NOVEL BAYESIAN CLUSTER ENUMERATION CRITERION FOR CLUSTER ANALYSIS WITH FINITE SAMPLE PENALTY TERM

Freweyni K. Teklehaymanot[1,2], Michael Muma[1], Abdelhak M. Zoubir[1,2]

[1] Signal Processing Group, Technische Universität Darmstadt, {ftekle, muma, zoubir}@spg.tu-darmstadt.de [2] Graduate School CE, Technische Universität Darmstadt, teklehaymanot@gsc.tu-darmstadt.de

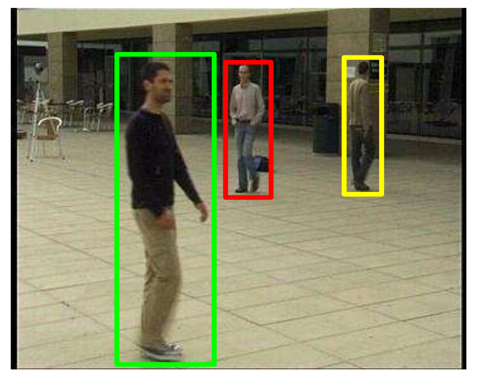
TECHNISCHE UNIVERSITÄT DARMSTADT

1 Motivation

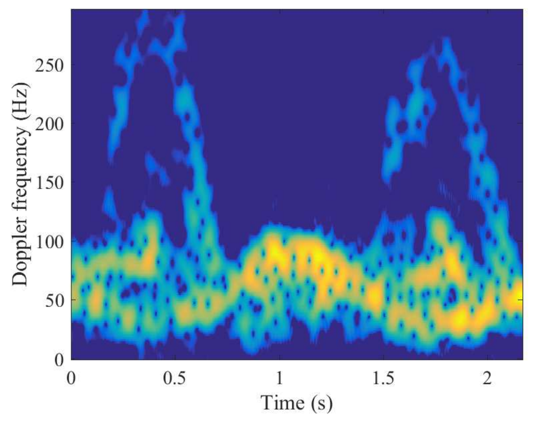
- Bayesian Information Criterion (BIC): extensively used in clustering.
- Prior to [1] BIC, for clustering, has not been derived from first principles.
- Finite-sample performance of asymptotic criterion is not satisfactory.

2 Contributions

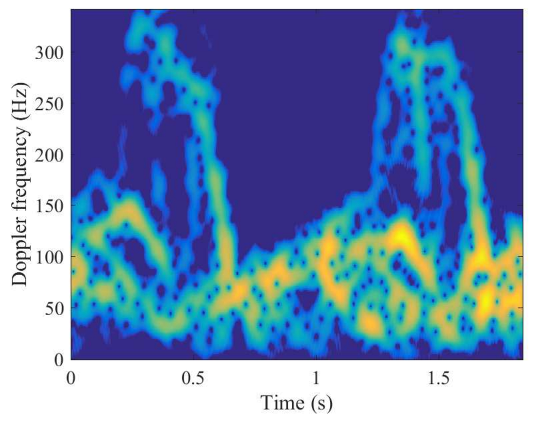
- Finite-sample BIC for clustering derived from first principles.
- Proposed criterion ($\mathrm{BIC}_{\mathrm{NF}}$) incorporates structure of the clustering problem and chooses model with maximum posterior probability.
- $\mathrm{BIC}_{\mathrm{NF}}$ successfully applied to camera networks [2] and radar [3].



Labeling humans in camera networks



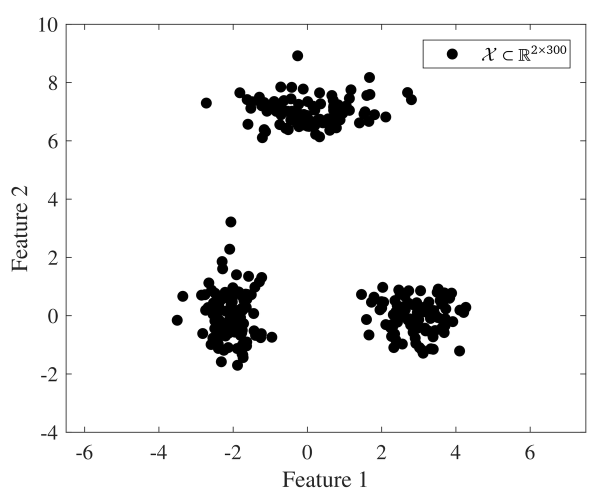
Doppler signature of Person A

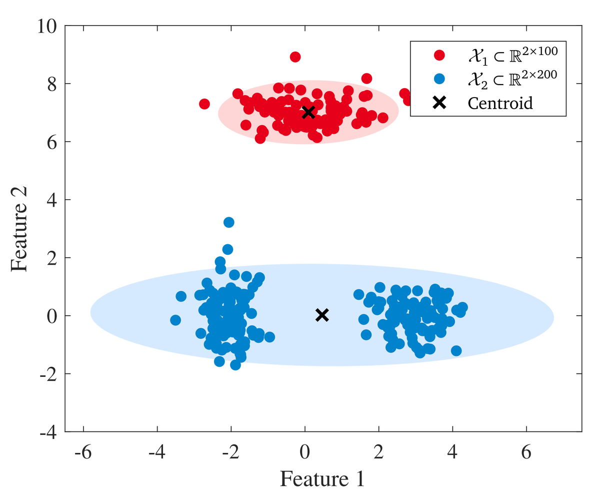


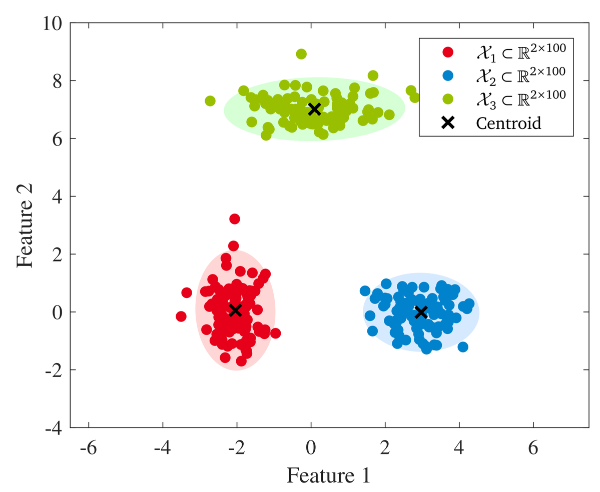
Doppler signature of Person B

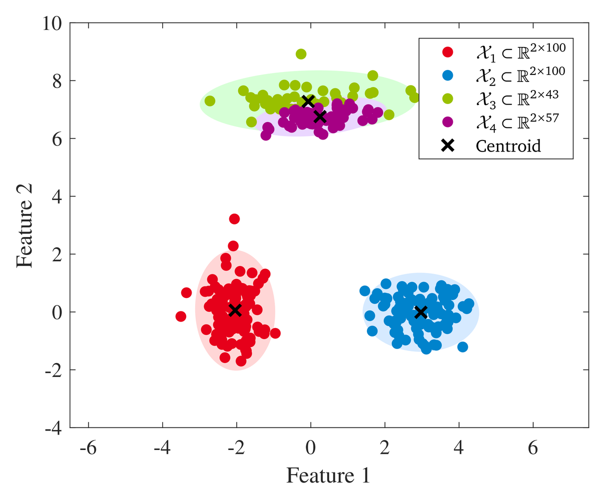
3 Problem Formulation

- $\boldsymbol{x}_k \sim \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$, $k \in \mathcal{K} \triangleq \{1,\ldots,K\}$: i.i.d Gaussian random variables; K: number of clusters; $\boldsymbol{\mu}_k \in \mathbb{R}^{r\times 1}$ and $\boldsymbol{\Sigma}_k \in \mathbb{R}^{r\times r}$: centroid and covariance matrix of the kth cluster
- $\mathcal{X}_k \subset \mathbb{R}^{r\times N_k}, k \in \mathcal{K}$: cluster containing realizations of $\boldsymbol{x}_k$
- $\mathcal{X} \triangleq \{\mathcal{X}_1,\ldots,\mathcal{X}_K\} \subset \mathbb{R}^{r\times N}$: observed data set; $N=\sum_{k=1}^{K} N_k$
- $\mathcal{M} \triangleq \{M_{L_{\min}},\ldots,M_{L_{\max}}\}$: family of candidate models
- $\mathcal{X}$ partitioned into $l = L_{\min},\ldots,L_{\max}$ clusters, using model M_l with parameters $\boldsymbol{\Theta}_l = [\boldsymbol{\theta}_1,\ldots,\boldsymbol{\theta}_l]$
- **Goal:** estimate the number of clusters in $\mathcal{X}$ given $\mathcal{M}$









4 Proposed Bayesian Cluster Enumeration Criterion With Finite Sample Penalty Term

- **Main idea:** maximization of posterior probability of candidate models $M_l \in \mathcal{M}$ given $\mathcal{X}$

$$M_{\hat{K}} = \underset{\mathcal{M}}{\arg\max}\ \log p(M_l|\mathcal{X})$$

$p(M_l|\mathcal{X})$: posterior probability of M_l given $\mathcal{X}$; $\hat{K}$: estimated number of clusters in $\mathcal{X}$

- New BIC for clustering derived from first principles in [1]: applicable to broad class of data distributions

$$\mathrm{BIC}_{\mathrm{G}}(M_l) \triangleq \log p(M_l|\mathcal{X}) \approx \log \mathcal{L}(\hat{\boldsymbol{\Theta}}_l|\mathcal{X}) - \frac{1}{2}\sum_{m=1}^{l}\log\left|\hat{\boldsymbol{J}}_m\right|$$

$\mathcal{L}(\hat{\boldsymbol{\Theta}}_l|\mathcal{X})$: likelihood function; $\hat{\boldsymbol{J}}_m$: Fisher information matrix of observations from the mth cluster; $|\cdot|$: determinant

$$\hat{\boldsymbol{J}}_m \triangleq -\left.\frac{d^2 \log \mathcal{L}(\boldsymbol{\theta}_m|\mathcal{X}_m)}{d\boldsymbol{\theta}_m d\boldsymbol{\theta}_m^\top}\right|_{\boldsymbol{\theta}_m=\hat{\boldsymbol{\theta}}_m} \in \mathbb{R}^{q\times q}$$

- Special case of [1]: $\mathcal{X}$ is distributed as multivariate Gaussian

$$\mathrm{BIC}_{\mathrm{N}}(M_l) = \sum_{m=1}^{l} N_m \log N_m - \sum_{m=1}^{l}\frac{N_m}{2}\log\left|\hat{\boldsymbol{\Sigma}}_m\right| - \frac{q}{2}\sum_{m=1}^{l}\log N_m$$

$\hat{\boldsymbol{\Sigma}}_m$: estimate of the covariance matrix of the mth cluster; N_m: number of data points in the mth cluster

- **Contribution:** derivation of the penalty term for the finite-sample regime

$$\mathrm{BIC}_{\mathrm{NF}}(M_l) = \mathrm{BIC}_{\mathrm{N}}(M_l) + \frac{1}{4}r(r+1)l\log 2 + \frac{1}{2}\sum_{m=1}^{l}\log\left|\hat{\boldsymbol{\Sigma}}_m\right| - \frac{1}{2}\sum_{m=1}^{l}\log\left|\boldsymbol{D}^\top\hat{\boldsymbol{F}}_m\boldsymbol{D}\right|$$

$$\hat{\boldsymbol{J}}_m = \begin{bmatrix} N_m\hat{\boldsymbol{\Sigma}}_m^{-1} & \boldsymbol{0}_{r\times\frac{1}{2}r(r+1)} \\ \boldsymbol{0}_{\frac{1}{2}r(r+1)\times r} & \frac{N_m}{2}\boldsymbol{D}^\top\hat{\boldsymbol{F}}_m\boldsymbol{D} \end{bmatrix}$$

$\boldsymbol{D} \in \mathbb{R}^{r^2\times\frac{1}{2}r(r+1)}$: duplication matrix; $\hat{\boldsymbol{F}}_m \triangleq \hat{\boldsymbol{\Sigma}}_m^{-1}\otimes\hat{\boldsymbol{\Sigma}}_m^{-1} \in \mathbb{R}^{r^2\times r^2}$

- Estimated number of clusters

$$\hat{K}_{\mathrm{BIC}_{\mathrm{NF}}} = \underset{l=L_{\min},\ldots,L_{\max}}{\arg\max}\ \mathrm{BIC}_{\mathrm{NF}}(M_l)$$

5 Results

- Data-1: Gaussian data set with $K=5$ clusters; Data-2: Gaussian data set with $K=6$ clusters
- $L_{\min}=1$ and $L_{\max}=2K$
- $\mathrm{BIC}_{\mathrm{O}}$: the original BIC

$$\mathrm{BIC}_{\mathrm{O}}(M_l) = \sum_{m=1}^{l} N_m\log N_m - \sum_{m=1}^{l}\frac{N_m}{2}\log\left|\hat{\boldsymbol{\Sigma}}_m\right| - \frac{ql}{2}\log N$$

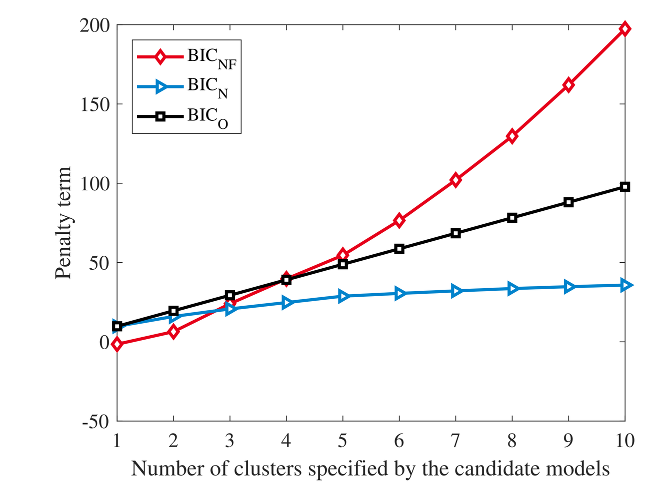
- $p_{\mathrm{det}} = \frac{1}{\mathrm{MC}}\sum_{s=1}^{\mathrm{MC}}\mathbb{1}_{\{\hat{K}_s=K\}}$, p_{det}: empirical probability of detection; MC: number of Monte Carlo experiments; $\mathbb{1}_{\{.\}}$: indicator function

Results for Data-1

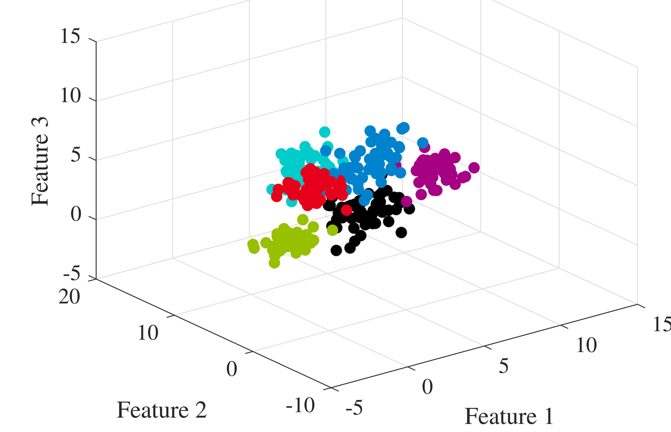
	N_k	10	50	100	1000
$p_{\mathrm{det}}(\%)$	$\mathrm{BIC}_{\mathrm{NF}}$	**77.6**	**100**	**100**	**100**
	$\mathrm{BIC}_{\mathrm{N}}$	0	77.8	96.2	**100**
	$\mathrm{BIC}_{\mathrm{O}}$	26.4	99.3	99.7	**100**

Results for Data-2

	N_k	50	100	250	1000
$p_{\mathrm{det}}(\%)$	$\mathrm{BIC}_{\mathrm{NF}}$	**82.1**	**96.7**	**98.7**	**99.3**
	$\mathrm{BIC}_{\mathrm{N}}$	64.7	92.9	98.1	**99.3**
	$\mathrm{BIC}_{\mathrm{O}}$	51.7	91.1	**98.7**	**99.3**



Penalty term for Data-1 when $N_k=10$



Data-2 when $N_k=50$

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