

## BDA group master project

Project title: Comparing PLSDA and SHM  
Duration: 4-6 months  
Number of ECs: 24-36  
Start: negotiable  
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### Project description

Many metabolomics studies are based on the discrimination between healthy individuals and individuals with a certain disease. The goal of such a study is to find those metabolites that are (statistically) different between the two groups. Partial Least Squares discriminant analysis is a multivariate discrimination method that is often used in such studies. This method is a 2-class discrimination model which is based on the assumption that the class of control and pathologic condition are intrinsically similar. However, for most complex diseases, the case where both the control and diseased groups are well-defined seldom occurs, particularly in clinical studies. In addition, while a similar response is expected during an experimental study, it might happen to observe a different response to the treatment (e.g., responders and non-responders), which can be unrecognized by using a two-class classification approach. Therefore, a 2-class method (such as PLSDA) might not always be the most appropriate approach. Another approach recently introduced is called Statistical Health Monitoring (SHM). Here a model of the control group is made, and then for each of the cases (being individuals with a disease or any perturbed situation) is examined for its deviation from the control situation. Such an approach could be beneficial when there are subgroups in the case group such as responders and non-responders or in case of different subgroups in the patient group. In this project we will use simulations and real data to explore the strength and weaknesses of the two methods.

Ref: <https://pubs.acs.org/doi/pdf/10.1021/acs.analchem.5b03078>