Non parametric methods

Course of Machine Learning
Master Degree in Computer Science
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Probability distribution estimates

- The statistical approach to classification requires the (at least approximate) knowledge of $p(\mathcal{C}_i|\mathbf{x})$: in fact, an item $\mathbf{x}$ shall be assigned to the class $\mathcal{C}_i$ such that

$$i = \underset{k}{\operatorname{argmax}}\, p(\mathcal{C}_k|\mathbf{x})$$

- The same holds in the regression case, where $p(y|\mathbf{x})$ has to be estimated.

Probability distribution estimates: hypotheses

What do we assume to know of class distributions, given a training set $\mathbf{X}, \mathbf{t}$?

- Case 1. The probabilities $p(\mathbf{x}|\mathcal{C}_i)$ are known: an item is assigned $\mathbf{x}$ to the class $\mathcal{C}_i$ such that
$$i = \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j|\mathbf{x})$$
where $p(\mathcal{C}_j|\mathbf{x})$ can be derived through Bayes' rule and prior probabilities, since $p(\mathcal{C}_k)|\mathbf{x}) \propto p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$

Probability distribution estimates: hypotheses

- Case 2. The type of probability distribution $p(\mathbf{x}|\boldsymbol{\theta})$ is known: an estimate of parameter values $\boldsymbol{\theta}_i$ is performed for all classes, taking into account for each class $\mathcal{C}_i$ the subset of $\mathbf{X}_i, \mathbf{t}_i$ of items belonging to the class, that is such that $t = i$. Different approaches to parameter estimation:
  1. Maximum likelihood: $\boldsymbol{\theta}_i^{ML} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, p(\mathbf{X}_i, \mathbf{t}_i|\boldsymbol{\theta})$ is computed. Item $\mathbf{x}$ is assigned to class $\mathcal{C}_i$ if
  $$i = \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j|\mathbf{x}) = \underset{j}{\operatorname{argmax}}\, p(\mathbf{x}|\boldsymbol{\theta}_j^{ML})p(\mathcal{C}_j)$$
  2. Maximum a posteriori: $\boldsymbol{\theta}_i^{MAP} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, p(\boldsymbol{\theta}|\mathbf{X}_i, \mathbf{t}_i)$ is computed. Item $\mathbf{x}$ is assigned to class $\mathcal{C}_i$ if
  $$i = \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j|\mathbf{x}) = \underset{j}{\operatorname{argmin}}\, p(\mathbf{x}|\boldsymbol{\theta}_j^{MAP})p(\mathcal{C}_j)$$
  3. Bayesian estimate: the distributions $p(\boldsymbol{\theta}|\mathbf{X}_i, \mathbf{t}_i)$ are estimated for each class and, from them,
  $$p(\mathbf{x}|\mathcal{C}_i) = \int_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X}_i, \mathbf{t}_i)d\boldsymbol{\theta}$$
  Item $\mathbf{x}$ is assigned to class $\mathcal{C}_i$ if
  $$i = \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j|\mathbf{x}) = \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j)p(\mathbf{x}|\mathcal{C}_j)$$
  $$= \underset{j}{\operatorname{argmax}}\, p(\mathcal{C}_j) \int_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X}_j, \mathbf{t}_j)d\boldsymbol{\theta}$$

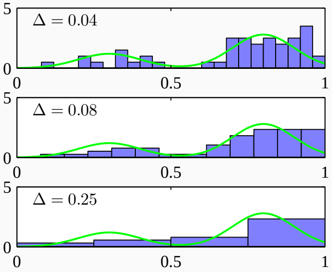
Probability distribution estimates: hypotheses

- Case 3. No knowledge of the probabilities assumed.
- The class distributions $p(\mathbf{x}|\mathcal{C}_i)$ are directly from data.
- In previous cases, use of (parametric) models for a synthetic description of data in $\mathbf{X}, \mathbf{t}$
- In this case, no models (and parameters): training set items explicitly appear in class distribution estimates.
- Denoted as non parametric models: indeed, an unbounded number of parameters is used

Histograms

- Elementary type of non parametric estimate
- Domain partitioned into m d-dimensional intervals (bins)
- The probability $P_{\mathbf{x}}$ that an item belongs to the bin containing item $\mathbf{x}$ is estimated as $\frac{n(\mathbf{x})}{n}$, where $n(\mathbf{x})$ is the number of element in that bin
- The probability density in the interval corresponding to the bin containing $\mathbf{x}$ is then estimated as the ratio between the above probability and the interval width $\Delta(\mathbf{x})$ (tipically, a constant Δ)

$$p_H(\mathbf{x}) = \frac{\frac{n(\mathbf{x})}{N}}{\Delta(\mathbf{x})} = \frac{n(\mathbf{x})}{N\Delta(\mathbf{x})}$$



Histograms: problems

- The density is a function of the position of the first bin. In the case of multivariate data, also from bin orientation.
- The resulting estimates is not continuous.
- Curse of dimensionality: the number of bins grows as a polynomial of order d: in high-dimensional spaces many bins may result empty, unless a large number of items is available.
- In practice, histograms can be applied only in low-dimensional datasets (1,2)

Kernel density estimators

- Probability that an item is in region $\mathcal{R}(\mathbf{x})$, containing $\mathbf{x}$

$$P_{\mathbf{x}} = \int_{\mathcal{R}(\mathbf{x})} p(\mathbf{z}) d\mathbf{z}$$

- Given n items $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$, the probability that k among them are in $\mathcal{R}(\mathbf{x})$ is given by the binomial distribution

$$p(k) = \binom{n}{k} P_{\mathbf{x}}^K (1 - P_{\mathbf{x}})^{n-k} = \frac{n!}{k!(n-k)!} P_{\mathbf{x}}^K (1 - P_{\mathbf{x}})^{n-k}$$

- Mean and variance of the ratio $r = \dfrac{k}{n}$ are

$$E[r] = P_{\mathbf{x}} \qquad \text{var}[r] = \frac{P_{\mathbf{x}}(1 - P_{\mathbf{x}})}{n}$$

- $P_{\mathbf{x}}$ is the expected fraction of items in $\mathcal{R}(\mathbf{x})$, and the ratio r is an estimate. As $n \to \infty$ variance decreases and r tends to $E[r] = P_{\mathbf{x}}$. Hence, in general,

$$r = \frac{k}{n} \simeq P(\mathbf{x})$$

- Let the volume of $\mathcal{R}(\mathbf{x})$ be sufficiently small. Then, the density $p(\mathbf{x})$ is almost constant in the region and

$$P_{\mathbf{x}} = \int_{\mathcal{R}(\mathbf{x})} p(\mathbf{z}) d\mathbf{z} \simeq p(\mathbf{x})V$$

  where V is the volume of $\mathcal{R}(\mathbf{x})$
- since $P_{\mathbf{x}} \simeq \frac{k}{n}$, it then derives that $p(\mathbf{x}) \simeq \frac{k}{nV}$

Two alternative ways to exploit the estimate $p(\mathbf{x}) \simeq \frac{k}{nV}$

1. Fix V and derive k from data (kernel density estimation)
2. Fix k and derive V from data (K-nearest neighbor).

It can be shown that in both cases, under suitable conditions, the estimator tends to the true density $p(\mathbf{x})$ as $n \to \infty$.

Kernel density estimation: Parzen windows

- Region associated to a point $\mathbf{x}$: hypercube with edge length h (and volume h^d) centered on $\mathbf{x}$.
- Kernel function $k(\mathbf{u})$ (Parzen window) used to count the number of items in the unit hypercube centered on u

$$k(\mathbf{u}) = \begin{cases} 1 & |u_i| \leq 1/2 \qquad\qquad i = 1, \dots, d \\ 0 & \text{otherwise} \end{cases}$$

- as a consequence, $k\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) = 1$ iff $\mathbf{x}'$ is in the hypercube of edge length h centered on $\mathbf{x}$
- the number of items in the hypercube is then

$$K = \sum_{i=1}^{n} k\left(\frac{\mathbf{x}-\mathbf{x}_i}{h}\right)$$

- The estimated density is

$$p(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{h^d}k\left(\frac{\mathbf{x}-\mathbf{x}_i}{h}\right)$$

- Since

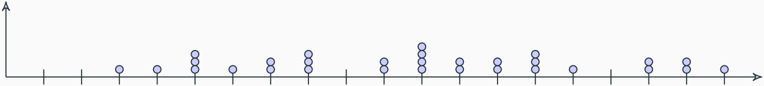
$$k(\mathbf{u}) \geq 0 \qquad \text{and} \qquad \int k(\mathbf{u})d\mathbf{u} = 1$$

  it derives

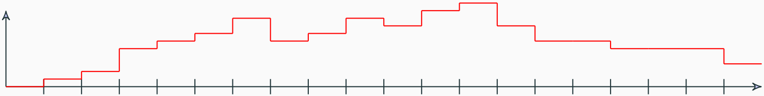
$$p(\mathbf{x}) \geq 0 \qquad \text{and} \qquad \int p(\mathbf{x})d\mathbf{x} = 1$$

  that is, $p_n(\mathbf{x})$ is a probability density
- Window size has a relevant effect on the estimate

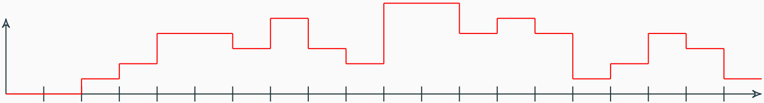
Kernel density estimation: Parzen windows



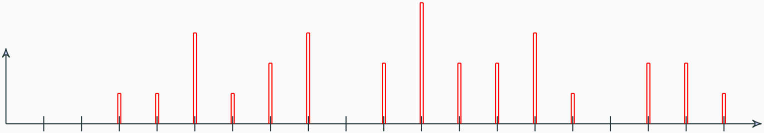
$h = 2$



$h = 1$



$h = \varepsilon$

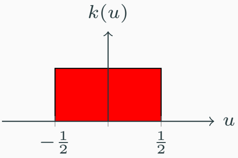


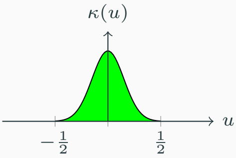
- Parzen windows drawbacks
  1. discontinuity of the estimates
  2. items in a region centered on $\mathbf{x}$ have uniform weights: their distance from $\mathbf{x}$ is not taken into account
- Solution: use of smooth kernel functions $\kappa(u)$

$$\int_{0^d}^{h^d} \kappa(\mathbf{x}) d\mathbf{x} = 1$$

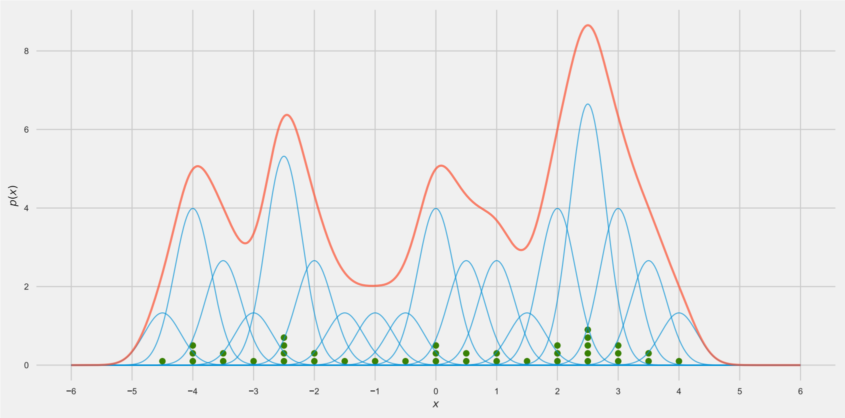
  1. usually radial functions (functions of the distance from the center)
  2. resulting estimate:

$$p(\mathbf{x}) = \frac{1}{nh^d} \sum_{i=1}^{n} \kappa\left(\frac{\mathbf{x} - \mathbf{x}_i}{h}\right)$$

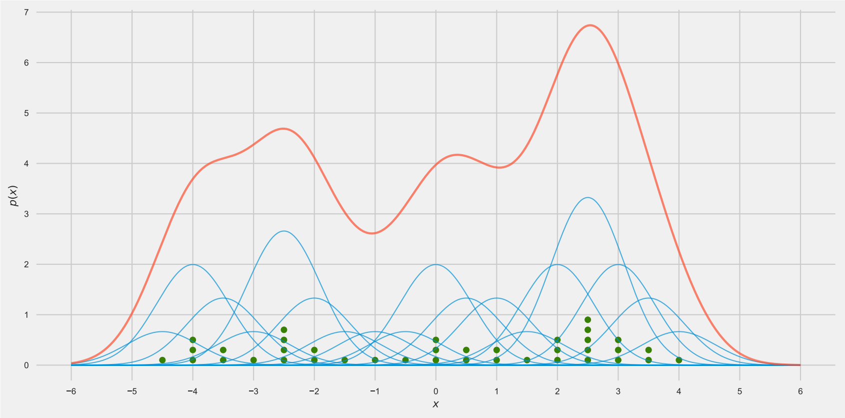




$h = 1$

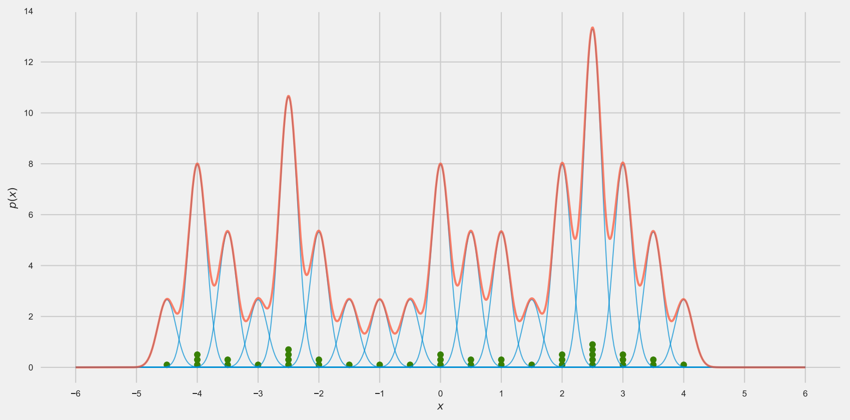


$h = 2$

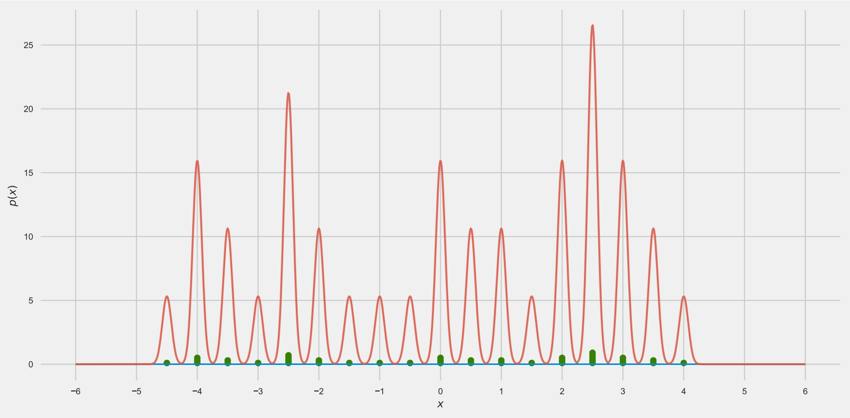


Kernels e smoothing

$h = .5$



$h = .25$



Density estimation through kNN

- The region around $\mathbf{x}$ is extended to include k items
- The estimated density is

$$p(\mathbf{x}) \simeq \frac{k}{nV} = \frac{k}{nc_d r_k^d(\mathbf{x})}$$

where:

  - c_d is the volume of the d-dimensional sphere of unitary radius
  - $r_k^d(\mathbf{x})$ is the distance from $\mathbf{x}$ to the k-th nearest item (the radius of the smallest sphere with center $\mathbf{x}$ containing k items)

Classification through kNN

- To classify $\mathbf{x}_i$, let us consider a hypersphere of volume V with center $\mathbf{x}$ containing k items from the training set
- Let k_i be the number of such items belonging to class $\mathcal{C}_i$. Then, the following approximation holds:

$$p(\mathbf{x}|\mathcal{C}_i) = \frac{k_i}{n_i V}$$

where n_i is the number of items in the training set belonging to class $\mathcal{C}_i$

- Similarly, for the evidence,

$$p(\mathbf{x}) = \frac{k}{nV}$$

- And, for the prior distribution,

$$p(\mathcal{C}_i) = \frac{n_i}{n}$$

- The class posterior distribution is then

$$p(\mathcal{C}_i|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_i)p(\mathcal{C}_i)}{p(\mathbf{x})} = \frac{\frac{k_i}{n_i V} \cdot \frac{n_i}{n}}{\frac{k}{nV}} = \frac{k_i}{k}$$

- Simple rule: an item is classified on the basis of similarity to near training set items
- To classify $\mathbf{x}$, determine the k items in the training nearest to it and assign $\mathbf{x}$ to the majority class among them
- A metric is necessary to measure similarity.