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CHOOSING THE CORRECT CHEMOMETRIC STRATEGY FOR QUALITY CONTROL AND AUTHENTICITY VERIFICATION: CONSOLIDATED APPROACHES AND RECENT TRENDS

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Qualitative data modelling is a fundamental branch of pattern recognition, with many applications in analytical chemistry, and embraces two main families: discriminant and class-modelling methods. The first strategy is appropriate when at least two classes are meaningfully defined in the problem under study, while the second strategy is the right choice when the focus is on a single class. For this reason, class-modelling methods are also referred to as one-class classifiers.

When quality or authenticity of a product have to be verified, the problem is often asymmetric, meaning that a class of interest (the one of the target product) has to be characterised against the rest of the world (i.e., the non-compliant samples). In these cases, since the interest is actually on a single target class (and the other class is not properly defined), class-modelling is the correct choice.

Nevertheless, discriminant approaches are very frequently applied for this purpose, claiming that class-modelling is less efficient in terms of model performances.

In the last years, some modified strategies that make use of discriminant methods for addressing asymmetric problems in a declared "one-class way" have been proposed. Such strategies define a dummy class, which can arise either from real measurements on dummy samples (blanks, solvents) or from random artificial calculations. Discriminant methods – including linear discriminant analysis (LDA) and partial least squares discriminant analysis (PLS-DA) – are then applied to discriminate the target class from the dummy class.

In the present study, these novel approaches are evaluated in depth, on real and simulated analytical datasets, and critically compared with standard class-modelling strategies, verifying whether they actually represent or not a reliable and more efficient alternative for addressing authentication problems.