# Small Dataset Acquisition for Machine Learning Analysis of Industrial Processes with Possible Uncertainties

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# About us

Xukuan Xu earned a Diplom degree in mechanical engineering from Technische Universität Dresden, Germany in 2020. He is currently pursuing a doctoral degree at Technische Hochschule Aschaffenburg, specializing in the field of small batch production with a focus on machine learning, process monitoring, and anomaly detection.

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TU Dresden

# BMBF Competence Cluster InZePro
# Project KIproBatt

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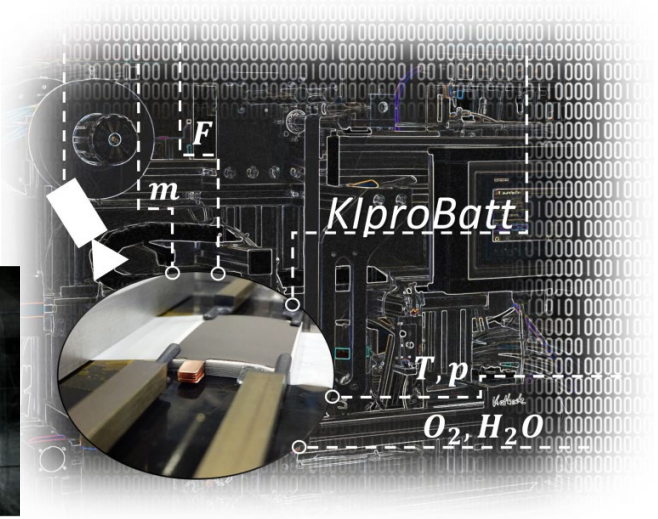
KIproBatt:
Intelligent Battery Cell Production with AI-based Process Monitoring based on a Generic System Architecture

Goal:
- Process modeling ---- Hybrid AI
- Representation of process correlations ---- Data-driven approach
- Process monitoring ---- Sensor hardware & dataspace

Specification:
- An intelligent battery cell production
- A production-oriented generic system architecture
- General applicability & transferability

Homepage: https://kiprobatt.de/wiki/Main_Page

# Aims and contributions of our paper

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- Data preparation is the bottleneck of ML applications according to a survey from Crowdflower [2]
- This problem is often overlooked. In most cases, the datasets are unthinkingly pre-existing
- The quality of the dataset determines the upper limit of data analysis

In our paper, we :

1) discussed the characteristics of small-data context with process uncertainties based on practical examples
2) developed an adapted design of experiments (DOE) aiming at preparing datasets for ML applications

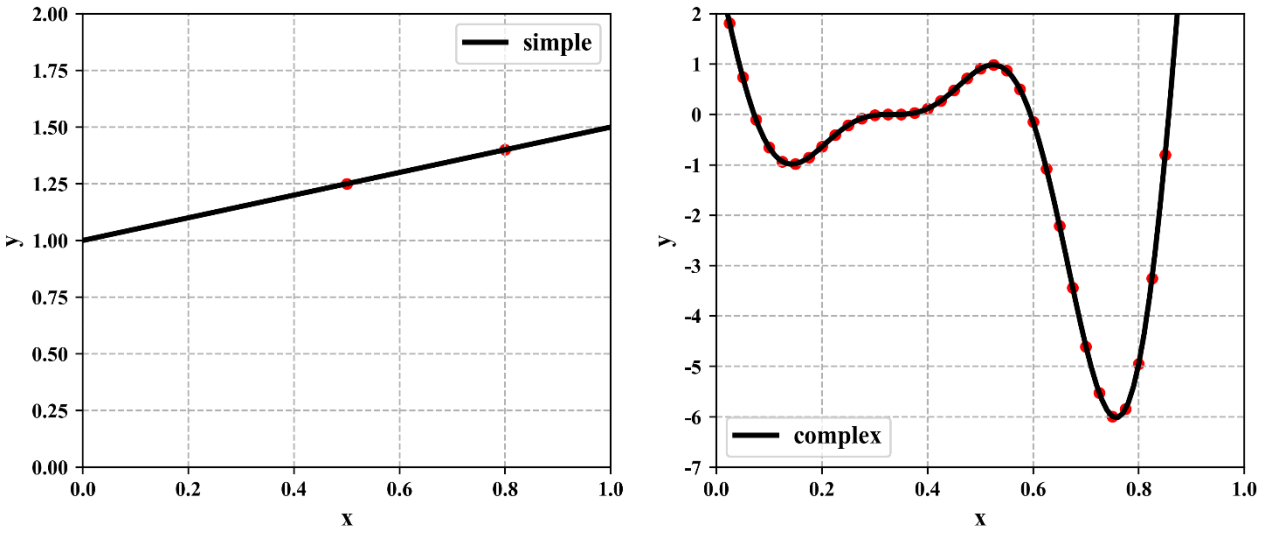
# a. Small-data problem

Under which circumstances will small-data problem appear:

- **Small-batch production** is often unavoidable in laboratory research, on a pilot production stage prior to upscaling, or in customer-specific (individualized) manufacturing [5]
- Data acquisition is limited by **budget or time constraints** to datasets with <1000 elements

However, the amount of data is not necessarily dominant factor

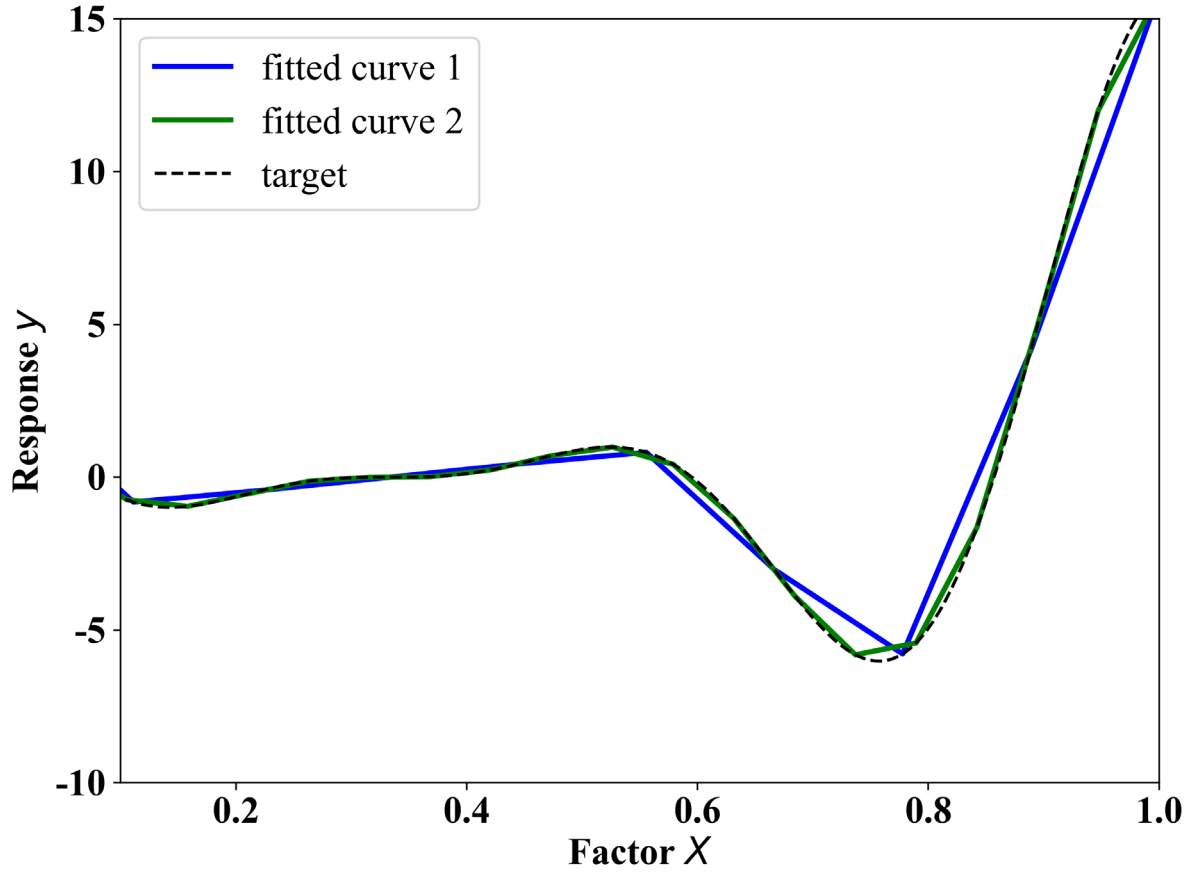
- The number of required data depends on the **complexity** of the process
- The particular **distribution** of selected data points affects the outcomes of analysis



# a. Small-data problem

the fundamental characteristics of small-data context:

- under-sampling of the parameter space
- a lack of convergence of the ML models.

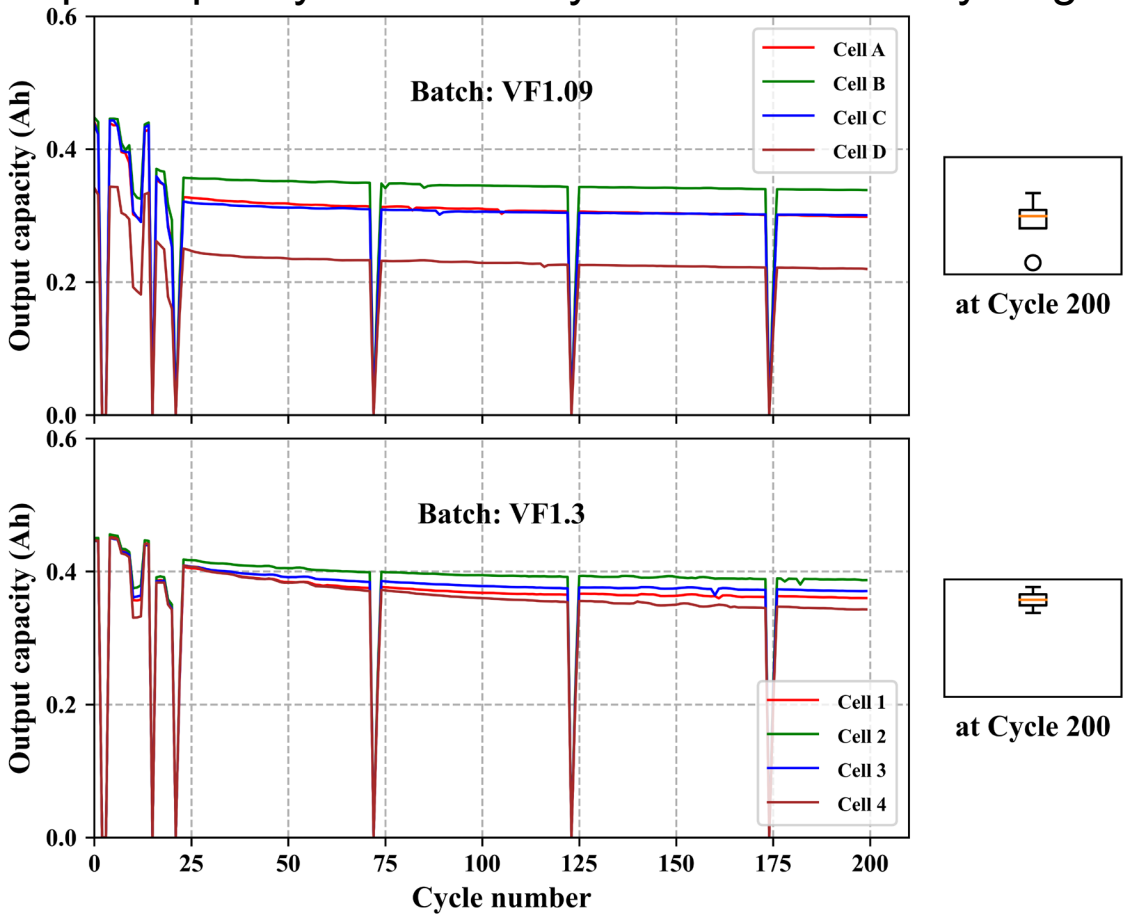


# b. Process uncertainties

**Process uncertainty:**
a statistical spreading in the target responses

- measurement uncertainties
- unavoidable fluctuations of the process parameters
- some potential variables uncontrolled
- human factor

Cell output capacity related to cycle number in a cycling test



# c. Existing DOE strategies

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According to DEAN et al. [3], the two main purposes of DOE are:

I. to find the control variables that give rise to an **optimal** response
II. to obtain **a mathematical description** for the pre-defined dataspace in order to predict further responses

Traditional DOE workflow:

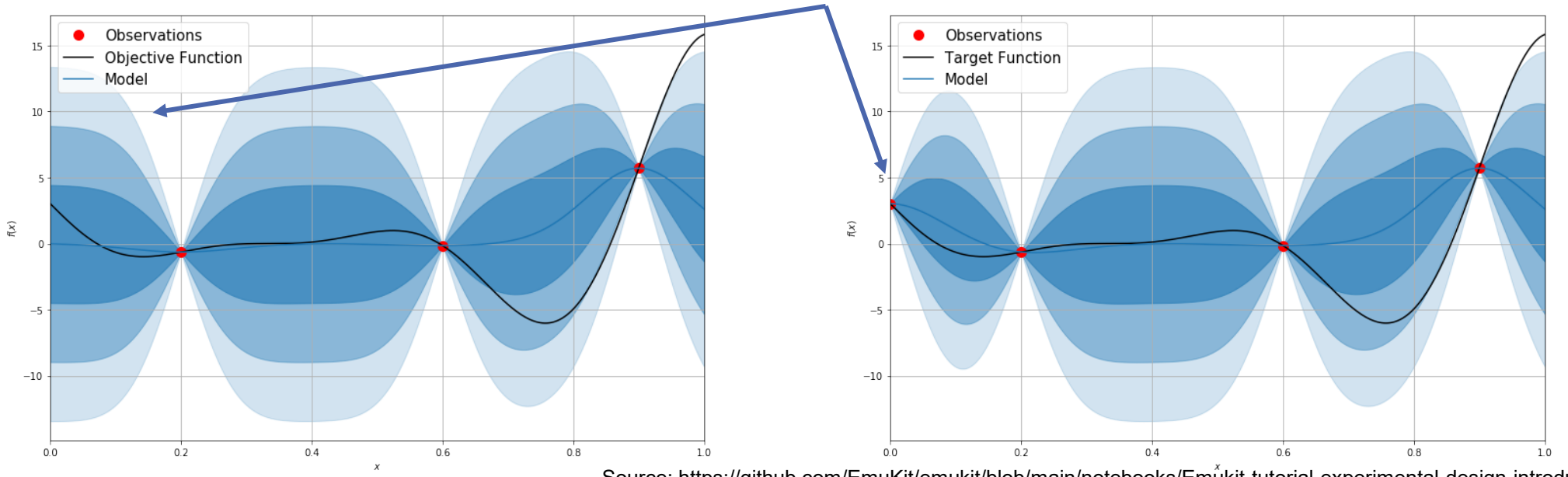
1. Determine the factors of interest and the response
2. Identify the significant factors
   - (fractional) factorial design: full factorial design, Plackett–Burman design
3. Establish a regression model
   - central composite design, Box-Behnken design

Drawbacks:
Inflated data volume with multiple factors
outdated analysis techniques ( in comparison with the development of ML )
Predetermined, non-adaptive

# d. Adaptive DOE strategy

Iterative data acquisition schemes have been discussed, e.g., Emukit [9] provides such a model-based iterative DOE scheme within a Bayesian optimization framework.
3 steps to generate data points:

- fit a prediction model to the existing data (initial dataset)
- find the next point with the highest marginal predictive variance as predicted by the prediction model
- add this new data point to the existing dataset




Source: https://github.com/EmuKit/emukit/blob/main/notebooks/Emukit-tutorial-experimental-design-introduction.ipynb

# e. Our proposed DOE strategy for small-data context

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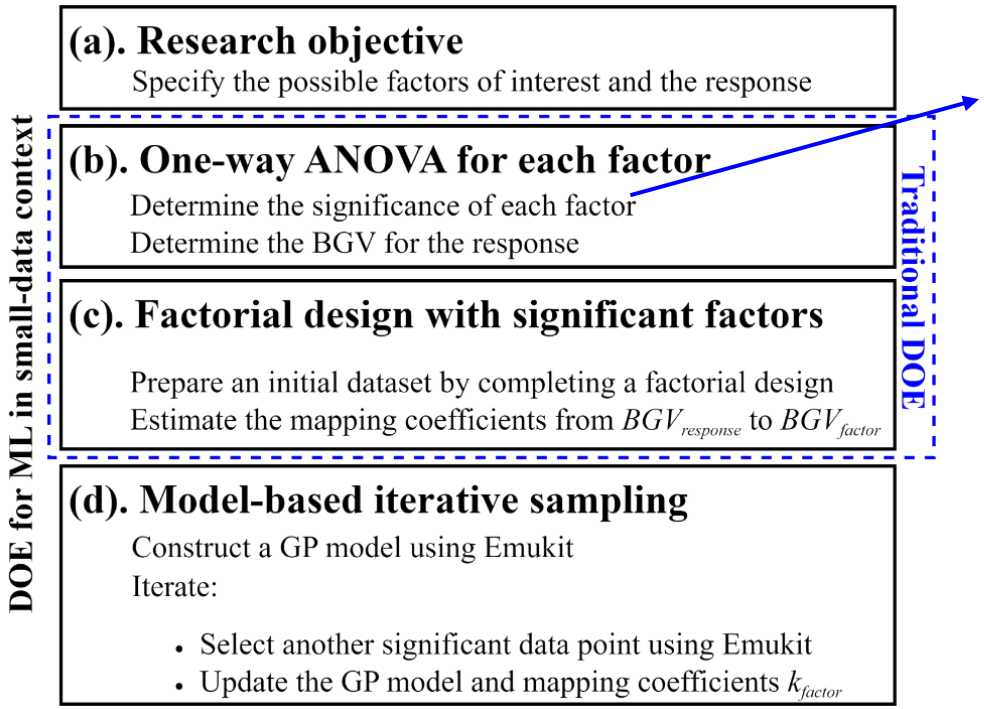
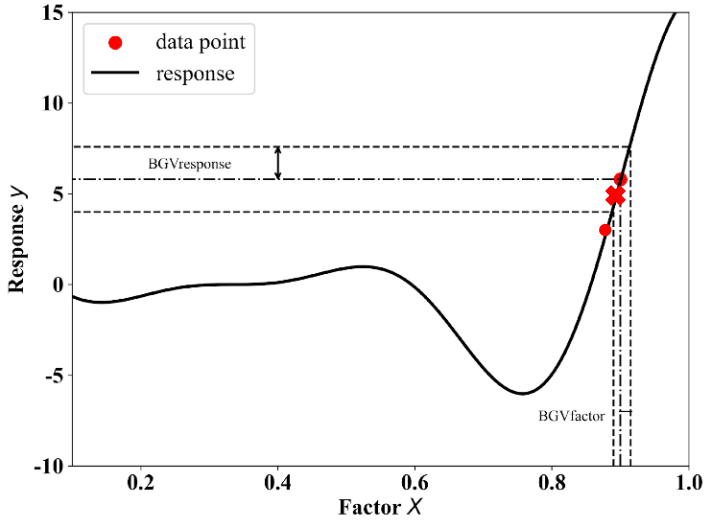
Proposed DOE workflow in small-data context




BGV: between-group variance
GP model: Gaussian Process model

Assuming that the levels we set for the one factor are too **close** to each other, then the statistical spreading due to within variance may limit the **distinguishability**.
In other words, once the P-value exceeds the predefined level of significance ($p > p_0$), the considered factor should be judged as insignificant within this interval.
If this principle is applied to select the next data point, it can determine whether this data point is valid for the considered factor.

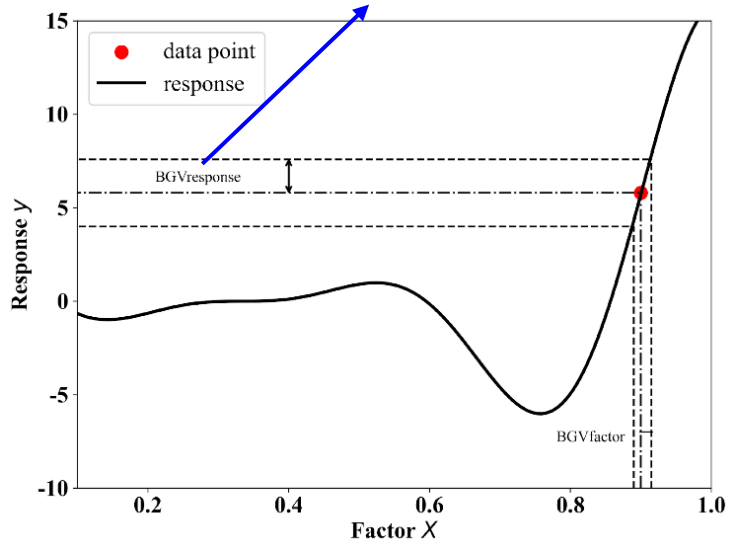


# e. Our proposed DOE strategy for small-data context

ANOVA: OC versus EV

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|---|---|---|---|---|---|
| Electrolyte | 1 | 0.011542 | 0.011542 | 8.16 | 0.029 |
| Error | 6 | 0.008482 | 0.001414 | | |
| Total | 7 | 0.020024 | | | |

$$BGV_{response,min} = \sqrt{F\ value_{1,6,a=0.05} * Adj\ MSE}$$




Next to the **Electrolyte Volume** (EV), experts believe [6] that **Drying Time** (DT), **Wetting Time** (WT), **Coating Defects** (CD) on electrodes, and **Stacking Accuracy** (SA) also have impact on the **Output Capacity** (OC):

$$OC_{cycle\ 200}(X_{EV}, X_{DT}, X_{WT}, X_{CD}, X_{SA})$$

$$k_{factor} = \frac{\partial OC_{cycle\ 200}}{\partial X_{factor}}$$

For instance:

$$OC_{cycle\ 200} = \sum_{i=1}^{5} k_i X_i + b$$

$$BGV_{factor,min} = \frac{BGV_{response,min}}{k_{factor}}$$

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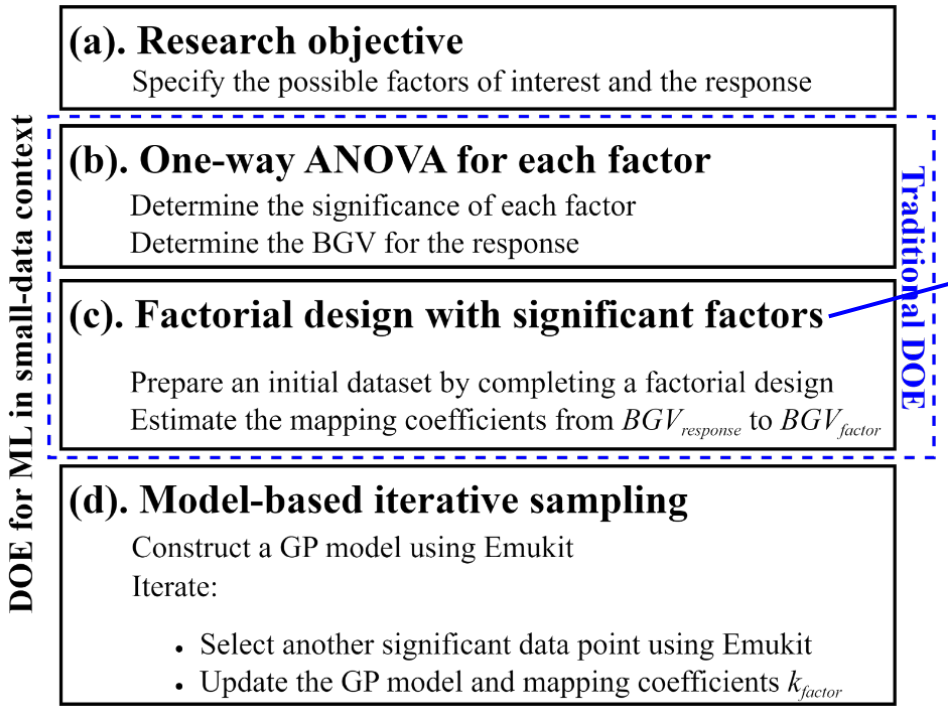


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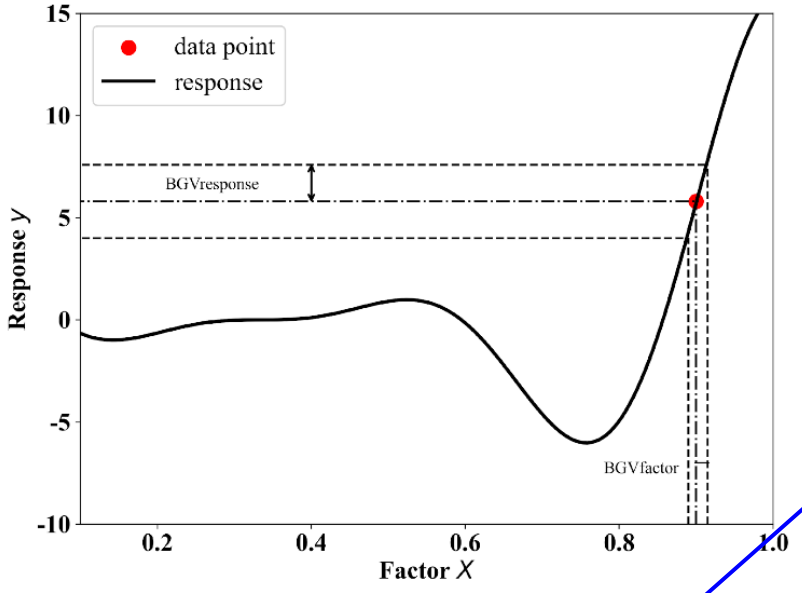


- $BGV_{factor,min}$ defines an environment around each factor value where no significant data points can be chosen
- Under this framework, we can proceed the iterative sampling in step (d) until all data points for a ML dataset have been collected
- Each new data point will be used to update the model and the mapping coefficients to determine a more accurate estimate for $BGV_{factor,min}$

# Future work

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- We will conduct a comprehensive analysis of our proposed DOE workflow with a FEM-simulation:
  - Collecting data by running the simulation with limited number of access
  - Add noise function to emulate process uncertainties
  - Comparing different sampling strategies by investigating the correlation between the sampling strategy used and it´s corresponding ML model's performance on the test data

- Our DOE strategy will be used to guide the production of cells in the KIproBatt program

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