CSCI567 Machine Learning (Spring 2021)

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Outline

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Logistics

- **Recognition for top teams** – Working with the department to get recognition for the top teams. *Keep up the good work!*

Outline

Density estimation

Given a training set $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$, **estimate a density function p that could have generated this dataset** (via $\boldsymbol{x}_n \stackrel{i.i.d.}{\sim} p$).

This is exactly the problem of *density estimation*, another important unsupervised learning problem.

Useful for many downstream applications such as clustering, we will look at a classification task today.

Parametric methods: generative models

Parametric estimation assumes a generative model parametrized by $\boldsymbol{\theta}$:

$$p(\boldsymbol{x}) = p(\boldsymbol{x}\,; \boldsymbol{\theta})$$

Examples:

- GMM: $p(\boldsymbol{x} \,|\boldsymbol{\theta}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ where $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}$
- Multinomial: a discrete variable with values in $\{1, 2, \ldots, K\}$ s.t.

  $$p(x = k\,; \boldsymbol{\theta}) = \theta_k$$

  where $\boldsymbol{\theta}$ is a distribution over K elements.

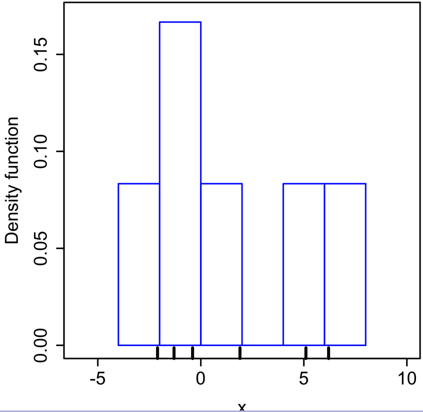
Size of $\boldsymbol{\theta}$ is independent of the training set size, so it's parametric.

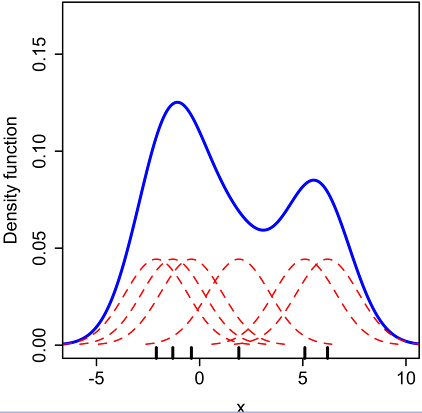
Nonparametric methods: High level idea

picture from Wikipedia

Construct something similar to a **histogram**:

- for each data point, create a "bump" (via a Kernel)
- sum up or average all the bumps





Kernel Density Estimation (KDE)

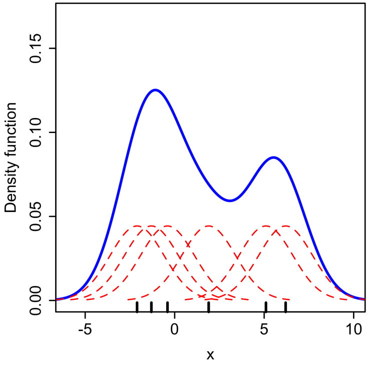
KDE with **a kernel** K: $\mathbb{R} \rightarrow \mathbb{R}$:

$$p(x) = \frac{1}{N} \sum_{n=1}^{N} K\left(x - x_n\right)$$

e.g. $K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{u^2}{2}}$, the standard Gaussian density

Kernel needs to satisfy:

- symmetry: $K(u) = K(-u)$
- $\int_{-\infty}^{\infty} K(u) du = 1$, makes sure p is a density function.



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Naive Bayes

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- a simple yet surprisingly powerful **classification** algorithm

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- a simple yet surprisingly powerful **classification** algorithm
- **density estimation** is one important part of the algorithm

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p is of course unknown, but we can estimate it, which is *exactly a density estimation problem!*

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This is *not a 1D problem* in general.

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More often this assumption is *unrealistic and "naive"*, but still Naive Bayes can work very well even if the assumption is wrong.

Example: discrete features

Height: $\leq$3', 3'-4', 4'-5', 5'-6', $\geq$6'
Vocabulary: $\leq$5K, 5K-10K, 10K-15K, 15K-20K, $\geq$20K
Age: $\leq$5, 5-10, 10-15, 15-20, 20-25, $\geq$25

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MLE estimation: e.g.

$$p(\text{Age} = \text{10-15}) = \frac{\#\text{examples with age 10-15}}{\#\text{examples}}$$

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$$p(\text{Height} = \text{5'-6'} \mid \text{Age} = \text{10-15})$$
$$= \frac{\#\text{examples with height 5'-6' and age 10-15}}{\#\text{examples with age 10-15}}$$

More formally

For a label $c \in [\mathsf{C}]$,

$$p(y = c) = \frac{|\{n : y_n = c\}|}{N}$$

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For each possible value k of a discrete feature d,

$$p(x_d = k \mid y = c) = \frac{|\{n : x_{nd} = k, y_n = c\}|}{|\{n : y_n = c\}|}$$

Continuous features

If the feature is continuous, we can do

- parametric estimation,

- or nonparametric estimation,

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- or nonparametric estimation, e.g. via a Kernel K and bandwidth h:

$$p(x_d = x \mid y = c) = \frac{1}{|\{n : y_n = c\}|} \sum_{n:y_n=c} K_h(x - x_{nd})$$

How to predict?

After learning the model

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&= \underset{c \in [\mathsf{C}]}{\operatorname{argmax}}\; \left(\ln p(y = c) + \sum_{d=1}^{\mathsf{D}} \ln p(x_d \mid y = c) \right)
\end{aligned}$$

Examples

For **discrete features**, plugging in previous MLE estimations gives

$$
\begin{aligned}
&\operatorname*{argmax}_{c\in[\mathsf{C}]} \; p(y=c \mid x) \\
&= \operatorname*{argmax}_{c\in[\mathsf{C}]} \; \left(\ln p(y=c) + \sum_{d=1}^{\mathsf{D}} \ln p(x_d \mid y=c) \right) \\
&= \operatorname*{argmax}_{c\in[\mathsf{C}]} \; \left(\ln |\{n : y_n = c\}| + \sum_{d=1}^{\mathsf{D}} \ln \frac{|\{n : x_{nd} = x_d, y_n = c\}|}{|\{n : y_n = c\}|} \right)
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Examples

For **continuous features** with a Gaussian model,

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which is *quadratic* in the feature $\boldsymbol{x}$.

What is naive Bayes learning?

Observe again the case for continuous features with a Gaussian model, if we **fix the variance for each feature to be σ** (i.e. not a parameter of the model any more), then the prediction becomes

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where we denote $w_{c0} = \ln|\{n : y_n = c\}| - \sum_{d=1}^{\mathsf{D}}\frac{\mu_{cd}^2}{2\sigma^2}$ and $w_{cd} = \frac{\mu_{cd}}{\sigma^2}$.

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\end{aligned}
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So what is different then? They **learn the parameters in different ways**:

- both via MLE, one on $p(y = c \mid x)$, the other on $p(x, y)$
- solutions are different: logistic regression has no closed-form, naive Bayes admits a simple closed-form

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Example	logistic regression	naive Bayes

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Remark		more flexible, can generate data after learning