

## Goal

Efficiently find optimal solutions with a minimal set of computer/physical experiments, and considering

- Multiple objectives
- Uncertainty in outputs
- Potential feasibility constraints (on inputs/outputs)

## Motivation

- In many real-life systems (engineering design, process design, supply chain design, etc.), the optimization problems studied are **multi-objective** (exhibiting *trade-offs* between individual objectives), and outputs observations are **noisy** (repeated experiments of the same inputs may yield different output observations).
- The input/output relationships for objectives and constraints are often a **black box: experimentation** is required to evaluate them. These (physical or computer) experiments can be **expensive (in terms of cost, time, etc)**, and the budget for experimentation is typically constrained.
- The goal then is to detect solutions with very high quality (optimal or near-optimal) **within as few experiments as possible**.
- Traditional optimization heuristics (genetic algorithms, evolutionary algorithms) **are ill-suited** to achieve this goal.
- **Machine learning (ML)** techniques (fit for use in settings with scarce data) combined with **optimization (OR)** insights and/or **statistical learning**, to achieve the goal.

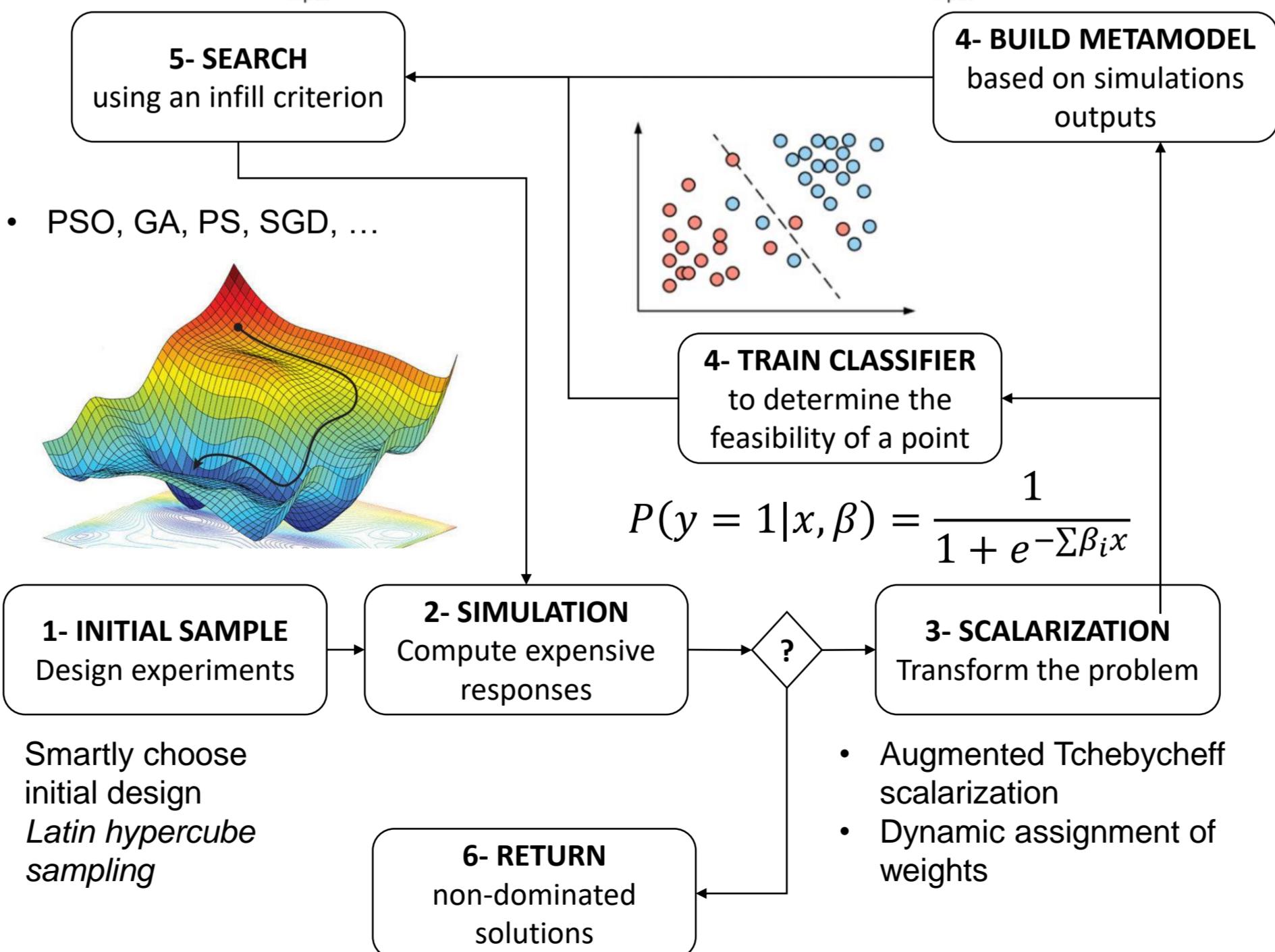
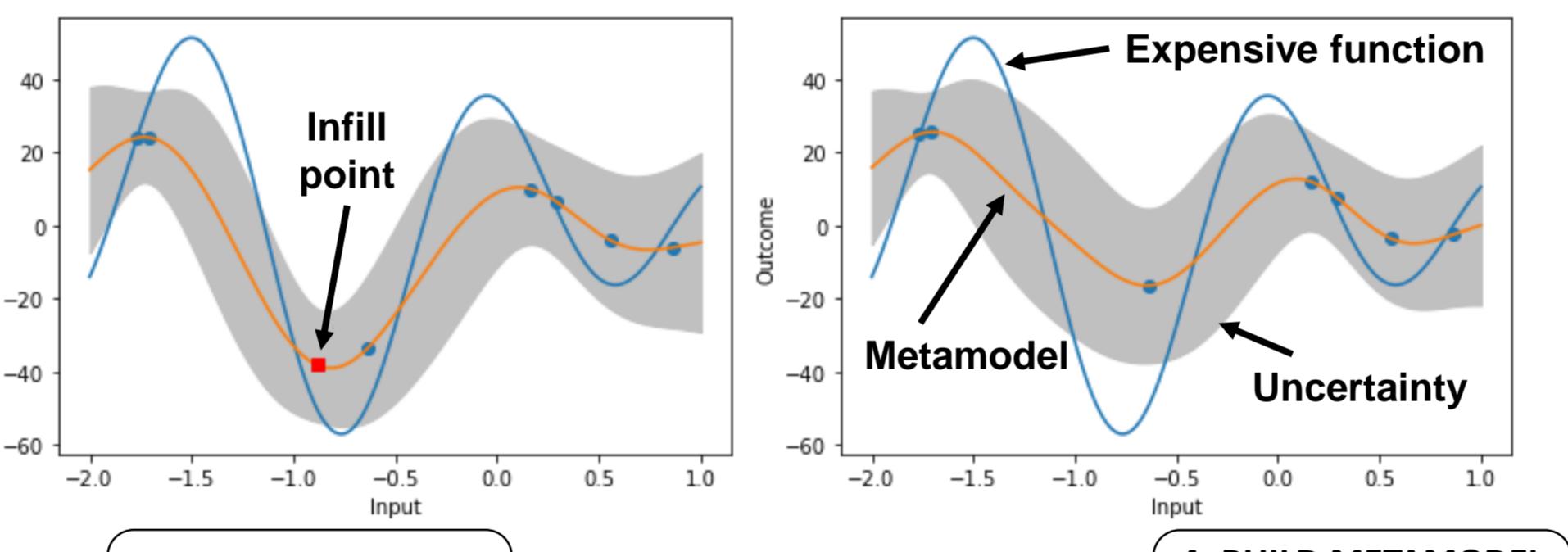
## Approach

- Model (expensive, black-box) continuous output functions  $f$  using **Gaussian Process Regression (GPR)** with heterogeneous noise (**stochastic kriging**) [1]. This allows us to obtain an estimation of the output value ( $\hat{f}$ ) at unobserved locations, along with an estimator for the **uncertainty** on this value ( $s^2$ , also referred to as the MSE). This MSE captures both **metamodel uncertainty** and **stochastic uncertainty**.

- Use **infill criterion (acquisition function)** to select next input combination to sample (**Bayesian optimization**).

### Infill criterion [2]

$$CMEI = \left[ (\hat{f}_{min} - \hat{f}) \Phi\left(\frac{\hat{f}_{min} - \hat{f}}{s}\right) + s \phi\left(\frac{\hat{f}_{min} - \hat{f}}{s}\right) \right] * P(y = 1|x, \beta)$$



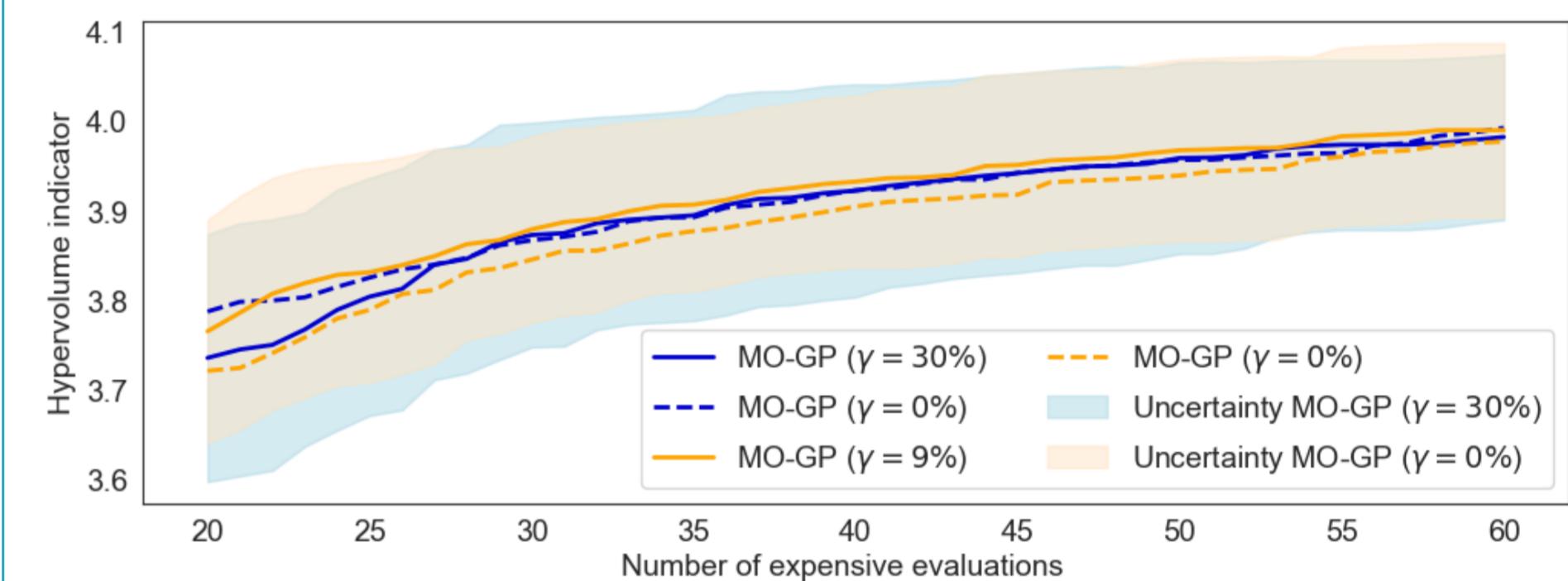
\*Algorithm based on the work presented in [3]

## Results

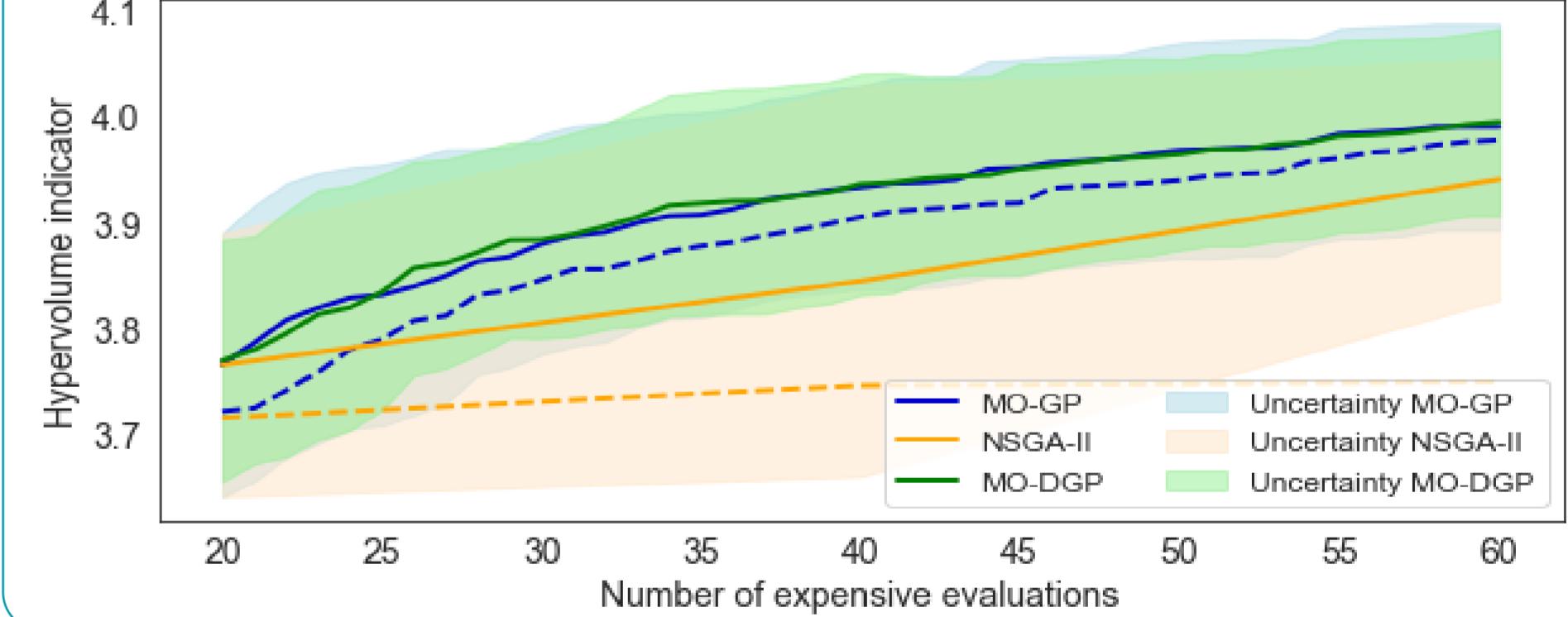
Parameter optimization for plasma process in adhesive bonding application (JMLab, Flanders Make)

- Maximize break strength and minimize production costs (bi-objective) by tuning 6 parameters
- Avoid configurations that lead to adhesive failure or visual damage of the sample

### Results MO-GP for low and moderate noise levels ( $\gamma$ )



### Outperforms common evolutionary algorithms (NSGA-II)



## Key take-aways

- Efficient and effective search for solutions to expensive optimization problems with noise
- Proposed (Bayesian) approach is shown to be robust to the noise level and clearly outperforms the well-known NSGA-II

## Further reading

- [1] <https://doi.org/10.1287/opre.1090.0754>
- [2] <https://doi.org/10.1080/0740817X.2012.706377>
- [3] <https://doi.org/10.1016/j.ejor.2019.12.014>