CSCI567 Machine Learning (Fall 2018)

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U of Southern California

Oct 24, 2018

Administration

HW 4 is available and is due on 11/04.

Today's plan: first finish clustering, then move on to more unsupervised learning problems

Outline

1. Density estimation

2. Naive Bayes

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- we have seen clustering already, will see more today
- these applications also *provide a way to measure quality of the density estimator*

Parametric methods: generative models

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- Multinomial for 1D examples with K possible values

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

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

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

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Again, we apply **MLE** to learn the parameters $\boldsymbol{\theta}$:

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For some other cases this admits a simple closed-form solution (e.g. multinomial).

MLE for multinomial

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where $z_k = |\{n : x_n = k\}|$ is **the number of examples with value k**.

The solution is simply

$$\theta_k = \frac{z_k}{N} \propto z_k,$$

i.e. the fraction of examples with value k.

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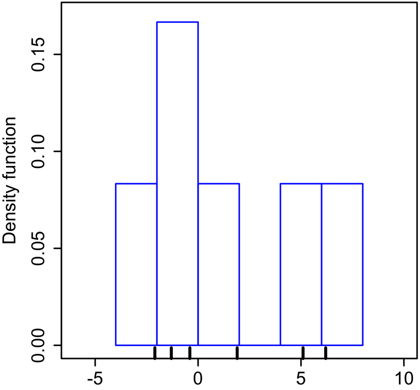
- here "kernel" means something different from what we have seen for "kernel function" (in fact it refers to several different things in ML)
- the approach is nonparametric: it keeps the entire training set
- we focus on the 1D (continuous) case

High level idea

picture from Wikipedia

Construct something similar to a **histogram**:



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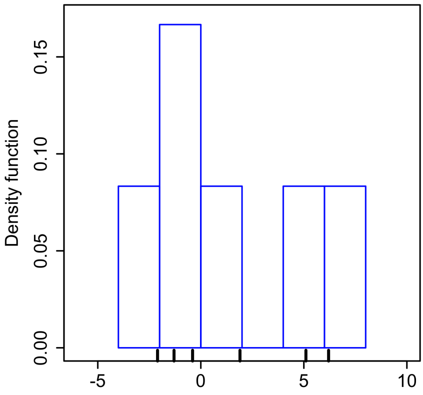

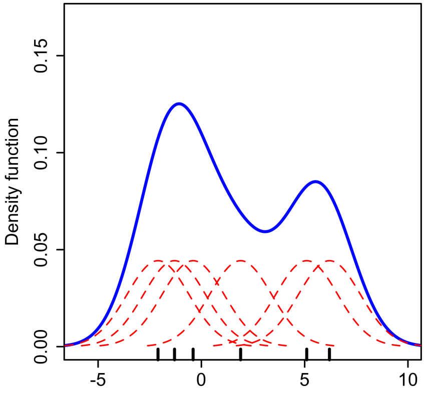

High level idea

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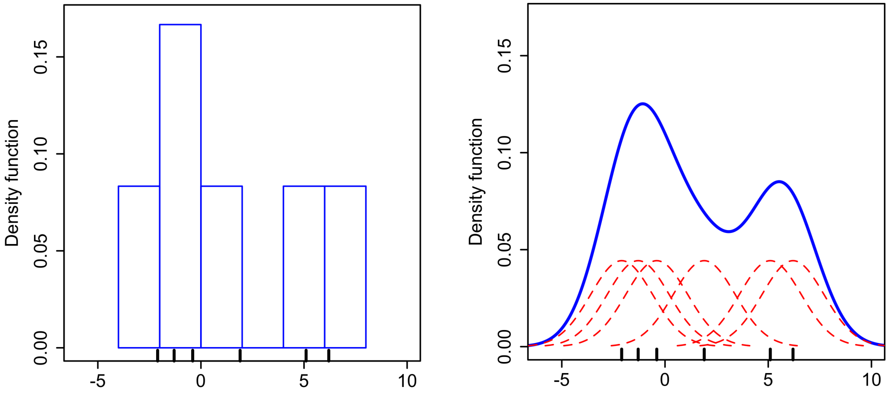
Construct something similar to a **histogram**:

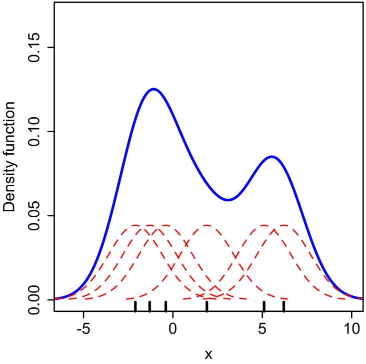
- for each data point, create a "bump" (via a Kernel)
- sum up all the bumps



Kernel

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

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



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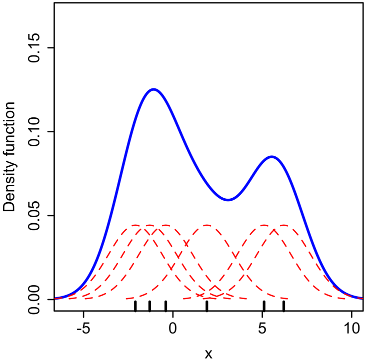

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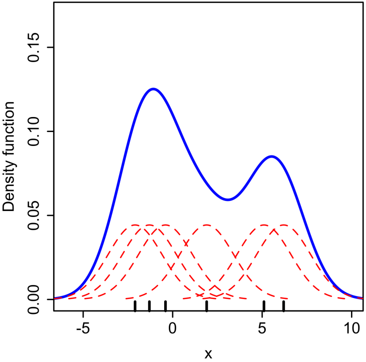

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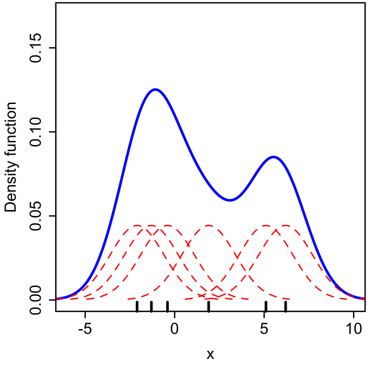
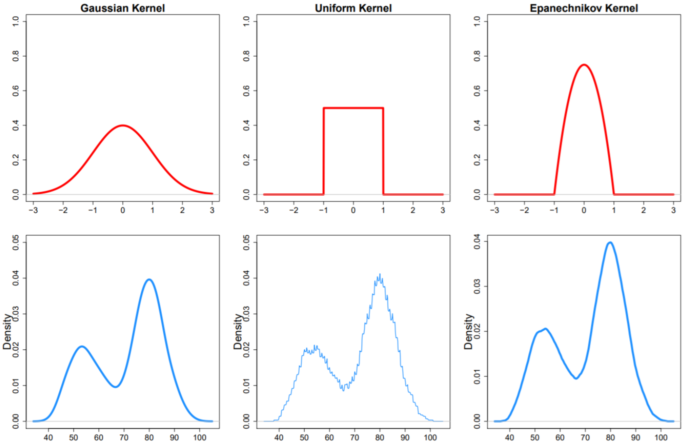
- $\int_{-\infty}^{\infty} K(u) du = 1$, makes sure p is a density function.



Different kernels $K(u)$

$$\frac{1}{\sqrt{2\pi}}e^{-\frac{u^2}{2}} \qquad \frac{1}{2}\mathbb{I}[|u| \leq 1] \qquad \frac{3}{4}\max\{1 - x^2, 0\}$$



Bandwidth

If $K(u)$ is a kernel, then for any $h > 0$

$$K_h(u) \triangleq \frac{1}{h} K\left(\frac{u}{h}\right) \qquad \text{(stretching the kernel)}$$

can be used as a kernel too (verify the two properties yourself)

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So general KDE is determined by both the kernel K and the bandwidth h

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

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- x_n controls the center of each bump
- h controls the width/variance of the bumps

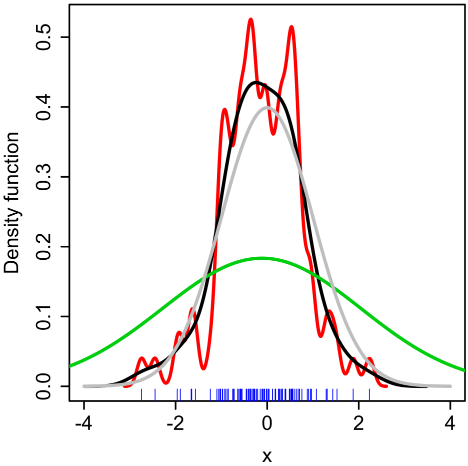
Effect of bandwidth

picture from Wikipedia

Larger h means larger variance and also smoother density

Gray curve is ground-truth

- Red: $h = 0.05$
- Black: $h = 0.337$
- Green: $h = 2$



Bandwidth selection

Selecting h is a deep topic

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- one can also do cross-validation based on downstream applications

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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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More formally

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For each possible value k of a discrete feature d,

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

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If the feature is continuous, we can do

- parametric 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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$$\begin{aligned} \operatorname*{argmax}_{c \in [\mathsf{C}]} \; p(y = c \mid x) &= \operatorname*{argmax}_{c \in [\mathsf{C}]} \; p(x, y = c) \\ &= \operatorname*{argmax}_{c \in [\mathsf{C}]} \; \left(p(y = c) \prod_{d=1}^{\mathsf{D}} p(x_d \mid y = c) \right) \end{aligned}$$

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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

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

Examples

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

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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 naive Bayes is 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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So what is different then? They **learn the parameters in different ways**:

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- solutions are different: logistic regression has no closed-form, naive Bayes admits a simple closed-form

Generative model v.s discriminative model

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Remark		more flexible, can generate data after learning