# Clustering-oriented selection of the amount of smoothing in kernel density estimation

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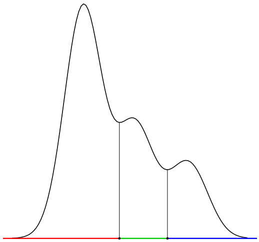
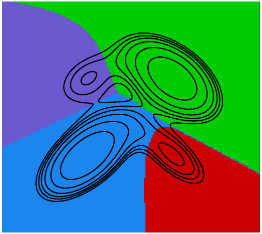
# Density-based clustering

- **Framework**: density-based clustering
  - Statistical formalization of the clustering problem;
  - Identifies a partition of the sample space and not only of the data points;
  - Definition of cluster based on features of the density underlying the data.

# Modal clustering

- **Nonparametric formulation**: clusters correspond to the domains of attraction of the modes of the density;
- Operationally required:
  - A density estimate;
  - A method to locate modal regions of the density.





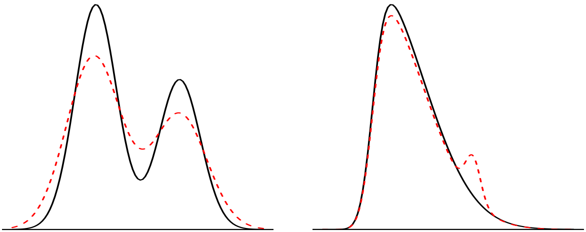
# Modal clustering

- Kernel density estimator (KDE) is usually considered to obtain a nonparametric density estimate;
- Let $\mathcal{X} = \{x_i\}_{i=1,\ldots,n}$, $x_i \in \mathbb{R}$ be a sample from a r.v. $X$ with density $f$. Define KDE as

$$\hat{f}_h(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right)$$

  - $K(\cdot)$ is the kernel function;
  - $h$ is the bandwidth.
- Bandwidth $h$ controls the amount of smoothing:
  $\rightarrow$ if wrongly chosen could lead to cover interesting features or highlight spurious ones.

# Aim and contribution



- Usual bandwidth selectors aim to obtain appropriate estimates of the density from a global perspective
  BUT $\longrightarrow$ Density estimation and clustering are different problems with different requirements;
- **Contribution**: propose an asymptotically optimal modal clustering-oriented bandwidth by minimizing a measure of distance.

# Distance between clusterings

- **Distance in measure** (DM) between clusterings $\mathcal{C}_0 = \{C_1, \ldots, C_r\}$ and $\hat{\mathcal{C}}_n = \{\hat{C}_r, \ldots, \hat{C}_r\}$

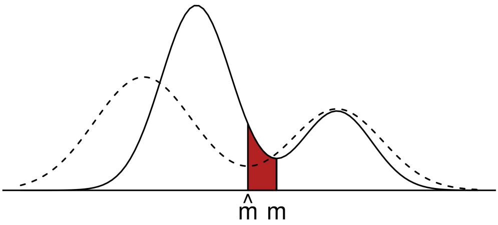
$$d(\mathcal{C}_0, \hat{\mathcal{C}}_n) = \frac{1}{2} \min_{\sigma \in \mathcal{P}_r} \left\{ \sum_{j=1}^{r} \mathbb{P}\left(C_j \Delta \hat{C}_{\sigma(j)}\right) \right\}$$

  - $\mathcal{P}_r$: set of permutations of $\{1, \ldots, r\}$;
  - $C \Delta \hat{C} = (C \cap \hat{C}^c) \cup (C^c \cap \hat{C})$;

- Easily generalizable for clusterings with different number of groups;
- Optimal bandwidth:

$$h_{opt} = \operatorname*{argmin}_h \mathbb{E}[d(\mathcal{C}_0, \hat{\mathcal{C}}_n)]$$

# Distance between clusterings




- **Interpretation**: minimal probability mass that has to be moved to transform one clustering to the other.
- For $n$ large DM is

$$d(\mathcal{C}_0, \hat{\mathcal{C}}_n) = \sum_{j=1}^{r-1} \left| F(\hat{m}_j) - F(m_j) \right| ,$$

  - $F$ cdf of $f$;
  - $\{m_j\}$ and $\{\hat{m}_j\} = \{\hat{m}_j(h)\}$ minima of $f$ and $\hat{f}_h$, $j = 1, \ldots, r$.

# Distance between clusterings

- **Asymptotic Expected Distance in Measure** (AEDM)

$$
\begin{aligned}
\mathbb{E}(d_P(\mathcal{C}_0, \hat{\mathcal{C}}_n)) &\simeq \sum_{j=1}^{r-1} \frac{f(m_j)}{f^{(2)}(m_j)} n^{-2/7} \psi(\mu, \sigma) \\
&\simeq \sum_{j=1}^{r-1} \frac{f(m_j)}{f^{(2)}(m_j)} n^{-2/7} \{2\sigma^2 \phi_\sigma(\mu) + \mu[1 - 2\Phi_\sigma(-\mu)]\}
\end{aligned}
$$

  - $\mu = \mu(h) = n^{2/7} h^2 f^{(3)}(m_j) \mu_2(K)/2$;
  - $\sigma^2 = \sigma^2(h) = R(K^{(1)}) f(m_j)/(n^{3/7} h^3)$;
  - $\phi_\sigma(\cdot)$ and $\Phi_\sigma(\cdot)$ density and cdf of $\mathcal{N}(0, \sigma^2)$;
  - $R(K^{(r)}) = \int_{\mathbb{R}} (K^{(r)}(x))^2 dx$ and $\mu_2(K) = \int_{\mathbb{R}} x^2 K(x) dx$;
- Two summands behaving as *Integrated Squared Bias* and *Integrated Variance* for the MISE;
- Problems:
  - Dependence on $f, f^{(2)}$ and $f^{(3)}$;
  - Not available a closed form for $h_{opt}$.

# Optimal bandwidth

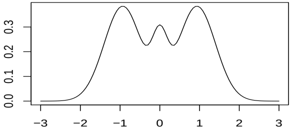
- Introduce two different upper bounds:

$$\begin{aligned}\psi(\mu,\sigma) &\leq \sigma\sqrt{2/\pi} + |\mu| \\ \psi(\mu,\sigma) &\leq \sigma\sqrt{2/\pi} + \mu^2/(\sigma\sqrt{2\pi}))\end{aligned}$$

- Minimization of the bounded versions of the AEDM leads to

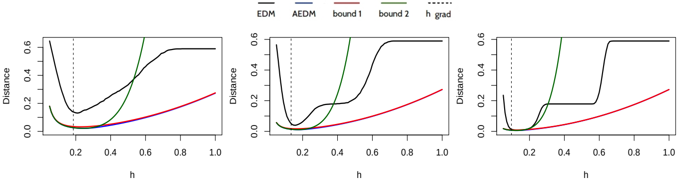
$$\begin{aligned} h_{opt,b_1} &= \left(\frac{3R(K')^{1/2}\sum_{j=1}^{r-1}\frac{f(m_j)^{3/2}}{f^{(2)}(m_j)}}{\mu_2(K)\sqrt{2\pi}\sum_{j=1}^{r-1}\frac{f(m_j)|f^{(3)}(m_j)|}{f^{(2)}(m_j)}}\right)^{2/7} n^{-1/7} \\ h_{opt,b_2} &= \left(\frac{24R(K')\sum_{j=1}^{r-1}\frac{f(m_j)^{3/2}}{f^{(2)}(m_j)}}{11\mu_2^2(K)\sum_{j=1}^{r-1}\frac{f(m_j)^{1/2}f^{(3)}(m_j)^2}{f^{(2)}(m_j)}}\right)^{1/7} n^{-1/7} \ . \end{aligned}$$

# Numerical results



| | n =100 | n=1000 | n=10000 |
|---|---|---|---|

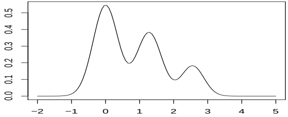
EDM approximation




DM estimate

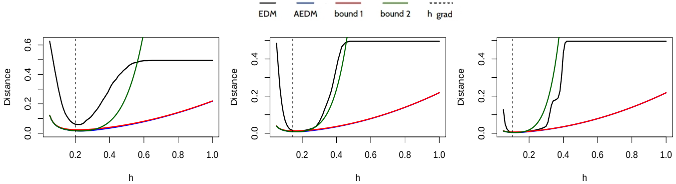
| | n =100 | n=1000 | n=10000 |
|---|---|---|---|
| $h_{aedm}$ | 0.265 (0.173) | 0.060 (0.070) | 0.010 (0.016) |
| $h_{bound1}$ | 0.237 (0.155) | 0.053 (0.066) | 0.011 (0.017) |
| $h_{bound2}$ | 0.257 (0.168) | 0.058 (0.069) | 0.010 (0.016) |
| $h_{grad}$ | 0.183 (0.031) | 0.092 (0.075) | 0.008 (0.005) |

# Numerical results




| | n =100 | n=1000 | n=10000 |
|---|---|---|---|

EDM approximation




DM estimate

| | n =100 | n=1000 | n=10000 |
|---|---|---|---|
| $h_{aedm}$ | 0.113 (0.131) | 0.017 (0.034) | 0.006 (0.007) |
| $h_{bound1}$ | 0.095 (0.114) | 0.017 (0.030) | 0.006 (0.007) |
| $h_{bound2}$ | 0.109 (0.128) | 0.017 (0.034) | 0.006 (0.007) |
| $h_{grad}$ | 0.136 (0.113) | 0.013 (0.009) | 0.005 (0.003) |

# Concluding remarks and future work

- We have obtained a good asymptotic approximation to the EDM $\longrightarrow$ problems in data-driven procedures due to plug-in strategies;
- Gradient bandwidth seems to be an appropriate choice when resorting to modal clustering;

- Directions of **future work**:
    - Find suitable nonparametric alternatives to better locate the minima and to estimate the features of the density at those points $\longrightarrow$ local bandwidth ?
    - Extend the results in multivariate situations.

# Relevant references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