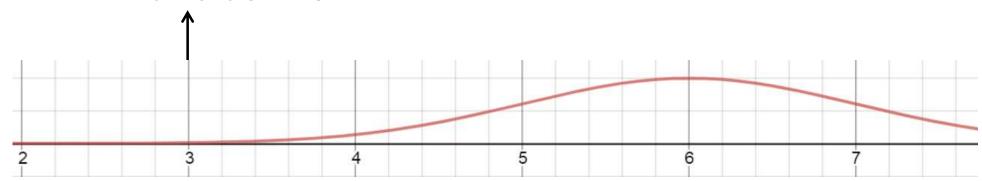


$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_4-x)^2}{2}\right)$$

$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(1-3)^2}{2}\right) = 0.054$$







$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_5-x)^2}{2}\right)$$

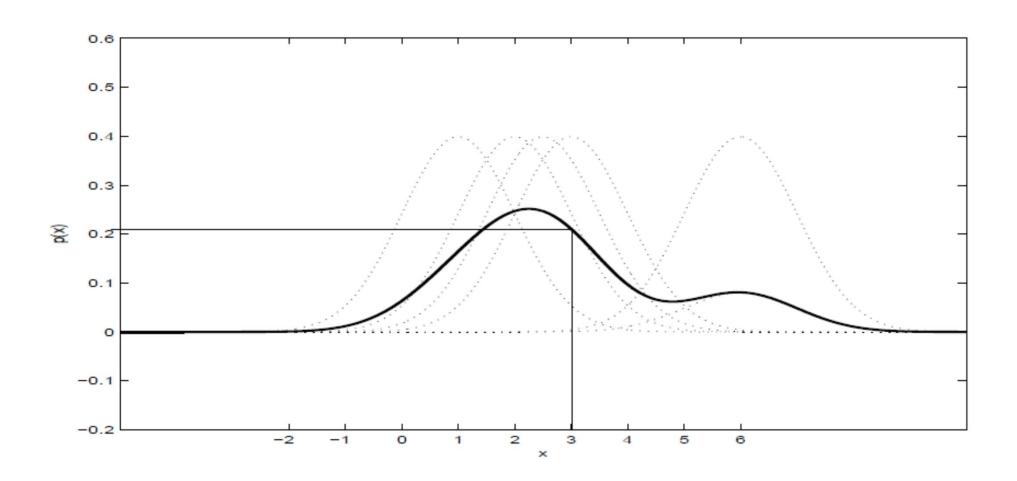
$$= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(6-3)^2}{2}\right) = 0.0044$$



$$p(x = 3) = (0.2420 + 0.3521 + 0.3989$$
  
+0.0540 + 0.0044)/5 = 0.2103



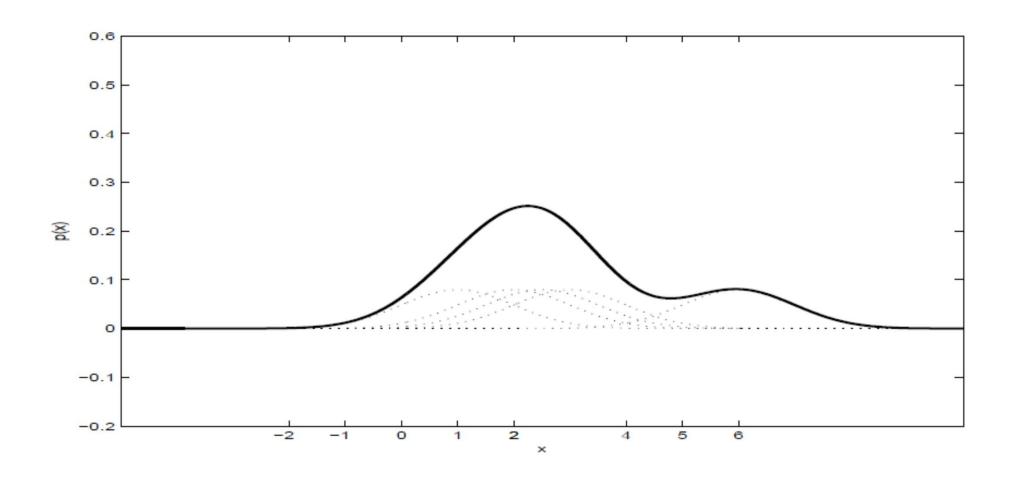
$$x1 = 2$$
,  $x2 = 2.5$ ,  $x3 = 3$ ,  $x4 = 1$  and  $x5 = 6$ 



What is p(3)? Answer is 0.21



Given: x1 = 2, x2 = 2.5, x3 = 3, x4 = 1 and x5 = 6



What is p(x) in general?
Answer is the estimated curve

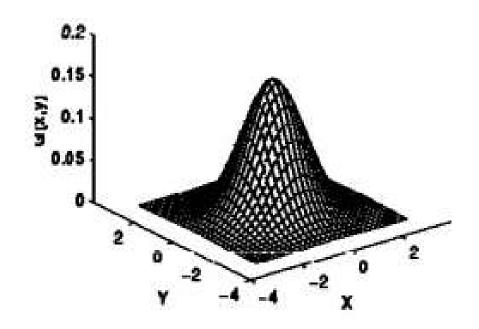


## If data is two dimensional ...<sup>1</sup>

 Use two dimensional Gaussian function to estimate PDF

$$G(x,y) = \frac{1}{2\pi\sigma^2} e^{-\frac{x^2+y^2}{2\sigma^2}}$$

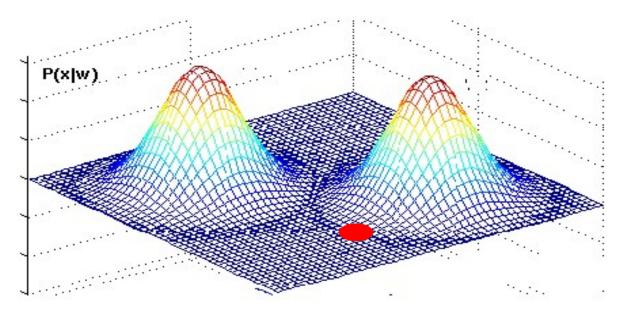
A graphical representation of the 2D Gaussian distribution with mean(0,0) and  $\sigma = 1$ 





## If data is two dimensional ...<sup>2</sup>

- Place the Gaussian @ various points
- Find their contributions @ the given point
- Sum up all the contributions
- Take average



- Assume we have3 points on a plane
- @ red color point the PDF is given by average contributions from other two Gaussians



#### Parzen Window

Number of data points (N)

## To calculate the density @ one point

- N Gaussian computations and then summing up
  - One  $\Sigma$

Information potential (IP)

- Need to know PDf @ N points and then summing up
  - One more  $\Sigma$
  - i.e. Two  $\Sigma$



Information Potential = 
$$V^{\alpha}(x) = \sum_{k=1}^{\infty} p_k^{\alpha}$$

 Quadratic information potential with Gaussian kernel

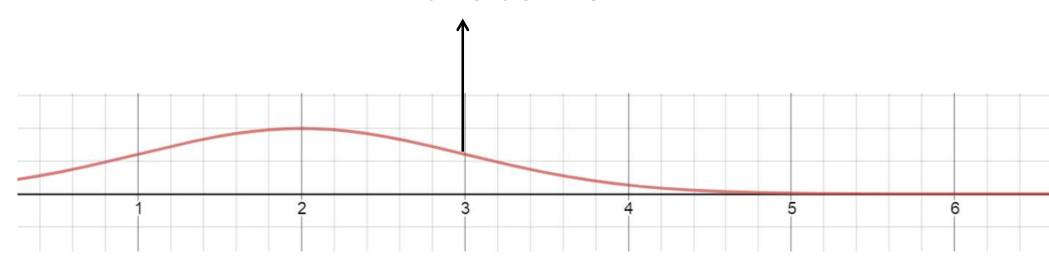
$$\left(\frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} G_{\sigma\sqrt{2}}(x_j - x_i)\right)$$

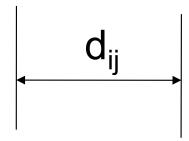
$$\hat{V}(X) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{V}_{i,j}$$

$$d_{i,j} = x_i - x_j$$
  
 $V_{ij} = G(d_{ij})$ 

# What is $G(d_{ij})$ ?

Find value x=3







## Information force

Information force on sample xj due to sample xi

$$\hat{F}(i) = \frac{-1}{2N\sigma^2} \sum_{j=1}^{N} \hat{V}_{i,j} d_{i,j}$$

 $d_{i,j} = x_i - x_j$ 

where

$$V_{ij} = G(d_{ij})$$

Total / information force acting on sample



# Information force and information potential

$$\hat{F}(i) = \frac{-1}{2N\sigma^2} \sum_{j=1}^{N} \hat{V}_{i,j} d_{i,j}$$

where  $1_{i,j} = x_i - x_j$ 

$$V_{ij} = G(d_{ij})$$

$$\hat{V}(X) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{j=1}^{N} \hat{V}_{i,j}$$



$$G(d_{ij})$$

- G(d<sub>ij</sub>) Gaussian placed @ x<sub>j</sub> point, and evaluated @ x<sub>i</sub> point
- G(d<sub>ii</sub>) is always positive
- Both IP and IF are functions of G(d<sub>ij</sub>)

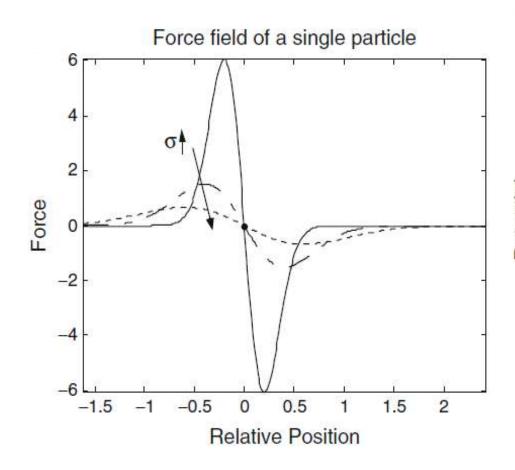
dij

- $d_{ij} = x_i x_j$
- Can be positive or negative
- IF =  $G(d_{ij}) \times d_{ij}$
- IF could be +ve or -ve

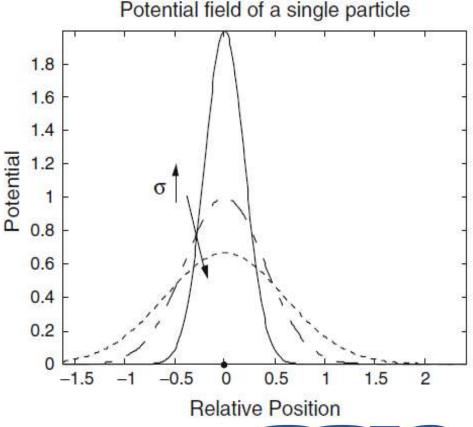


#### IP and IF

- IF +ve and -ve
- IF depends on both
   G(d<sub>ij</sub>) & d<sub>ij</sub>



- IP always +ve
- IP depends on G(d<sub>ii</sub>)





## IF for two dimensional

## **Dimension X**

- $d_{ij} = x_i x_j$
- $IF_x = G(d_{ij}) \times d_{ij}$

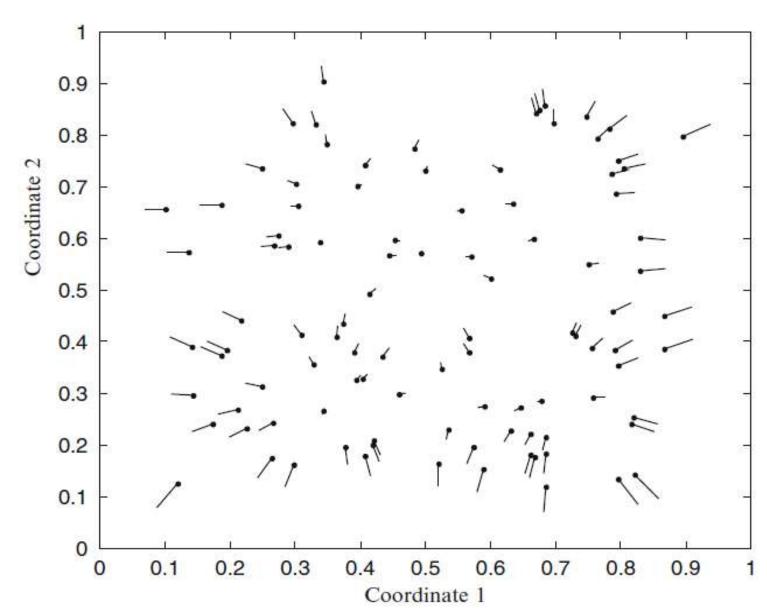
## **Dimension Y**

- $d_{ij} = y_i y_j$
- $IF_y = G(d_{ij}) \times d_{ij}$

- Combine IF<sub>x</sub> and IF<sub>y</sub>
- Vector sum
- · Produces magnitude as well as direction



# Quadratic information forces on 2 featured data points





## Information forces for clustering

- Some points become center of cluster
- IF of many surrounding points oriented towards them



#### Directed tree

- Create graph out of N nodes
- Use their IF as cost
- More the IF better the connection

General constraints

- $d_{ij} < 3\sigma$
- |F| > 0

