

PhD research topic proposal

BME, Doctoral School of Mathematics and Computer Science

Name and degree of supervisors :

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No

Title of the topic:

New Methods for Overcoming Challenges in Data Learning and Optimization with Applications in Experiment-design

Short description:

High-dimensional feature space combined with a relatively low number of samples may make data learning and optimization problems difficult. This problem can be tackled by reducing the dimensionality of the feature space or by information-rich sample generation. This latter is often necessary in numerous fields of science and engineering as well.

For example, in numerous industries, such as fine chemicals or pharmaceuticals, the number of specific experiments that can be performed for process development is limited. By designing more informative experiments, the number of experiments, material needs, overall costs, and market time can also be reduced. This will not only translate to significant cost savings, but it can also be life-saving in the case of critical drug products. The question to answer in this case is: how many experiments need to be performed, what are the experimental conditions, and what kind of sampling strategy should be adopted? Answering these questions requires interdisciplinary research based on mathematical modeling, multivariate statistics, and machine learning that supports them.

From a scientific perspective, the question can be formulated as follows: knowing that N experiments can be performed, what experimental conditions should be applied (multivariate optimization), and at which sampling instance should we take discrete measurements (further decision variables) to extract the maximum experimental information (information theory)? All of these start from the dynamic modeling of the underlying process (differential equations and numerical solutions). Exploring how machine learning, e.g., physics-informed neural networks, can help answer these questions is also an objective. Finally, a mathematical model can be constructed using these optimally designed experiments, which can be used further in engineering.

Requirements: An MSc degree in mathematics or engineering with a solid background in machine learning; Python programming skills; Chemical engineering background is an advantage.

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Place of work:

BME,TTK respectively BME, VBK