HEURISTIC AND EVOLUTIONARY ALGORITHMS LABORATORY

# Improving the Flexibility of Shape-Constrained Symbolic Regression with Extended Constraints

## Eurocast 2022 - Theory and Applications of Metaheuristic Algorithms

**David Piringer**, Stefan Wagner, Christian Haider, Gabriel Kronberger, Armin Fohler, Siegfried Silber, Michael Affenzeller

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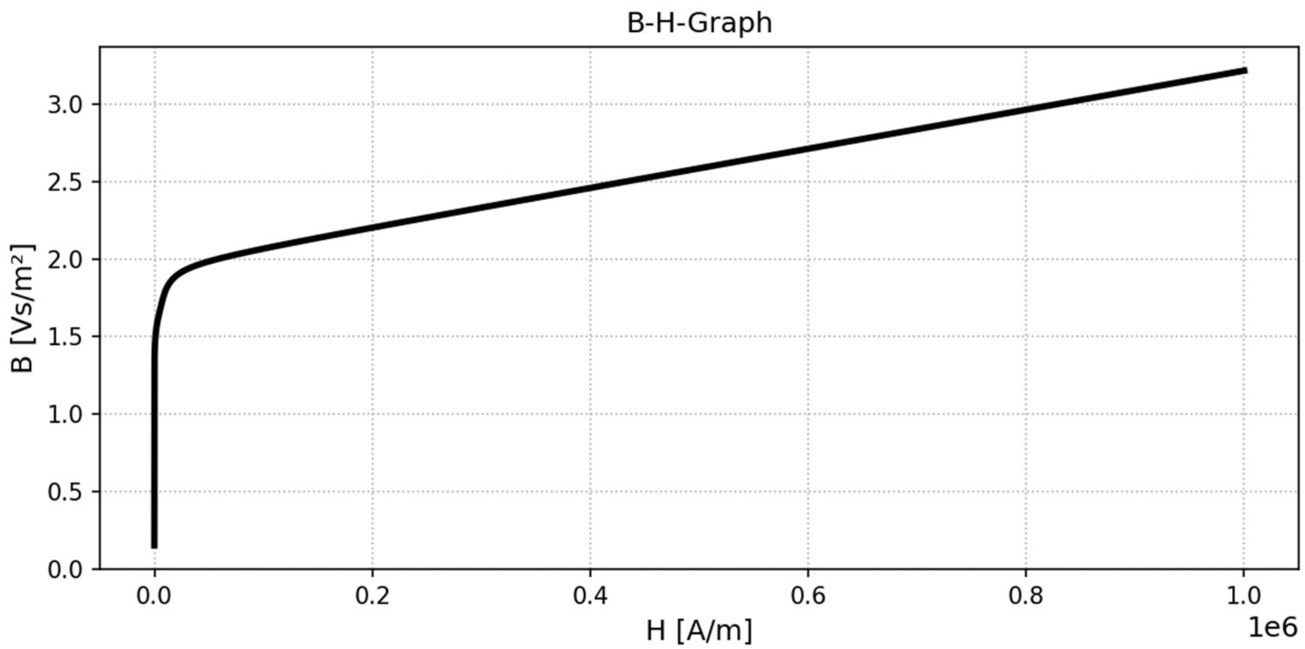
UNIVERSITY OF APPLIED SCIENCES UPPER AUSTRIA

# Overview

- Problem Formulation
- Shape Constraints
- Motivation
- Extended Constraints
- Experiment Configuration
- Applied Constraints
- Preliminary Results
- Conclusion & Outlook

# Problem Formulation



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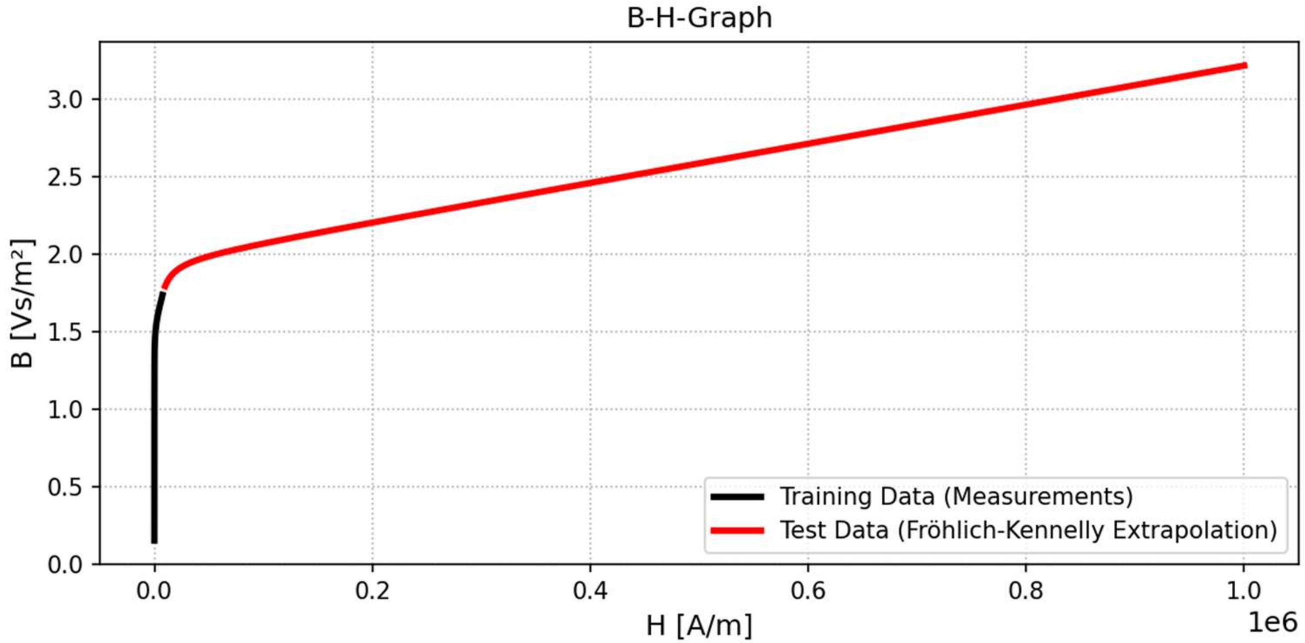
# Problem Formulation



# Problem Formulation

- Constant slope of $4\pi 10^{-7}$(permeability of vacuum)
- 2nd derivative is negative
- Magnetic polarization (J) has an upper limit (saturation polarization)
  - Material dependent
- Relative permeability ($\mu_r$) has a lower limit of one
- Peak of relative permeability ($\mu_r$) is contained inside the measurements

# Shape Constraints

## Previous Work

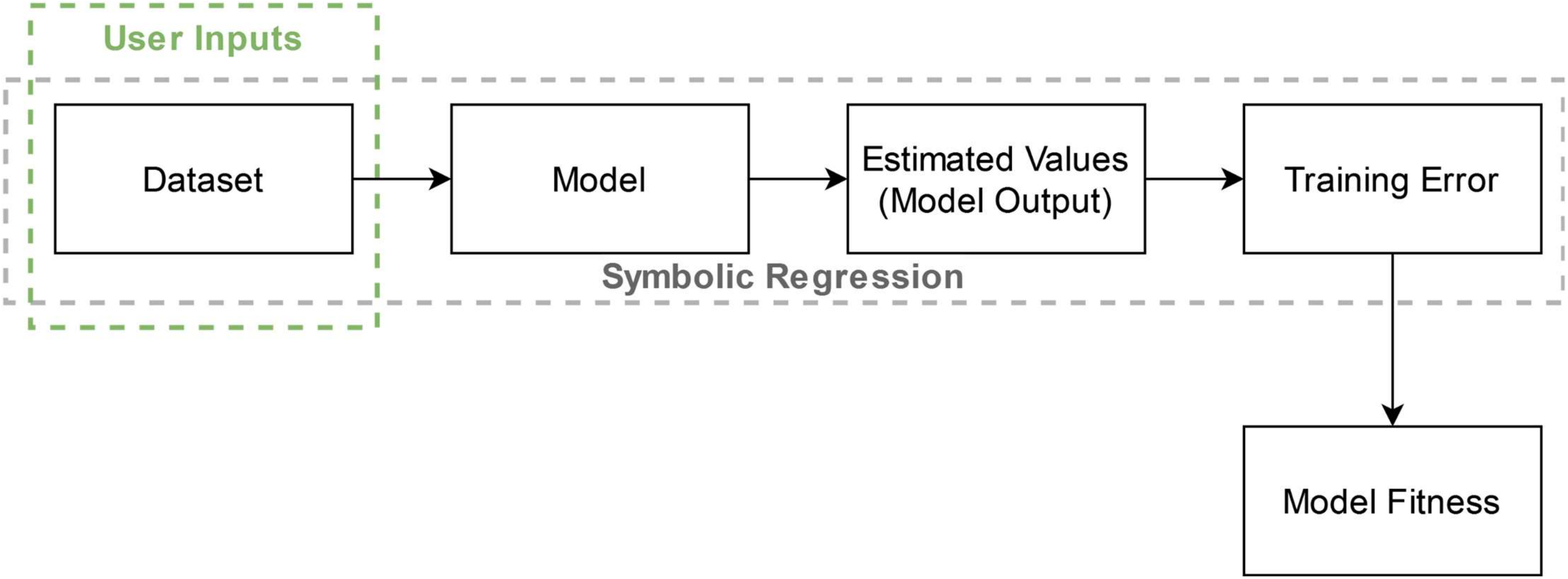
- Introduces additional domain knowledge in Symbolic Regression [1,2]
- Define constraints for
  - the shape of the function
  - derivations of any order of the function
- Each constraint can be limited to specific ranges for each input variable
- Examples:
  - $y \in [1, 5]$
  - $\frac{\partial y}{\partial x} \in [0, \text{inf.}]$ where $x \in [0, 100]$


[1] Kronberger, G., de France, F.O., Burlacu, B., Haider, C., Kommenda, M.: Shape-constrained Symbolic Regression – Improving Extrapolation with Prior Knowledge. Evolutionary Computation pp. 1-24 (04 2021)

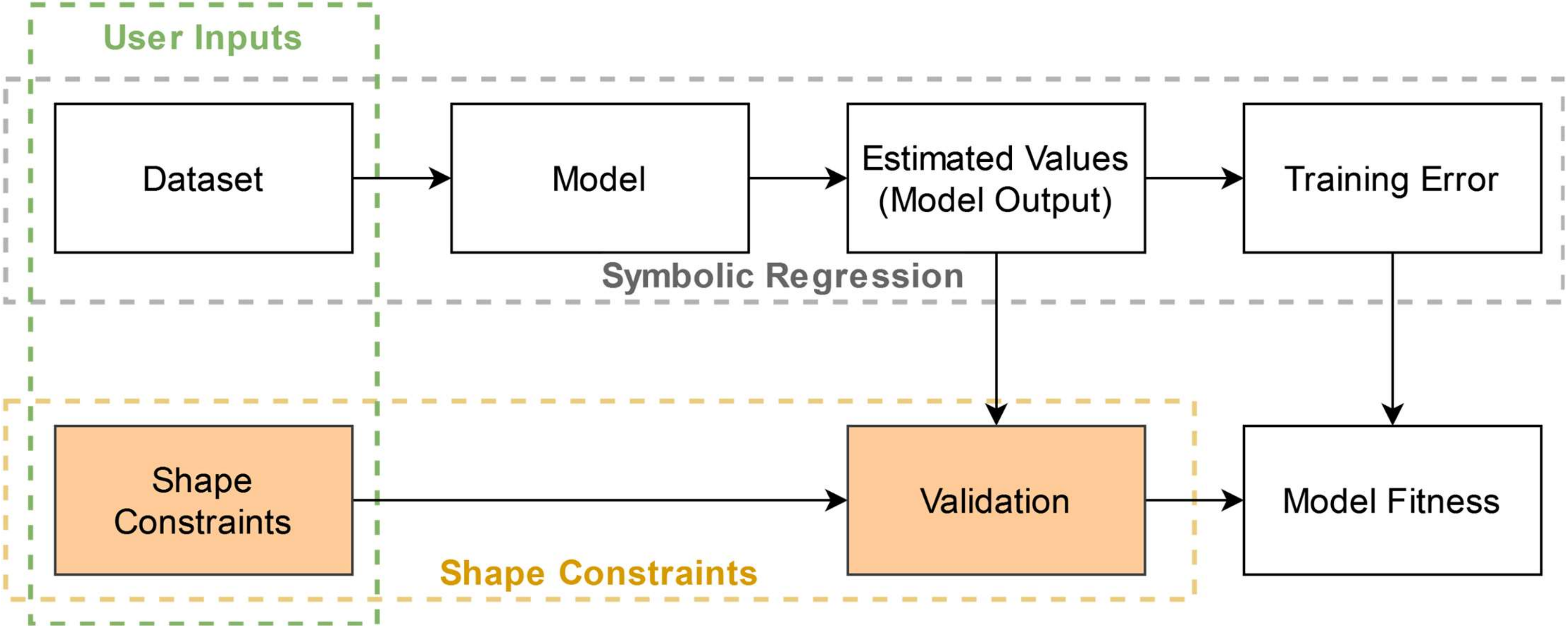
[2] Haider, C., de Franca, F.O., Burlacu, B., Kronberger, G.: Using shape constraints for improving symbolic regression models. arXiv preprint arXiv:2107.09458 (2021)

# Shape Constraints

## Previous Work



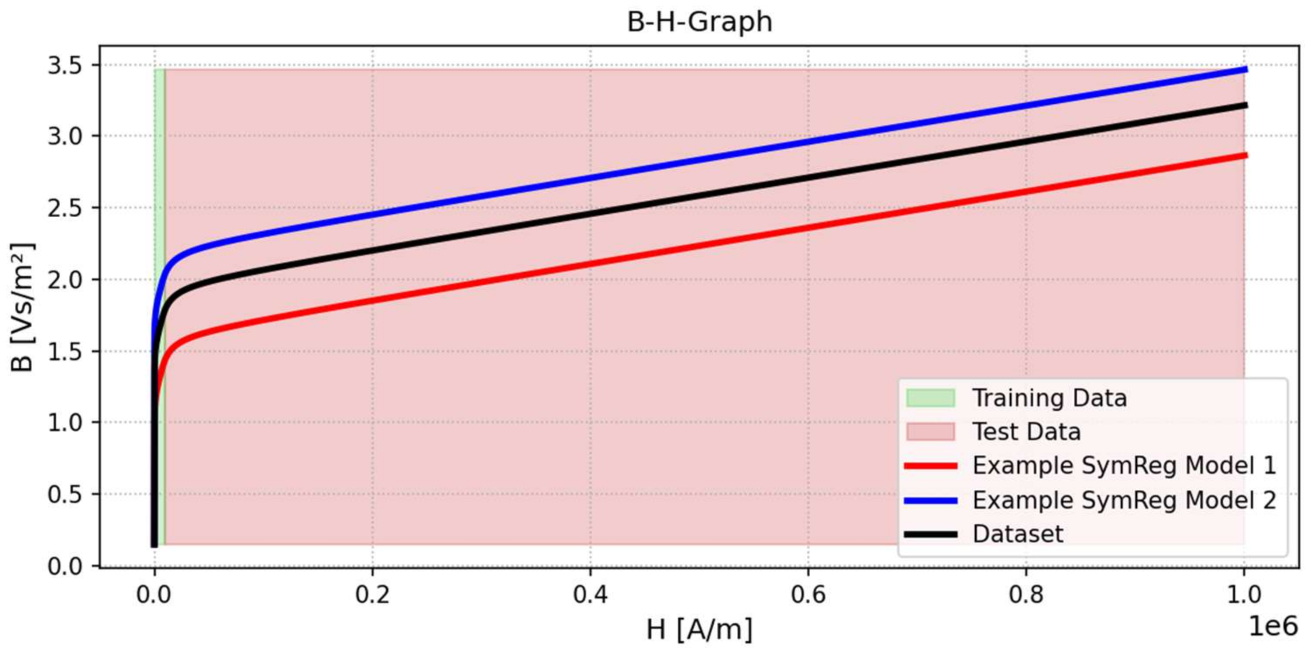
# Shape Constraints
## Previous Work



# Shape Constraints

## Difficulties

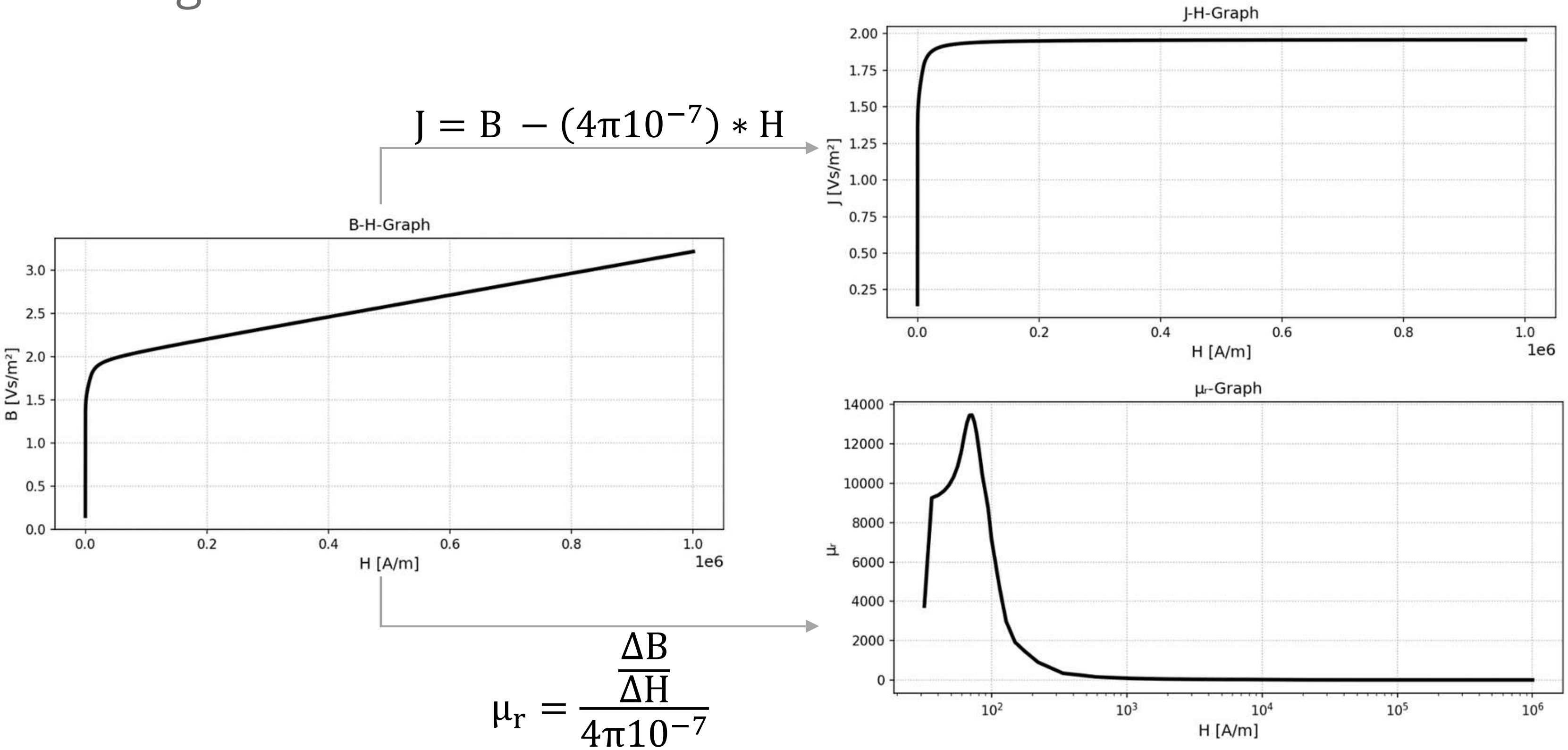
- Information about the magnetic polarization (J) and relative permeability ($\mu_r$) cannot be utilized



# Motivation

- Utilize additional information about the system for the algorithmic search

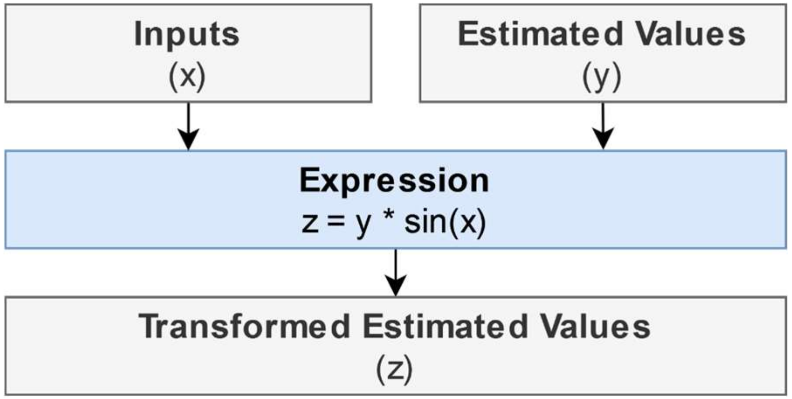
$$J = B - (4\pi 10^{-7}) * H$$




$$\mu_r = \frac{\frac{\Delta B}{\Delta H}}{4\pi 10^{-7}}$$

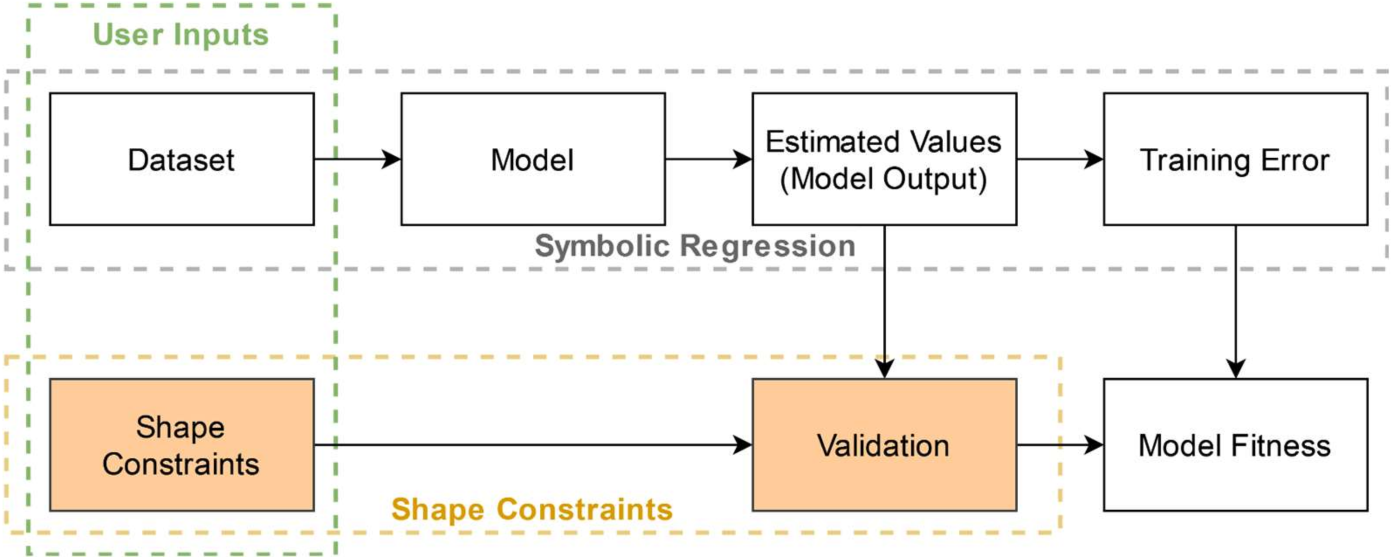
# Extended Constraints

- An additional way to define a broader spectrum of domain knowledge
- Has an expression to transform the estimated values of a model into a new temporary data

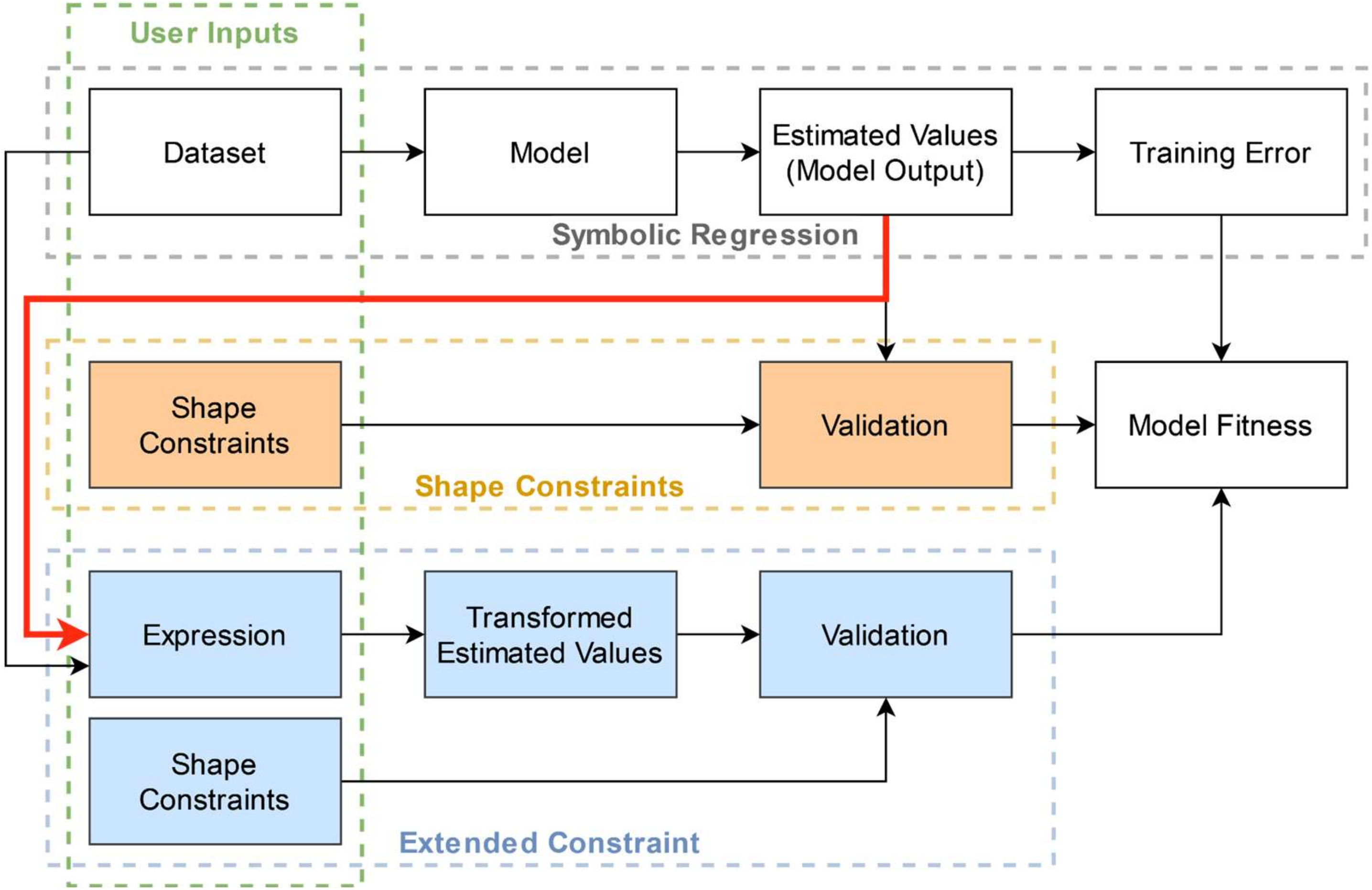



- Has a set of shape constraints
- Shape constraints are applied onto the transformed estimated values

# Extended Constraints



# Extended Constraints



# Experiment Configuration

- Defined shape constraints for
  - B-H-Function
  - J-H-Function ($J = B - (4\pi 10^{-7}) * H$)
  - $\mu_r$-Function ($\mu_r = \frac{\frac{\Delta B}{\Delta H}}{4\pi 10^{-7}}$)
- Tested with three different types of GA's
  - Genetic Algorithm (GA)
  - Offspring Selection Genetic Algorithm (OSGA) [1]
  - Age-Layered Population Structure Genetic Algorithm (ALPS GA) [2]
- Executed with and without extended constraints for comparison
- 30 runs per combination


[1] Affenzeller, M., Wagner, S.: Offspring Selection: A New Self-Adaptive Selection Scheme for Genetic Algorithms. Adaptive and natural Computing Algorithms pp. 218-221 (2005)

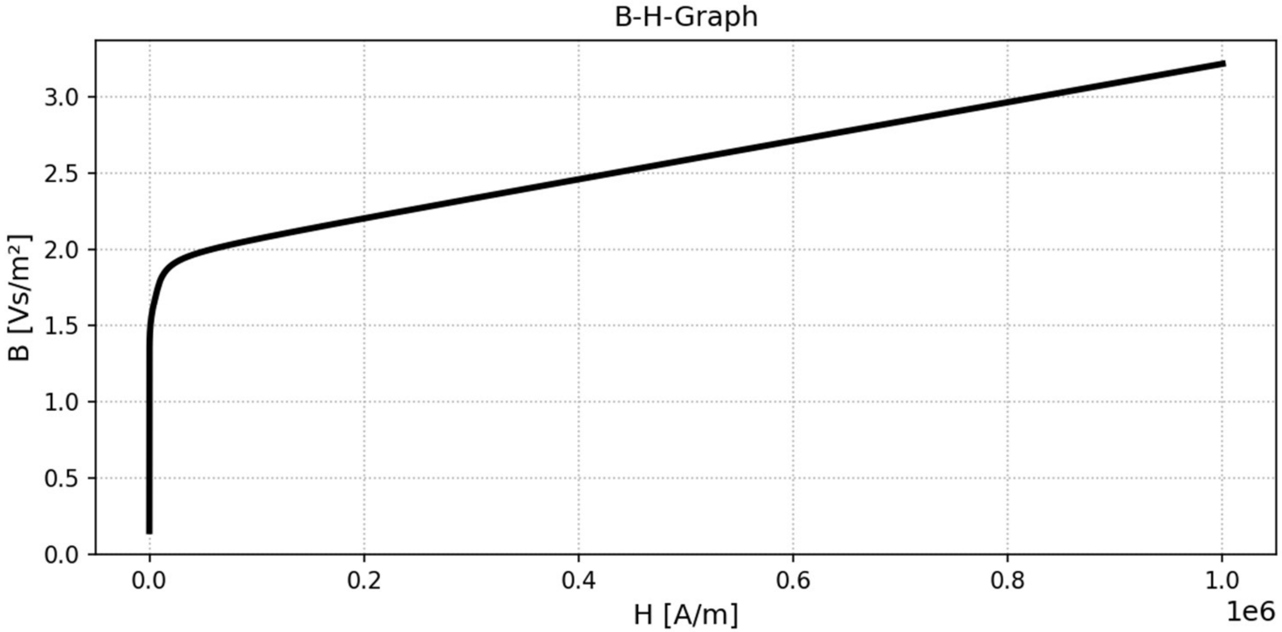
[2] Hornby, G. S.: The age-layered population structure (ALPS) evolutionary algorithm. Proceedings of the 9th annual conference on Genetic and evolutionary computation. (2009)

# Applied Constraints

## B-H-Graph

$$\frac{\partial B}{\partial H} \in [4\pi 10^{-7}, 4\pi 10^{-7}] \text{ where } H \in [800000, 1000000]$$

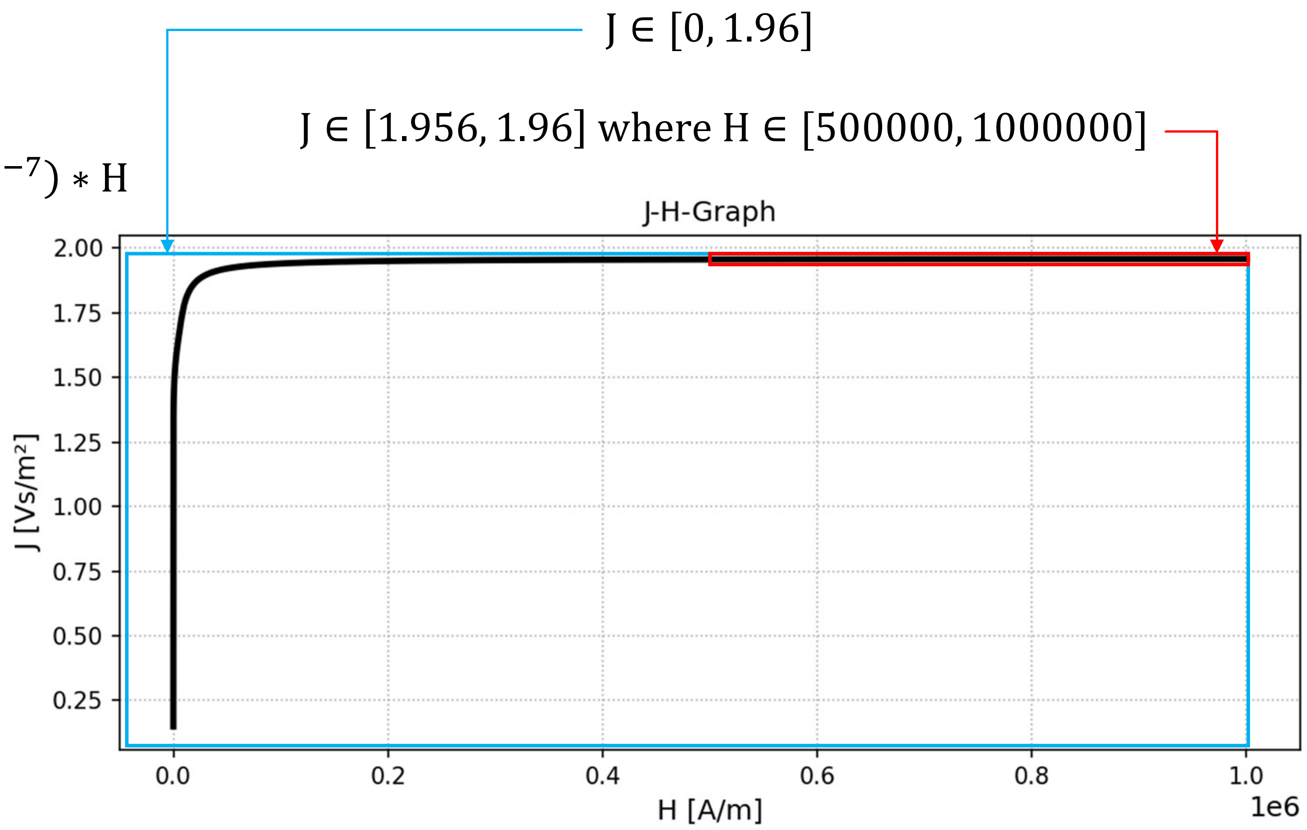
$$\frac{\partial B^2}{\partial H^2} \in [-10, 0] \text{ where } H \in [15000, 1000000]$$



# Applied Constraints

## J-H-Graph

$J = B - (4\pi 10^{-7}) * H$



# Applied Constraints

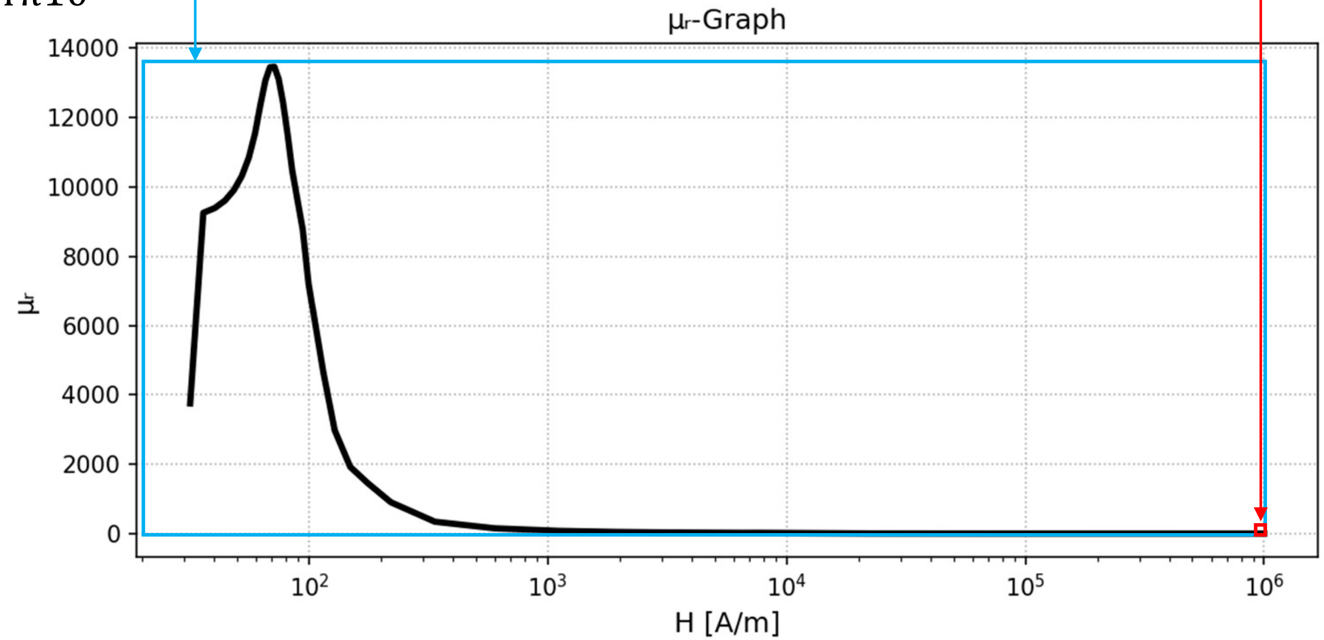
## $\mu_r$-Graph

$$\mu_r \in [1, 13500]$$

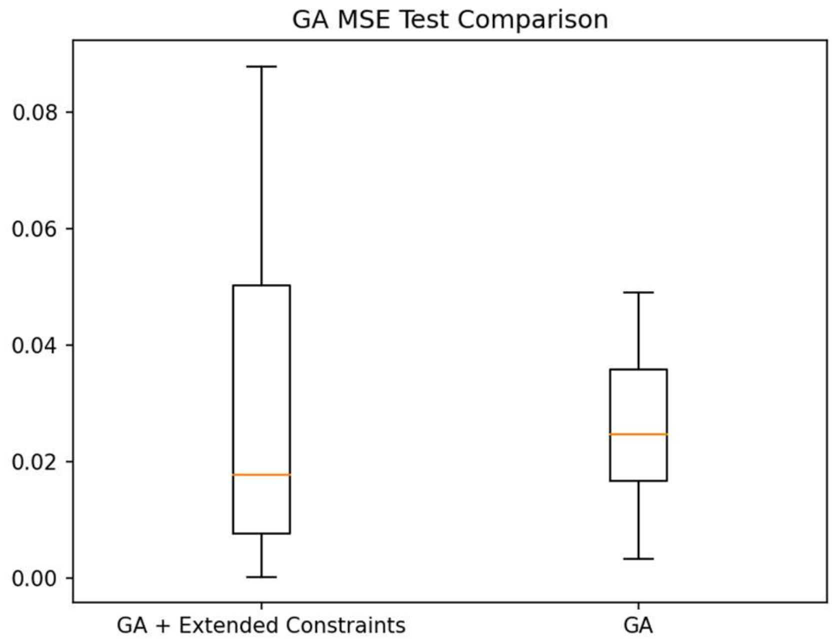
$$\mu_r \in [1, 1.005] \text{ where } H \in [90000, 1000000]$$

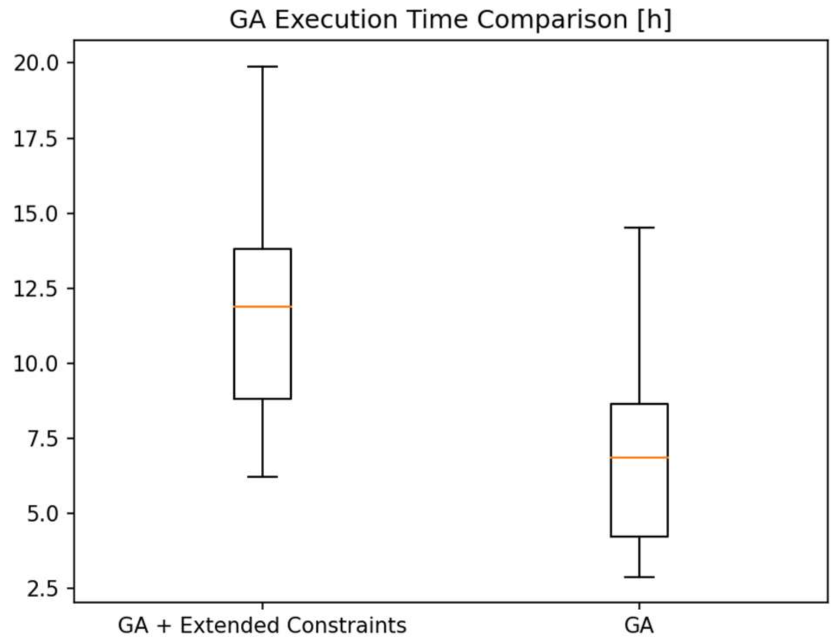
$$\frac{\partial \mu_r}{\partial H} \in [-100000, 0] \text{ where } H \in [80, 1000000]$$

$$\mu_r = \frac{\frac{\Delta B}{\Delta H}}{4\pi 10^{-7}}$$



# Preliminary Results
## Genetic Algorithm



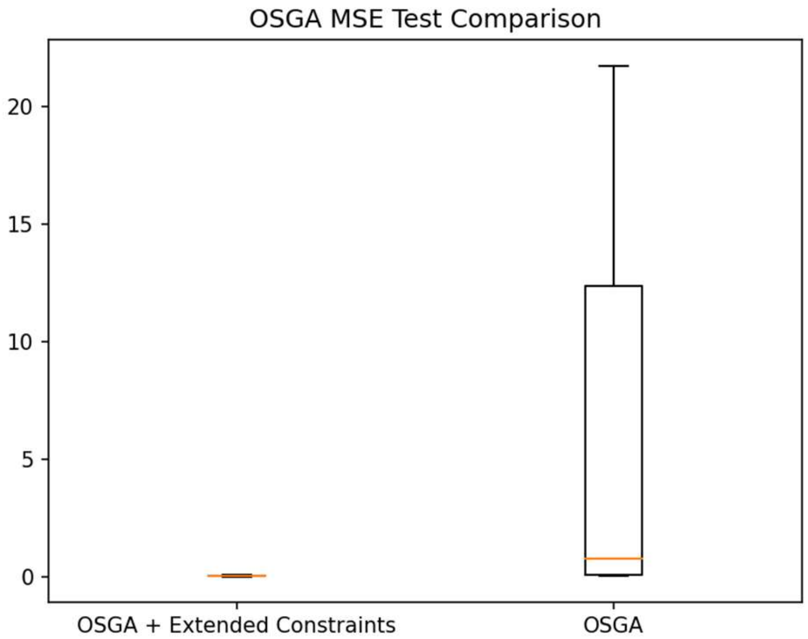



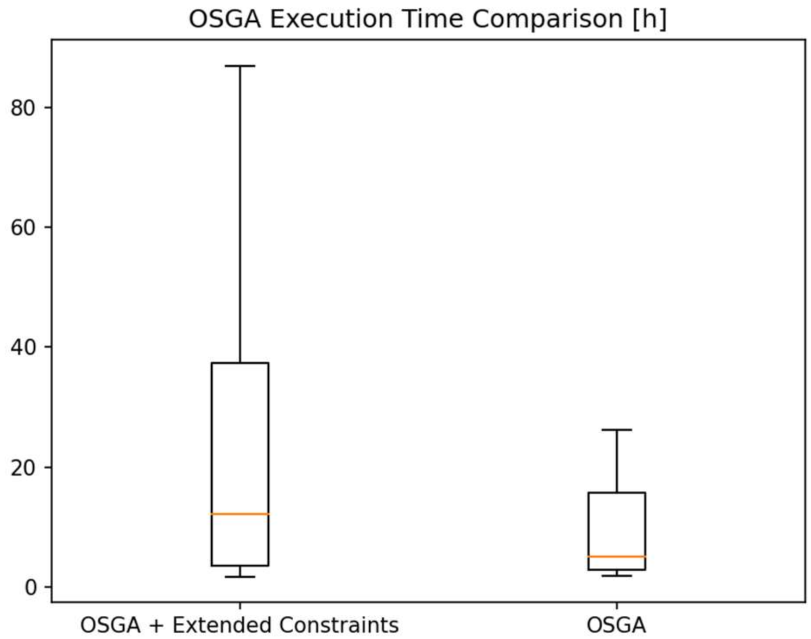

| **MSE Test Median** | |
|---|---|
| GA + Extended Constraints | GA |
| 0.018 | 0.025 |

| **Execution Time Median [s]** | |
|---|---|
| GA + Extended Constraints | GA |
| 42727 | 24627 |

# Preliminary Results

## Offspring Selection Genetic Algorithm

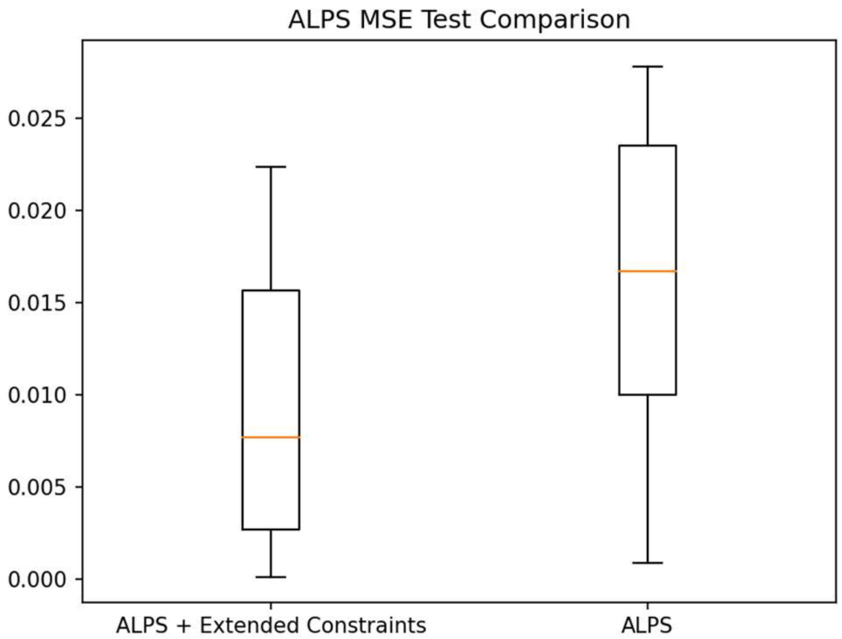


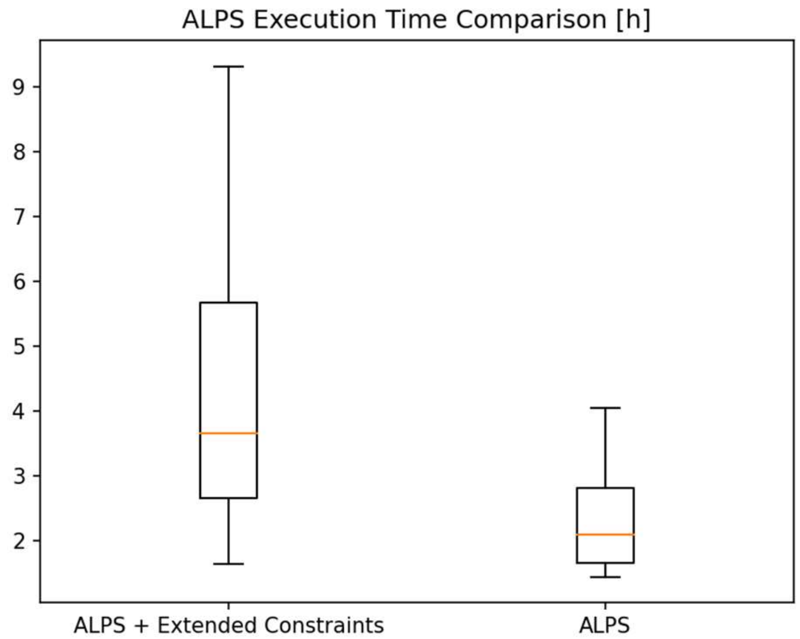




| **MSE Test Median** | |
|---|---|
| OSGA + Extended Constraints | OSGA |
| 0.024 | 0.756 |

| **Execution Time Median [s]** | |
|---|---|
| OSGA + Extended Constraints | OSGA |
| 43953 | 18422 |

# Preliminary Results
## Age-Layered Population Structure Genetic Algorithm




| **MSE Test Median** | |
|---|---|
| ALPS + Extended Constraints | ALPS |
| 0.008 | 0.017 |

| **Execution Time Median [s]** | |
|---|---|
| ALPS + Extended Constraints | ALPS |
| 13167 | 7573 |

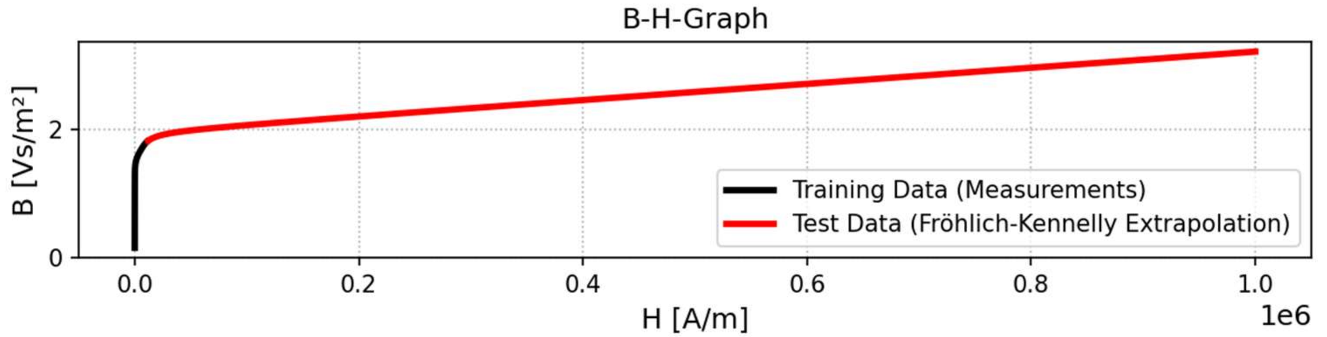
# Conclusion & Outlook

- With extended constraints is it possible to utilize a broader spectrum of domain knowledge
- Additional knowledge leads to better test qualities
- A promising way to reduce human calculation effort for extrapolating magnetization curves

- Experiments with additional materials for final paper
- Combination of extended shape constraints with structure template GP

# Problem Formulation

- Fit magnetization curves of ferromagnetic materials
  - Describes the relation between magnetic flux density B and magnetic field strength H
- Only small number of measured data points
- Manually extended with the Fröhlich-Kennelly extrapolation
- Goal: Find an automated way to search robust models, which fit the characteristics of magnetization curves with only the measured data points



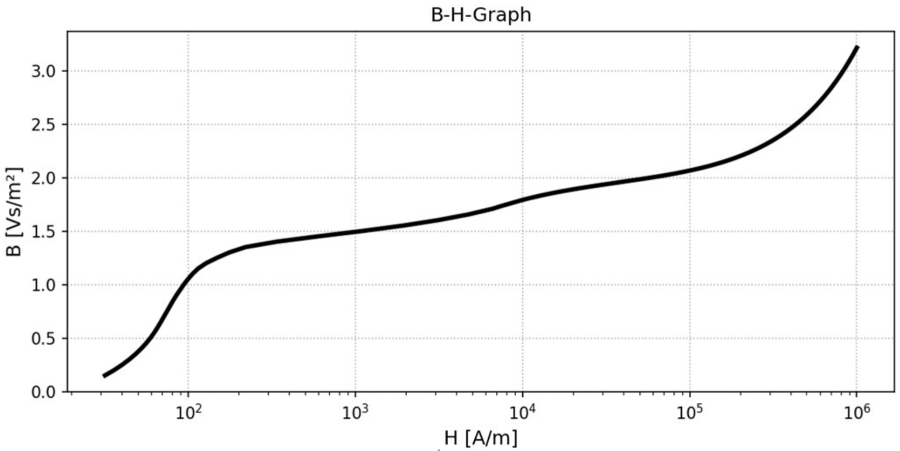
# Applied Algorithms

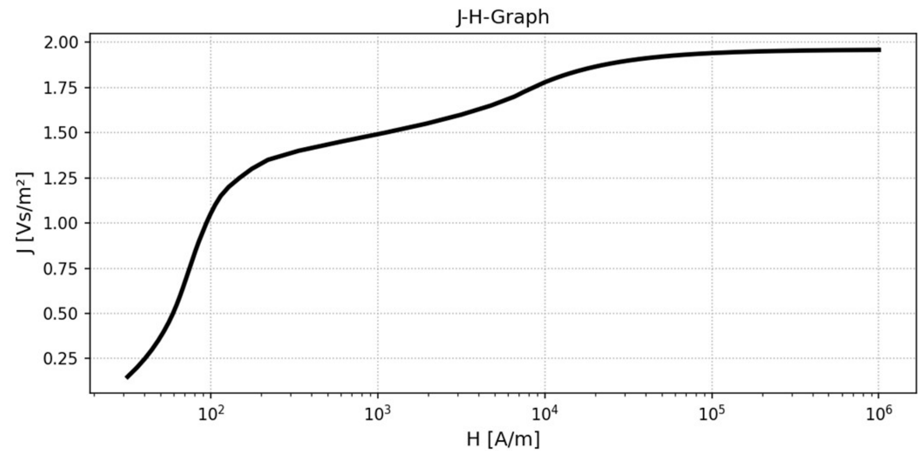
- Genetic Algorithm
- Offspring Selection Genetic Algorithm [1]
  - Additional selection mechanism after reproduction
  - Offspring must outperform its parents
  - Self-adaptive control of selection pressure
  - Terminates when maximum selection pressure is reached
  - Supports creation of larger building blocks in the population
- Age-Layered Population Structure Genetic Algorithm [2]
  - Population is split into different age layers
  - Each age-layer is a separate GA run
  - Each age-layer has its own maximum age for individuals
  - Continuous flow of new genetic material to prevent premature convergence

[1] Affenzeller, M., Wagner, S.: Offspring Selection: A New Self-Adaptive Selection Scheme for Genetic Algorithms. Adaptive and natural Computing Algorithms pp. 218-221 (2005)

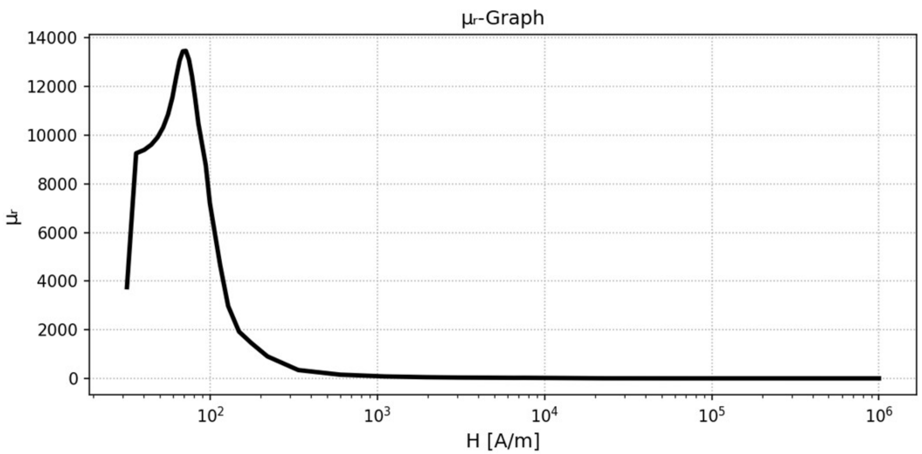
[2] Hornby, G. S.: The age-layered population structure (ALPS) evolutionary algorithm. Proceedings of the 9th annual conference on Genetic and evolutionary computation. (2009)

$$J = B - (4\pi 10^{-7}) * H$$



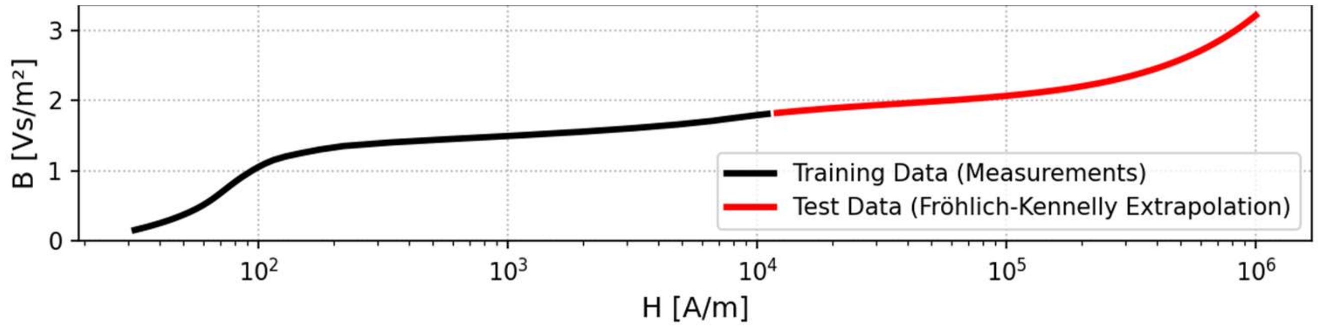




$$\mu_r = \frac{\frac{\Delta B}{\Delta H}}{4\pi 10^{-7}}$$



# Problem Formulation

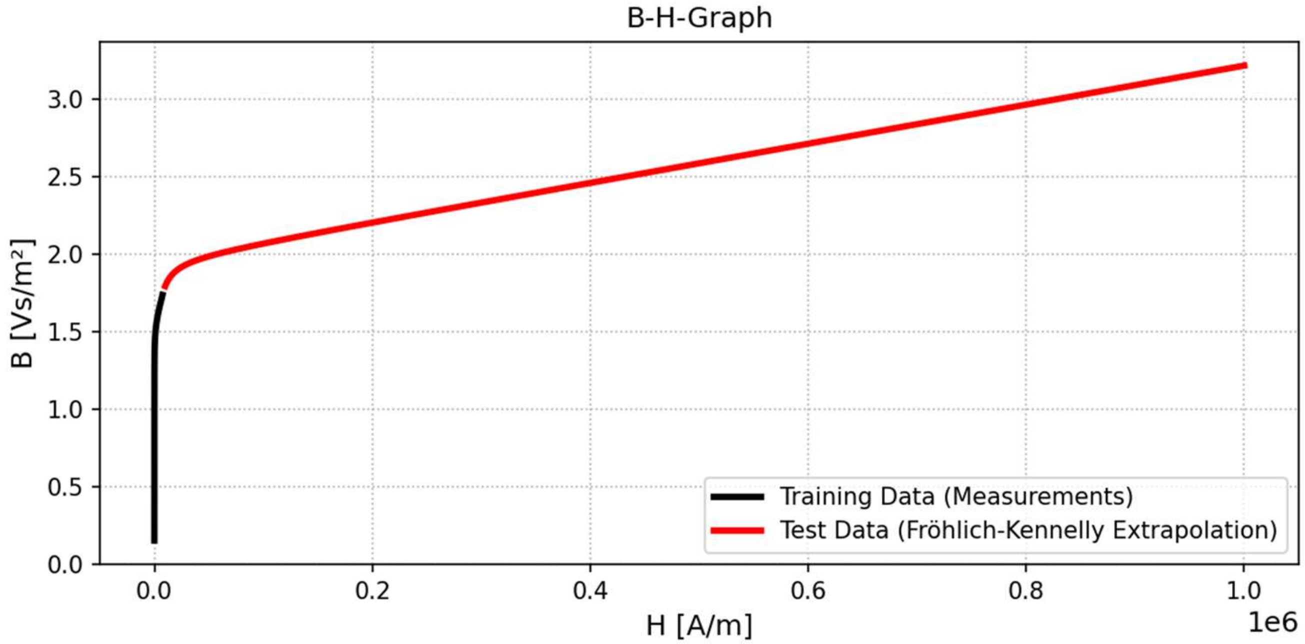
- fit magnetization curves of ferromagnetic materials
  - describes the relation between magnetic flux density B and magnetic field strength H
  - at a specific point (saturation point) B is growing linearly
- only small number of measured data points
- the measured data points are far below the saturation polarization
- Goal: find a way to search robust models, which fit the characteristics of magnetization curves with only a few data points



# Problem Formulation

- Goal: find an automated way to search robust models, which fit the characteristics of magnetization curves with only the measured data points

# Problem Formulation



# Shape Constraints - Previous Work

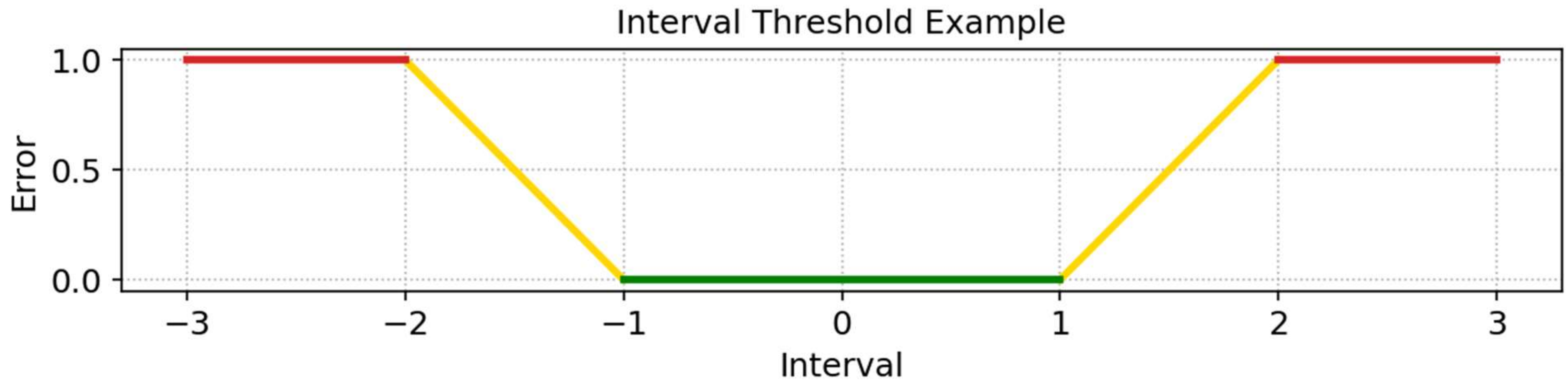
- introduces additional domain knowledge in Symbolic Regression [1,2]
- uses interval notation for definition
  - e.g.: y in [0, 5]
- uses interval arithmetic for calculation and validation
  - inputs are intervals
  - output is an interval which needs to fit inside the target interval of the shape constraint
- possible to constrain the model output as well as the shape of the function using derivations of any order
- each constraint can be limited to specific ranges for each input variable
  - e.g.: y in [0, 5] for x in [10, 20]

[1] Kronberger, G., de France, F.O., Burlacu, B., Haider, C., Kommenda, M.: Shape-constrained Symbolic Regression – Improving Extrapolation with Prior Knowledge. Evolutionary Computation pp. 1-24 (04 2021)

[2] Haider, C., de Franca, F.O., Burlacu, B., Kronberger, G.: Using shape constraints for improving symbolic regression models. arXiv preprint arXiv:2107.09458 (2021)

# Shape Constraints - Previous Work

- there exist hard and soft constraints for single-objective problems
  - hard constraints: each violation leads to a fixed fitness (NMSE = 1.0)
  - soft constraints:
    - for each interval bound exists a predefined threshold
    - the error is capped to 1.0 if the violation exceeds the threshold
    - if the violation is inside the range of the interval bound and the corresponding threshold, the error is linear between 0 and 1



# Shape Constraints - Previous Work

- each constraint can be limited to specific ranges for each input variable
  - e.g.: y in [0, 5] for x in [10, 20]

# Shape Constraints - Previous Work

- introduces additional domain knowledge in Symbolic Regression
- uses interval arithmetic to describe the additional knowledge
- possible to constrain the model output as well as the shape of the function using derivations of any order

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# Extended Constraints

- adds a way (on top of existing shape constraints) to define a broader spectrum of domain knowledge
- defines an expression to convert the estimated outputs of a model into a new symbol
- a set of defined constraints are applied onto the new symbol

```
Target = y
Input = x
Model = Symbolic Regression Solution
Shape Constraints:
- y in [0; 5]
- y' in [0;inf.]
```

```
Expression = y / (x*x)
Target = z
Input = y,x
Constraints:
- z in [0; 5]
- y' in [0;inf.]
```

# Extended Constraints

- adds a way (on top of existing shape constraints) to define a broader spectrum of domain knowledge
- defines an expression to convert the estimated outputs of a model into a new symbol
  - has access to all inputs and the calculated model estimations
  - calculated line-by-line
  - uniformly distributed samples are generated if ranges are used
- a set of defined constraints are applied onto the new symbol
  - Calculation
  - interval arithmetic is used
  - evaluated by calculating

# Experiment Configuration

| Parameter | Value |
| --- | --- |
| maximum Tree Size | 50 |
| maximum Tree Depth | 25 |
| allowed Symbols | +, -, *, tanh, number, variable |
| | |

# Results

## OSGA Training Qualities