Project Proposal – Bayesian Optimization for Material Properties, BOMP-R2B

1. Introduction

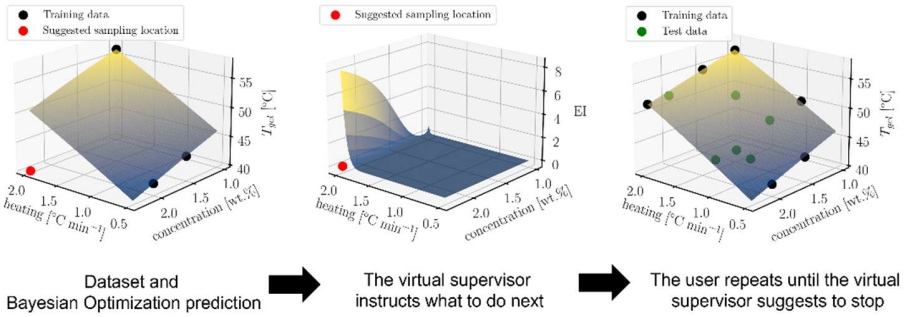

Figure 1: Bayesian optimization of material properties using Gaussian surrogate function and utility function to guide discovery of material properties. This example is what an R&D department would do with BOMP when looking for a novel material in the shortest time.

The Artificial Intelligence (AI) and Machine Learning (ML) megatrend is forcing entities to include modern algorithms in their processes. **This project addresses the need for low-cost, fast, adaptable, reliable and easy-to-use optimization algorithms for material properties and processes.** Our ML solution not only offers superior performance but also replaces the need for consultants and analysts in industrial decision making. It reduces the cost and increases profitability of production lines as well as reduces the usage of raw materials as the same properties of the end product can be achieved using recycled or side streams.

Inspired by automated decision-making and the need for fast exploration of a parameter space, we propose **BOMP framework, a Machine Learning tool for speeding up the exploration of complex scientific problems in materials industries.** In its current state, BOMP is a working principle that enables the user to explore the effect of multiple variables on a target response, thus finding optimal measurement points, locating extreme values, and creating novel materials with less labor. The same principles are transferrable from the laboratory scale to the industrial scale (i.e., from small to large entities). For example, BOMP helps identify the best material composition for optimal strength and cost-effective production. Our tool can be tailored to optimize raw materials, environmental impact, price, time, or any combination.

To meet this challenge, we rely on a novel idea that creates an easy-to-use and adaptable “virtual consultant”: BOMP — Bayesian optimization for material properties. The hard-core science and proofs-of-principles are tested in the laboratory environment**. BOMP is a framework based on Bayesian probabilistic reasoning, which allows gaining significant savings in multidisciplinary labor. It reduces the number of tests and requires fewer senior researchers’ input on designing novel unforeseen materials and processes**.

2. Project goals

In the project, a laboratory version using command line interface is improved and converted into a distributable software package. The tasks include:

- Creating a graphical user interface
- Compiling and converting existing python script with dependencies to third party libraries into one standalone package
- Creating a demo case with real data that is simple to use

- adding features, reservations for future features or mock-up features (chat GPT, material database, cold vault operation, cloud service mode)

The tasks can be adjusted depending on the background of the students.

3. Technologies

Modular approach in architecture is preferable e.g. Model-View-Controller model. This also makes it possible to create standalone version without internet connection (for sensitive data) and cloud-based solution where data and algorithm is running in a cloud service (e.g. for public material property data).

Controller: Current backend software is implemented with python and scikit-learn library. We'd like to keep python but change the library (e.g. to BOTorch).

View: GUI and frontend framework is to be decided (node-red, Qt, web-based, etc.).

Model: Local and global database architecture (proprietary, python dictionary, SQL, etc.) for long term storage is to be chosen. Using Memcached (or similar) for message passing and short term storage is encouraged.

Support and examples of previous similar software can be provided on MVC, Memcached, node-red, python and python-scikit.

4. Requirements for the students

Desired skills include familiarity with python and creating user interfaces. Difficulty can be adjusted on the student skills. Interest in AI, machine learning and commercial aspects is a plus.

5. Legal Issues

All IPRs to all Results will be transferred to the Client. The client will not share any confidential information with the students.

6. Client

BOMP is a Research to Business project, hosted by Department of Applied Physics at Aalto University, and funded by Business Finland. The goal of the project is to convert the laboratory tested (TRL 2) Machine Learning software into a proof-of-concept product suitable for smooth operation in real operating environment (TRL5+). The BOMP project will be converted into a startup at the beginning of 2026. We are looking for co-founders and first employees.

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The main communication and support would be handled through weekly or bi-weekly meetings. Cloud services can be arranged through Aalto or third parties.