Skript Pattern Analysis Sommersemester 2017

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1 Density Estimation

Let $p(\vec{x})$ denote a probability density function pdf then:

1. $p(\vec{x}) \geq 0$
2. $\int_{-\infty}^{\infty} p(\vec{x})\, d\vec{x} = 1$
3. $p(\vec{a} \leq \vec{x} \leq \vec{b}) = \int_{\vec{a}}^{\vec{b}} p(\vec{x})\, d\vec{x}$

The task of density estimation is to obtain a continous representation of the underlying pdf from a set of discrete samples (massumants). Note: that if we have the pdf we can do statistical analysis.

Parametric density estimation (mostly Pattern Recognition)
Make an assumption about the underlying distribution (e.g. Gausian, GMM) and determine the best fitting distribution parameters from the data. (ML estimation, MAP estimation)

Non-parametric density estimation We make no assumption of the underlying Model.

1.1 Parzen-Rosenblatt estimator

???Idea: Quantify the number of samples with a window

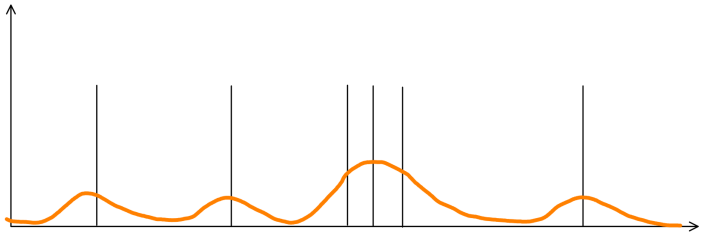


Figure 1: A PDF describing the distribution of measurements

The Parzen window estimator interpolates the pdf from the observations in the neighbourhood of a position x, using an appropriate kernel/window function.

Short derivtion: Let p_R denote the probability that $\vec{x}$ lies within region R:

$$p_R = \int_R p(\vec{x})\, d\vec{x}$$

Now assume that $p(\vec{x})$ is approximately constant in R.

$$p_R \approx p(\vec{x}) \int_R d\vec{x}$$

For example, let R be a d-dimensional hypercube with side length h, then its volume[1][2] is h^d

$$p_R \approx p(\vec{x}) V_R$$

Let $p_R = \frac{k_R}{N}$, we determine the probability of making observations in region R by counting the samples in R ($= k_R$) and dividing by the total number of samples. Note: p_R is also called the "relative frequency"

$$p(\vec{x}) = \frac{p_R}{V_R} = \frac{k_R}{V_R N}$$

Let's write the parzen window estimator as a function of a kernel[3] $k(\vec{x}; \vec{x_i})$, then

$$p(\vec{x}) = \frac{1}{h^d N} \sum_{i=1}^{N} k(\vec{x}; \vec{x_i})$$

where[4]

$$k(\vec{x}; \vec{x_i}) = \begin{cases} 1 & \text{when } \frac{|x_{i,k} - x_k|}{h} \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

equivalently, if we use a (multivariate) gaussian kernel:

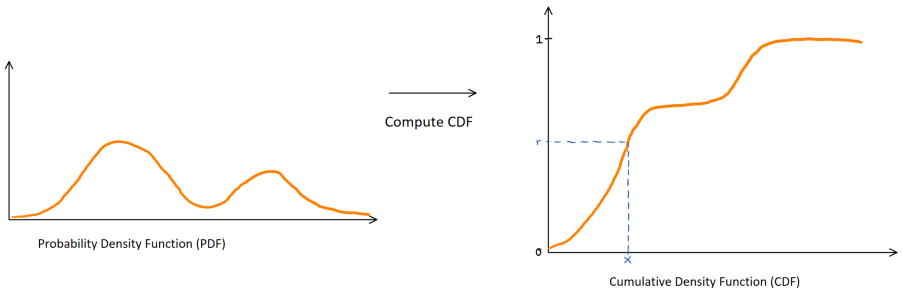
$$k(\vec{x}; \vec{x_i}) = \frac{1}{(2\pi)^d |\Sigma|} e^{-(\vec{x}-\vec{x_i})^T \Sigma^{-1} (\vec{x}-\vec{x_i})}$$

A note on applications

- General remark: We obtain a continuous pdf, i.e. desity estimation converts a list of measurments to a statistical model
- Specific example: We can sample from a pdf. This means that we have a princeple way of generating new / more / ... data that behaves / looks / ... similary to the observations.

[1] $\int_R d\vec{x}$ is just the volume of R
[2] We also write V_R for the volume
[3] Omit h^d if the kernel is gaussian
[4] $\vec{x_i}$ and $\vec{x}$ are not father apart then $0.5h$ in any dimension k

Q: How can we (practically) sample from a pdf?



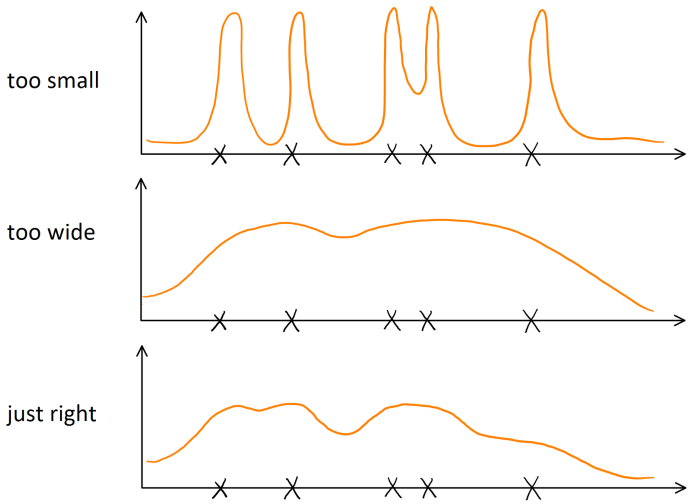
Compute through discretisation of the pdf $cdf[i] = cdf[i-1] + pdf[i]$. Then draw a uniformly distributed number (r) between 0 and 1. The sampled value is x where $cdf[x] = r$

Q: How can we determine a good window / kernel width h?
Let's do ML est. with a cross-vaslidation (cv) (e.g. leave-one-sample-out cv)

$$p^j_{h,N-1}(\vec{x}) = \frac{1}{h^d N} \sum_{i=1(i\neq j)}^{N} k(\vec{x}; \vec{x_i})$$

We estimate the pdf from all samples except $\vec{x_j}$. $\vec{x_i}$ will be used to evaluate the quality of the pdf using window siye h.

Q: How do the results change with varing window size?



$$\hat{h} = \arg\max_h L(h) = \arg\max_h \prod_{j=1}^{N} p^j_{h,N-1}(\vec{x_j}) = \arg\max_h \sum_{j=1}^{N} \log p^j_{h,N-1}(\vec{x_j})$$

The position of the maximum does not change, because the logarithm is a strictly monotonic function.

2 Mean Shift Algorithm

Purpose: Find maximum in pdf without actually performing a full density estimation. [5]

Potential applications: Clustering, segmentation, ...

Idea: Maxima can be found, where the gradient of the pdf is zero. (Assume that we have a full density estimator.)

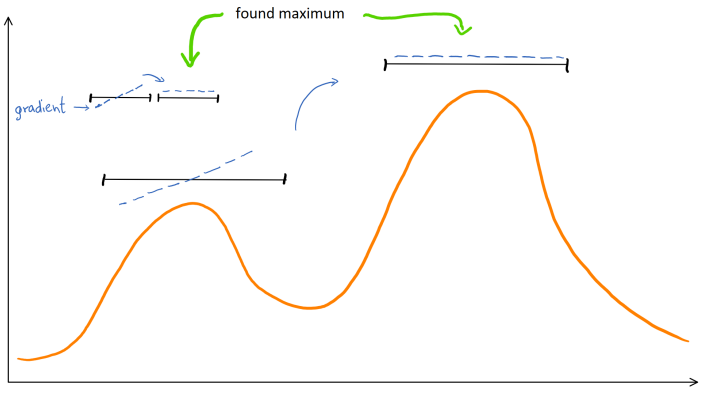


Figure 2: The kernel size indirectly controls the number of indentified maxima

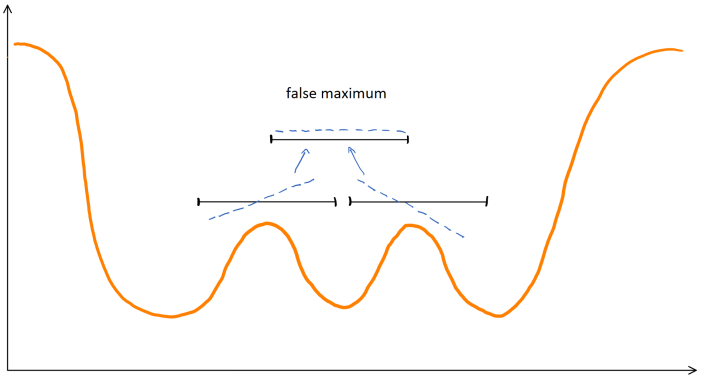


Figure 3: One of the issues is, the case when a zero gradient is just between two finer maxima

[5] This applies only in some cases, e.g. quickly finding clusters through particle tracing or with a downsampled PDF (see section 2)

Let

$$p(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} k_h(\vec{x};\vec{x_i})$$

denote the multivariate kernel density estimation. A local maxium of the pdf can be assumed where the gradient vanishes $\nabla p(\vec{x}) = 0$.

$$\nabla p(\vec{x}) = \nabla(\frac{1}{N}\sum_{i=1}^{N} k(\vec{x};\vec{x_i})) = \frac{1}{N}\sum_{i=1}^{N} \nabla k(\vec{x};\vec{x_i})$$

Let's assume that k_h is a radially symmetric kernel, i.e.

$$k(\vec{x};\vec{x_i}) = c_d k_h(||\vec{x_i} - \vec{x}||^2)$$

$$\frac{\partial k_h(S)}{\partial S} = k_h'(S)$$

$$\frac{\partial S}{\partial \vec{x}} = \frac{\partial(\vec{x_i} - \vec{x})^T(\vec{x_i} - \vec{x})}{\partial \vec{x}} = -2(\vec{x_i} - \vec{x})$$

$$\nabla p(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} c_d k_h(||\vec{x_i} - \vec{x}||^2)(-2(\vec{x_i} - \vec{x})) \doteq \vec{0}$$

$\frac{1}{N}$ and c_d can be dropped then multiply out

$$\sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)\vec{x_i} - \sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)\vec{x} = \vec{0}$$

Then we get the mean shift vector

$$\frac{\sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)\vec{x_i}}{\sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)} - \vec{x} = \vec{0} \tag{1}$$

To perform a gradient acsend, compute the gradient, walk one step, re-compute the gradient, walk a step, ...

Mean shift algorithm (formalized)

1. Compute the mean shift vector $m(\vec{x}^{(t)})$ (see 1)
2. Update $\vec{x} : \vec{x}^{(t+1)} = \vec{x}^{(t)} + m(\vec{x}^{(t)}) = \frac{\sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)\vec{x_i}}{\sum_{i=1}^{N} k_h'(||\vec{x_i} - \vec{x}||^2)}$

Q: Why is it called "mean shift"?
If we plug in for k_h the Epanechnikov kernel. Then the computation breks down to the mean of the samples in a circular (hyperspherical) around $\vec{x}^{(t)}$

Epanechnikov kernel

$$k_E(\vec{x}) = \begin{cases} c(1 - \vec{x}^T\vec{x}) & \text{when } \vec{x}^T\vec{x} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

Abstract example: Assume we have a 2-D feature space

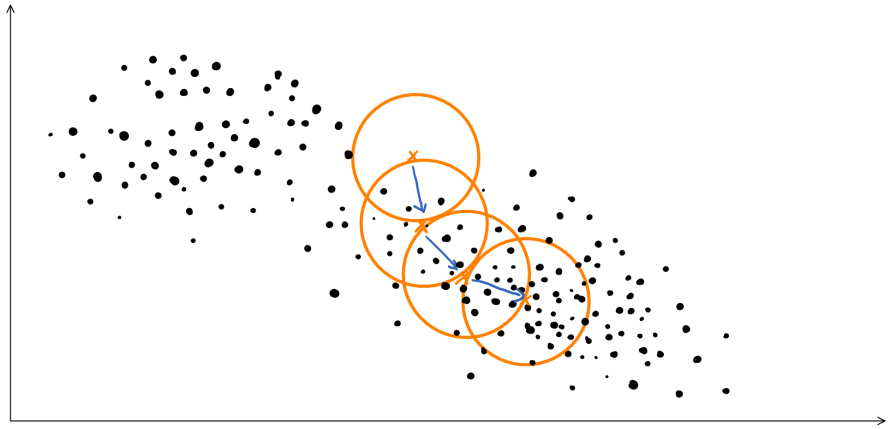


Figure 4: Mean Shift iterations with an Epanechnikov kernel

Specific example:

- (Color) quantization
  - Note: the RGB colorspace is not perceptually uniform (Lab or Luv are used in practice)
- (Color) segmentation
  - Similar in result to a super pixel segmentation: operate locally in the image
  - Incorporate the position of each pixel

Remarks on the found maxima:

- Different trajectories typically coverage only to **almost** the same peak, thus, we will have to post process the peaks and somehow reduce them.
- We don't have a guarentee to sit on top of a maximum when reaching a 0-gradient. This is due to the finite window size and the discrete representation of our density (see figure 2).

- If the amount of data is large, then it may become extremly costly to iteratively evaluate the "neighbourhood finder". In that case we have to help ourself, either with a smart data structure (oct-tree or a generalisation for many dimensions) or locality sensitve hashing (LSH).