UNIMORE
UNIVERSITÀ DEGLI STUDI DI
MODENA E REGGIO EMILIA

DIPARTIMENTO DI SCIENZE CHIMICHE E GEOLOGICHE

Modena 10/09/2022

To Whom It May Concern:

SUBJECT: Report on the PhD thesis of Zuzanna Małyjurek

The thesis **"Optimization, validation and applicability of one-class classification methods"** submitted by Mrs. Zuzanna Małyjurek is focused on the development and applicability of class modeling approaches. In particular, the SIMCA method, which is by far the most widely used. The Thesis very well and deeply framed the context and the state of art, then focused on some of the critical issues and formulated some proposals on how they can be solved. In general, the different steps involved in class modeling are revised and comparative studies are have been undertaken to point out the best optimization strategy and applicability domain of the different implementations. A new two-steps approach has been developed in case of authentication task with several product categories strongly overlapping. Guidelines were also derived on the most suitable methodology to cope with heterogeneous class distribution, a topic whose impact on classification results is often under evaluated.

On the applicative side, the developed, or recommended methodology, has been applied to food authentication field, namely to herbal teas. As a side, but not less interesting, outcome an evaluation of strategies for calibration and test sets splitting is given.

The thesis is structured as a collection of papers preceded by a wide introductory Chapter were state of art is revised and discussed. An overview of Thesis' aim and organization is then provided. A final Chapter, after the papers, summon up, the main results and conclusions reached.

Overall, the works is clearly presented and organized making the reading fluent. The objectives are clearly stated and well framed with respect to the state of art, which is well accounted in the cited literature. The Thesis style and content demonstrates that the candidate has acquired a broad knowledge of the covered topics. In fact, all the different aspects are thoroughly discussed, and the outlined objectives were fulfilled. Moreover, it clearly emerges that the PhD candidate has developed skills in programming chemometrics algorithms and analysis of different type of data. Few lines about future directions and development could eventually be added, but this is just a suggestion, not a requirement.

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The implementation of PFM method in SIMCA classification and the novel two steps approach as soft classification approach combining class modeling and discrimination are interesting and results how their suitability for challenging situation. Thus, starting from the state of art, the Candidate was able to develop an original tool and critically assess its performance. Overall, he gave a relevant contribution to the field.

It is also highly appreciated how the PhD candidate acquired also a deep understanding of the structure and limitations of the current methods in use.

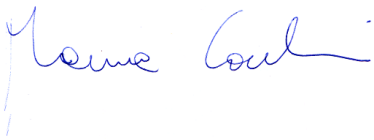
The outcome of the research described in this Thesis has been finalized into 5 papers, four published and one under minor revisions, in high quality peer reviewed international journals, among the most reputed in chemometrics and analytical chemistry. The PhD candidate is the first author in all of them, showing that significantly contributed both to conceptualization, writing and code development (as also reported on page 107).

Moreover, the Candidate received the best oral talk awards in the prestigious international conference 17th Scandinavian Symposium in Chemometrics. She has been presenting authors of oral communication in five international conferences. In addition, to several oral and poster communications in national context.

For all these reasons, I can affirm that the Thesis meets the highest quality standards for a graduate research and therefore it is fully adequate to be presented in the PhD defense.

It is my opinion that the amounts of work undertaken, the overall achievements, the rigor of the scientific approach as well as the clearness of both organization and Thesis language, are above the average level of a PhD student.

Sincerely yours,



(Prof. Marina Cocchi)

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