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Mathematical Modelling and learning in electro-physiology.

Damiano Lombardi[1], **Fabien Raphel**[2]

[1] Inria Paris, 2, rue S. Iff, damiano.lombardi@inria.fr
[2] Inria Paris, 2, rue S. Iff, fabien.raphel@inria.fr

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The present work deals with a classification problems arising in the context of safety pharmacology. The goal is to understand if a molecule, at a given concentration, disrupts the functioning of some of the ion channels of the cells. The application at hand motivates the use of machine learning methods in order to provide a fast prediction. However, we are in the regime called *high-dimensional/low sample size*, which is particularly critical. Furthermore, we are often in the case in which the available experimental data do not cover all the possible meaningful scenarios for the phenomenon under investigation.

We will present two different contributions related to these methodological issues. First, we will propose a method to systematically construct a training set by integrating a set of numerical simulations to the available experiments. The method is solely based on the knowledge of a validation set and selects, among sets of possible simulations, the ones which are the most promising in view of constructing a robust classifier. The method is featured by bias rejection, making it robust to the eventual model error. The second contribution is a goal-oriented model reduction method. In this, we will introduce a double-greedy method to construct the classifiers input by maximising a functional related to the classification performances. By proceeding in this way, we will reduce the classifier input dimension without deteriorating the classification performances. Some theoretical results on both these methods will be presented. Several realistic test-cases will be detailed and commented.