

11th Scientific Meeting of the SIS Group
"Statistics for the Evaluation and Quality in Services"

BOOK OF **SHORT PAPERS**

Editors

Andrea Bucci

Alfredo Cartone

Adelia Evangelista

Andrea Marletta



**STATISTICAL METHODS
FOR EVALUATION AND QUALITY:
TECHNIQUES, TECHNOLOGIES AND TRENDS (T³)**

**IES 2023 - Statistical Methods for Evaluation and Quality:
Techniques, Technologies and Trends (T³)**

BOOK OF SHORT PAPERS

Editors: Andrea Bucci, Alfredo Cartone, Adelia Evangelista and Andrea Marletta

Book of Short papers
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Statistical Methods for Evaluation and Quality: Techniques, Technologies and
Trends (T³)

University 'G. d'Annunzio' of Chieti-Pescara



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Adelia Evangelista University 'G. d'Annunzio' of Chieti-Pescara
Andrea Marletta University of Milan 'Bicocca'



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Preface

Statistical thinking, design and analysis play a crucial role in social life and are useful to society at large. Besides, promoting advanced methodological research is useful to facilitate the dissemination of ideas related to various fields of interest. For this purpose, experts in statistics, data analysis, data mining, statistical methods for decision making, machine learning and related methods come together to understand and analyse phenomena through data.

In line with this objective, the Statistics Group for the Evaluation and Quality of Services (SVQS; www.svqs.it) of the Italian Statistical Society (SIS) has been organizing the Innovation and Society (IeS) conference biennially since 2009, focusing on new developments and ideas in statistics applied to the evaluation and quality of public and private services, attracting national and international statisticians and data scientists. The meeting contributes to spot light on the main statistical approaches and methodologies for the evaluation of public services currently in use in different contexts, as well as to facilitate discussion on the impact of innovative statistical evaluation systems for these services, involving various economic and social policy actors.

The conference “Statistical Methods for Evaluation and Quality: Techniques, Technologies and Trends (T³)” recorded valuable contributions that are reported in this volume. The papers underscore how the growing availability of data has tasked social and economic actors, organizations, and researchers with the management and analysis of large volumes of unstructured and heterogeneous data. In recent years, many tools for both qualitative and quantitative models have been developed to better describe and understand complex systems and their underlying behaviors, and the papers reported in this volume bear witness to this.

Techniques, technologies and trends: the study of data complexity presents the potential to provide analyses with increased frequency and timeliness, accuracy and objectivity, and to define sustainable models. Traditional quantitative methods for capturing socioeconomic data have often shown limitations in their ability to examine underlying systems, and with the three ‘T’ just mentioned, the outlines of future developments are starting to emerge.

The volume reports 127 contributions in the following areas:

- Advanced statistical methods for pattern recognition
- Advances in statistical learning from high-dimensional data
- Data analysis for web sources
- Distance and depth-based statistical learning methods for robust data analysis

- Economics and environment
- Education and labour
- Inequalities in the labour market
- Innovations and challenges in official statistics
- Labour market: trends, perspectives and new challenges
- Methodological and applicative contributions for evaluating sustainable development
- Methodological developments and applications for the assessment of student competencies
- Networks data analysis: new perspectives and applications
- New advanced statistical methods for data science
- Recent advances in statistical learning and data analysis
- Statistical analysis and modeling of environmental pollution data
- Statistical methods and complexity for evaluation in finance
- Statistical methods and composite indicators for healthcare
- Statistical methods and models for land monitoring with spatio-temporal data
- Statistical methods for environmental monitoring and sustainability
- Statistical methods for the analysis of university student choices and academic performance
- Statistical methods for the assessment of transport services and sustainable emissions
- Statistical methods for education and educational services
- Statistics in sports
- Tourism and territory.

The Conference event attracted many contributions as well as numerous Authors, not just from Italy but also from abroad. Over the three-day meeting, the Community has the opportunity to witness some of the state-of-the arts, new trajectories, and methodological challenges in 24 solicited sessions, 7 sessions of free contributes, two round tables - organized by Maurizio Vichi and Matilde Bini respectively - and three keynotes sessions with Ron S. Kennet of Samuel Neaman Institute of Israel, Luigi D'Ambra of Federico II University of Naples, and the former Minister Enrico Giovannini from University of Tor Vergata.

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Solicited Session SS16 - *Recent advances in statistical learning and data analysis*

Session of the SIS-CLADAG organized by Domenico Vistocco and Pietro Coretto

Chair: Marcella Niglio

Discussant: Cristina Davino

1. *A Predictive Functional Principal Component Analysis of Well-Being Data* (Marcis L., Pagliarella M.C. and Salvatore R.)
2. *Detecting the partition in the extended hierarchy of a dendrogram: an application on biomedical data* (Policastro V., Palazzo L. and Vistocco D.)
3. *Concordance measure for rankings* (Bissiri P.G. and Nai Ruscone, M.)
4. *Quadratic discriminant scoring for selecting clustering solutions* (Coraggio L. and Coretto P.)

Quadratic discriminant scoring for selecting clustering solutions

Funzione discriminante quadratica per la selezione di soluzioni di clustering

Luca Coraggio and Pietro Coretto

Abstract Selecting an optimal clustering solutions is a difficult problem. There exist many data-driven validation strategies in the literature to perform this task. In this paper, we focus on a recent proposal, based on quadratic discriminant scores and bootstrap resampling, namely the BQH and BQS from Coraggio and Coretto [4]. These strategies proved to be extremely successful with elliptic-symmetric clusters and, in general, when clusters can be separated by quadratic boundaries. In this work, we review the BQH and BQS strategies, and try to shed more light on their functioning, by comparing them with alternative likelihood-based validation indexes, and with different resampling schemes.

Abstract *La selezione di soluzioni di clustering ottimali è un problema complesso. In letteratura, esistono molte strategie di validazione per svolgere questo compito. In questo lavoro, ci concentriamo su una proposta recente, basata su funzioni di discriminante quadratica e tecniche di ricampionamento bootstrap, ovvero i metodi BQH e BQS proposti in Coraggio and Coretto [4]. Queste strategie si sono dimostrate estremamente efficaci con cluster ellittico-simmetrici e, più in generale, quando i cluster possono essere separati da confini quadratici. In questo lavoro, riprendiamo le strategie BQH e BQS, e indaghiamo il loro funzionamento in uno studio comparativo, utilizzando nuovi indici di validazione, basati sulla funzione di verosimiglianza, assieme a schemi di ricampionamento alternativi.*

Key words: Cluster validation, Mixture models, Model-based clustering, Resampling methods

Luca Coraggio
Department of Economics and Statistics, University of Naples Federico II, e-mail:
luca.coraggio@unina.it

Pietro Coretto
Department of Economics and Statistics, University of Salerno e-mail: pcoretto@unisa.it

1 Introduction

Typically, in cluster analysis, the researcher produces many solutions, running several clustering algorithms with various settings. The problem is that, while a single final solution may be required, it may well be the case that multiple of them provide a good description of the data, according to different clusters' concepts [17]. Recently, in [4], we proposed a novel validation index aimed at selecting clustering solutions in cases where clusters can be expected to have elliptic-symmetric shapes, or to be separable by quadratic boundaries. The proposed strategy proved to be effective in conjunction with a bootstrap resampling strategy that hedges against overoptimism in the selection process, and helps avoid choosing overly-complex solutions. In this paper, we review this methodology and investigate the different components that make it successful. We do this by comparing it with an alternative likelihood-based validation index, and combining it with different resampling schemes. The outline of the paper is as follows. Section 2 reviews the BQH and BQS indexes, and introduces the alternative strategies; Section 3 presents the empirical analysis; Section 4 concludes.

2 Quadratic Discriminant Scoring

Let \mathbb{X}_n be an observed sample of size n , with feature vectors $\mathbf{x}_i \in \mathbb{R}^p$. Let $\mathcal{G}^{(m)} = \{G_k^{(m)}, k = 1, \dots, K_m\}$ be a clustering solution, allocating the n objects into K_m groups; $\mathcal{G}^{(m)}$ is obtained from a clustering method $m \in \mathcal{M}$. We assume that $\mathcal{G}^{(m)}$ can be meaningfully described by a collection of K_m triplets $\boldsymbol{\theta}^{(m)} = \{\boldsymbol{\theta}_k^{(m)}, k = 1, \dots, K_m\}$,

where each $\boldsymbol{\theta}_k^{(m)}$ collects unique elements of the following objects: (i) π_k : the expected fraction of points belonging to the k -th group; (ii) $\boldsymbol{\mu}_k \in \mathbb{R}^p$ is the k -th cluster's center; (iii) $\boldsymbol{\Sigma}_k \in \mathbb{R}^{p \times p}$ is a positive definite scatter matrix that either coincides with or is proportional to the k -th cluster's covariance matrix. $\boldsymbol{\theta}^{(m)}$, together with K_m , provides a description of the m -th clustering configuration $m \in \mathcal{M}$.¹

For a point \mathbf{x} and a triplet $\boldsymbol{\theta}_k$, we define the quadratic scoring of point \mathbf{x} for the k -th cluster as

$$\text{qs}(\mathbf{x}, \boldsymbol{\theta}_k) = \log(\pi_k) - \frac{1}{2} \log(\det(\boldsymbol{\Sigma}_k)) - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \quad (1)$$

The quadratic score is inspired to Quadratic Discriminant Analysis, where (1) represents the optimal classification boundaries under the Gaussian assumption (e.g., see [10]). It can be seen as a measure of how well point \mathbf{x} is accommodated into

¹ Depending on m , the triplets $\boldsymbol{\theta}_k^{(m)}$ may be taken to coincide with elements defined by the approach itself (e.g., in model-based clustering, each triplet coincides with the parameters of one mixture component; e.g., see [13]), or can be estimated with sample quantities, computing within-cluster empirical counterparts (using estimated point-to-cluster assignments).

cluster k (higher values correspond to a better fit). Using (1) we define the quadratic partition, \mathcal{Q} , as

$$\mathcal{Q} = \{Q_k, k \in \{1, \dots, K\}\}, \quad Q_k = \left\{ \mathbf{x} \in \mathbb{R}^P : k = \arg \max_{k \in \{1, \dots, K\}} \text{qs}(\mathbf{x}, \boldsymbol{\theta}_k) \right\}. \quad (2)$$

Finally, for a given $\boldsymbol{\theta}$ we define the hard and smooth quadratic scoring criteria respectively as

$$H(\boldsymbol{\theta}^{(m)}; \mathbb{X}_n) = \frac{1}{n} \sum_{\mathbf{x} \in \mathbb{X}_n} \sum_{k=1}^{K^{(m)}} s_H(\mathbf{x}, \boldsymbol{\theta}^{(m)}) = \frac{1}{n} \sum_{\mathbf{x} \in \mathbb{X}_n} \sum_{k=1}^{K^{(m)}} \mathbb{I} \left\{ \mathbf{x} \in Q_k(\boldsymbol{\theta}^{(m)}) \right\} \text{qs}(\mathbf{x}, \boldsymbol{\theta}_k^{(m)}); \quad (3)$$

$$T(\boldsymbol{\theta}^{(m)}; \mathbb{X}_n) = \frac{1}{n} \sum_{\mathbf{x} \in \mathbb{X}_n} \sum_{k=1}^{K^{(m)}} s_T(\mathbf{x}, \boldsymbol{\theta}^{(m)}) = \frac{1}{n} \sum_{\mathbf{x} \in \mathbb{X}_n} \sum_{k=1}^{K^{(m)}} \tau_k(\mathbf{x}, \boldsymbol{\theta}^{(m)}) \text{qs}(\mathbf{x}, \boldsymbol{\theta}_k^{(m)}), \quad (4)$$

where τ_k defines a smooth weight of point-to-cluster membership as measured by the quadratic score:

$$\tau_k(\mathbf{x}, \boldsymbol{\theta}) = \frac{\text{qs}(\mathbf{x}, \boldsymbol{\theta}_k)}{\sum_{k=1}^K \text{qs}(\mathbf{x}, \boldsymbol{\theta}_k)}.$$

2.1 Likelihood-based validation

The quadratic score (1) is strongly connected to likelihood theory, and it is easy to show that it is proportional to the Gaussian density function [4]. Thus, a natural alternative to the scoring criteria (3) and (4) appears to be the likelihood function of a Gaussian mixture model. A similar proposal was also made by Smyth [16], used in combination with cross-validation. Thus, the data log-likelihood can be used to score a clustering solution (solutions achieving higher likelihood are preferred), and is defined as:

$$l(\boldsymbol{\theta}^{(m)}; \mathbb{X}_n) = \frac{1}{n} \sum_{\mathbf{x} \in \mathbb{X}_n} \log \left(\sum_{k=1}^{K^{(m)}} \pi_k^{(m)} \phi(\mathbf{x}, \boldsymbol{\theta}_k^{(m)}) \right), \quad (5)$$

where $\phi(\mathbf{x}, \boldsymbol{\theta}_k^{(m)})$ is the density function of a multi-variate Gaussian distribution with mean $\boldsymbol{\mu}_k$ and covariance $\boldsymbol{\Sigma}_k$. Note that, differently from (3) and (4), the usage of (5) is only justified for model-based clustering, where a probabilistic model is assumed, and it is needed to motivate the construction of the likelihood function.

Algorithm 1 Bootstrap quadratic scoring

input: observed sample \mathbb{X}_n (with ecdf \mathbb{F}_n), $\alpha \in (0, 1)$; clustering method $m \in \mathcal{M}$; integers $B > 0$

output: bootstrap quadratic scoring for method m : $\tilde{L}_n^{(m)}$.

(to ease notation, dependence on m is dropped and reintroduced in step 3)

for $b \in \{1, \dots, B\}$ do

(step 1.1) $\mathbb{X}_n^{(b)} \leftarrow$ non-parametric bootstrap resample from \mathbb{X}_n (sample of size n from \mathbb{F}_n)

(step 1.2) $\hat{\theta}_n^{(b)} \leftarrow$ triplets of parameters from clustering solution m fitted on $\mathbb{X}_n^{(b)}$

(step 1.3) $S_n^{(b)} \leftarrow$ score solution on points in \mathbb{X}_n not in $\mathbb{X}_n^{(b)}$

$$S_n^{(b)} = H(\hat{\theta}_n^{(b)}; \mathbb{X}_n) \quad \text{or} \quad S_n^{(b)} = T(\hat{\theta}_n^{(b)}; \mathbb{X}_n) \quad \text{or} \quad S_n^{(b)} = l(\hat{\theta}_n^{(b)}; \mathbb{X}_n)$$

end for

(step 2) $\tilde{W}_n \leftarrow \frac{1}{B} \sum_{b=1}^B S_n^{(b)} \quad R_n^{(b)} \leftarrow \sqrt{n} (S_n^{(b)} - \tilde{W}_n)$

(step 3) Compute $(\alpha/2)$ -level and $(1 - \alpha/2)$ -level empirical quantiles:

$$\tilde{L}_n^{(m)} \leftarrow \inf_t \left\{ \frac{1}{B} \sum_{b=1}^B \mathbb{I} \{ R_n^{*(b)} \leq t \} \geq \frac{\alpha}{2} \right\}; \quad \tilde{U}_n^{(m)} \leftarrow \inf_t \left\{ \frac{1}{B} \sum_{b=1}^B \mathbb{I} \{ R_n^{*(b)} \leq t \} \geq 1 - \frac{\alpha}{2} \right\}$$

2.2 Resampling schemes

Choosing the solution that maximizes (3) or (4) may give poor results: since the sample data \mathbb{X}_n is used both for estimation and scoring, overly-complex solutions may be selected due to overoptimism in the evaluation process. It is well known that increasingly complex solutions can fit the data better, and many selection methods takes this into account in several ways. For example, information criteria typically include a penalization term for the model's complexity (e.g., BIC [15] and ICL [3]). To cope with this issue, in Coraggio and Coretto [4], we propose to estimate clustering solutions on non-parametric bootstrap resamples [7] from \mathbb{X}_n , and to evaluate (3) and (4) on \mathbb{X}_n . The procedure is reviewed in Algorithm 1, and here we extend it to include a likelihood-based scoring, using (5) as the scoring function.

3 Empirical analysis

The experimental analysis is a scaled-down version of that in Coraggio and Coretto [4], using the Iris, Olive and Banknote data sets [1, 9, 8]. Since we are going to compare the quadratic scores with likelihood-based ones, \mathcal{M} includes only model-based clustering methods: (i) 140 model-based clustering methods, using Gaussian mixture models with parsimonious representation of the covariance matrices [2], implemented with the Mclust software [14] (setting $K = 1, \dots, 10$, and 14 covariance models); (ii) 180 model-based clustering methods, using Gaussian mixture models with eigen-ratio constraints (ERC; [12]), implemented with Otrimle software

Table 1: Selected clustering solution by selection criteria (left-most column). Each sub-table shows results from a real data set: the first column shows the selected solution, and the second column reports its ARI, computed against true classes.

Criterion	(b) Iris		(c) Olive		(d) Banknote	
	Selected m	ARI	Selected m	ARI ¹	Selected m	ARI
QH	Otrimle, $K=10, \gamma=10^4$	0.44	Mclust, $K=10, VVV$	0.54	Otrimle, $K=10, \gamma=10^4$	0.26
QS	Otrimle, $K=10, \gamma=10^4$	0.44	Mclust, $K=10, VVV$	0.54	Otrimle, $K=10, \gamma=10^4$	0.26
LK	Otrimle, $K=10, \gamma=10^4$	0.44	Mclust, $K=10, VVV$	0.54	Otrimle, $K=10, \gamma=10^4$	0.26
CVQH	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=6, VVV$	0.79	Mclust, $K=4, VVE$	0.68
CVQS	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=6, VVV$	0.79	Otrimle, $K=3, \gamma=10$	0.86
CVLK	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=9, VEE$	0.65	Mclust, $K=4, VVE$	0.68
BQH	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=8, VVV$	0.86	Otrimle, $K=3, \gamma=10$	0.86
BQS	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=8, VVV$	0.86	Otrimle, $K=3, \gamma=10$	0.86
BLK	Otrimle, $K=3, \gamma=10^2$	0.90	Mclust, $K=8, VVV$	0.86	Mclust, $K=6, EEE$	0.47

(Olive) 1. refers to the finer 9-regions classification.

[5, 6] (setting $K \in \{1, \dots, 10\}$, ERC $\gamma \in \{1, 5, 10, 10^2, 10^3, 10^4\}$, and 3 initialization methods). The criteria compared to select optimal solutions are respectively based on equations (3), (4), and (5), and are divided as follows. QH, QS, and LK: clustering solutions are estimated and scored using the full data, \mathbb{X}_n ; CVQH, CVQS, CVLK: clustering solutions are estimated on a “train set” and scored on a non-overlapping “test set”, using a 10-fold cross-validation scheme, as in [16]. BQH, BQS, BLK: clustering solution are estimated and scored according to Algorithm 1, selecting the method m maximizing $\tilde{L}_n^{(m)}$. For each criterion, the selected solutions are evaluated against the true class labels, reporting the achieved Adjusted Rand Index (ARI, [11]).

Results are presented in Table 1. The comparison gives a better understanding on the mechanism that lies behind the effectiveness of the BQH and BQS criteria. First, notice that all criteria where solutions are estimated and scored on the full data (QH, QS, LK) always select poor, overly-complex solutions: this is because of the problem discussed in Subsection 2.2. On the contrary, both resampling mechanisms choose lower complexity solutions, acting similar to complexity penalization. However, the cross-validation scheme produces poor (Olive) or inconsistent (Banknote) results, with respect to the bootstrap scheme. This is likely due to the fact that 10-fold cross-validation splits leave too few shared information between train and test sets, and is less adequate for clustering where, differently from prediction settings, the goal is to select a clustering method that has a good in-sample performance. This is also true for the likelihood-based criteria, CVLK and BLK, which perform worse with respect to the quadratic score criteria. Indeed, it can be shown that compared to the likelihood function, the quadratic scores add extra penalization for overlapping clusters. Overall, both the quadratic scores, (3) and (4), and the resampling scheme in Algorithm 1 seem equally important to consistently achieve good results.

4 Conclusion

In this paper, we reviewed the BQH and BQS procedures from [4]. We ran an empirical analysis comparing it with a likelihood-based validation index, and testing different resampling schemes. Our experiments show that neither the bootstrap resampling scheme in Algorithm 1 nor the quadratic discriminant score in (1), alone, are sufficient to obtain good results. Rather, both of them contribute to the procedure in different ways. The comparison with likelihood-based alternatives highlights that the extra penalty that the quadratic scores impose on overlapping clusters is needed to select better solutions in cases where clusters are not well separated. Similarly, the comparison with the 10-fold cross-validation shows that the bootstrap resampling scheme is better suited for cluster analysis, where the final goal is to describe the data at hand, rather than predicting cluster membership for unseen points.

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The papers, which had been selected through a refereeing process, contain topics on statistical approaches and methodologies for the evaluation of public services in different contexts, and cover the areas of digital transition, e-commerce and digital marketing, enterprises, environment and territory, healthcare and wellness, finance, bank and FinTech, justice system, labour market, official statistics, public administration, food and wine, school, education and training, social, sports, sustainability, tourism, transport, university and research, well-being and welfare.

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