SymReg

JOSEF RESSEL CENTER FOR
SYMBOLIC REGRESSION

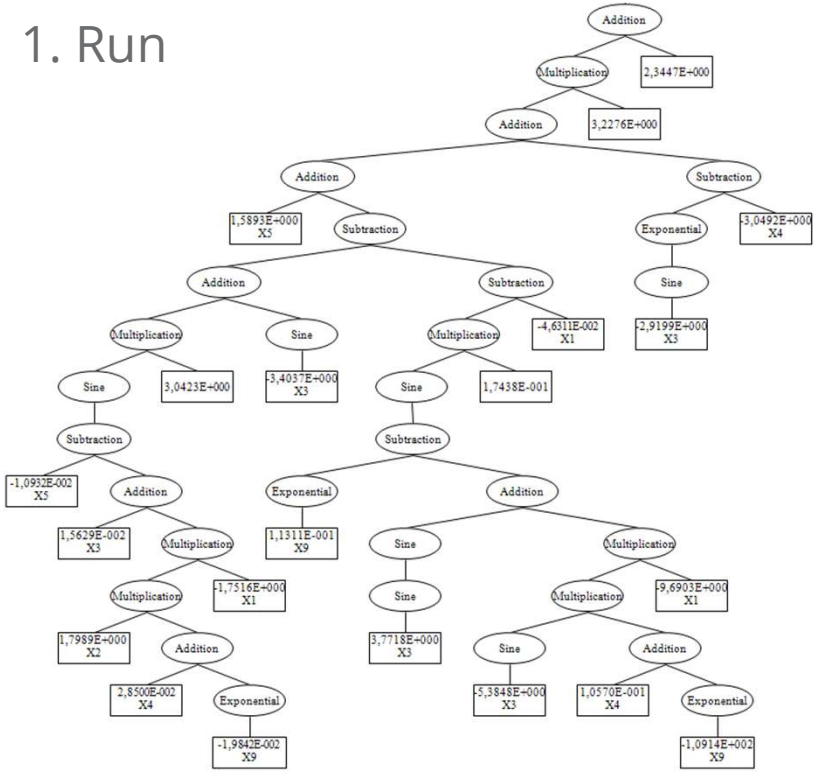
Empirical Analysis of Variance for GP based Symbolic Regression

Lukas Kammerer

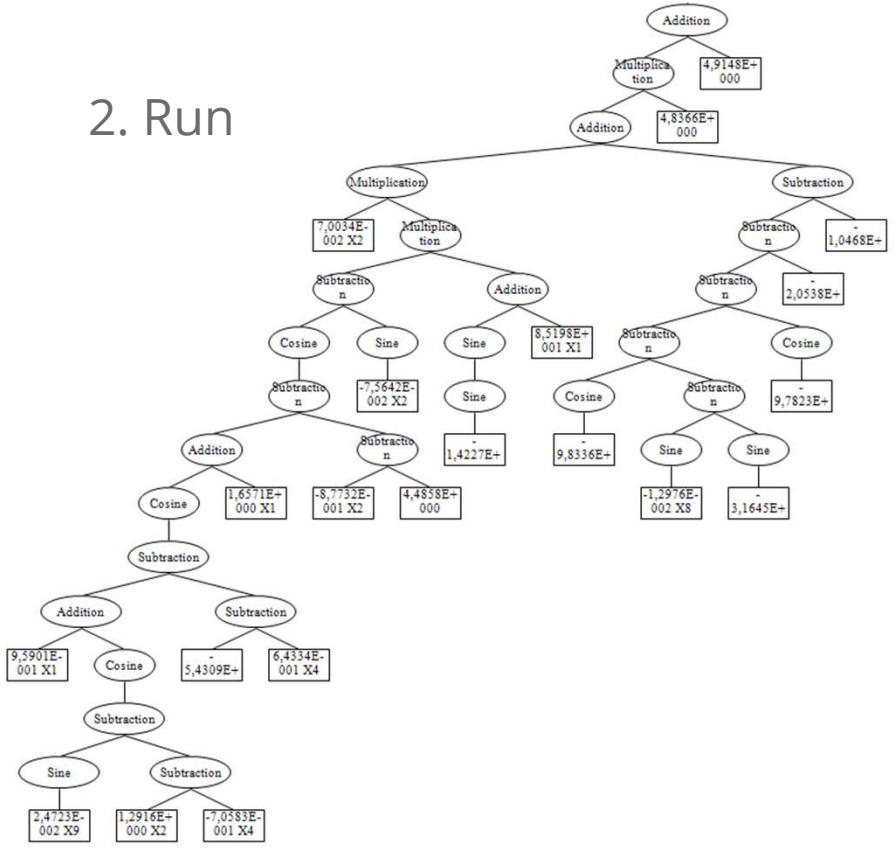
JRZ SymReg Workshop
24.02.2021

Motivation

1. Run



2. Run



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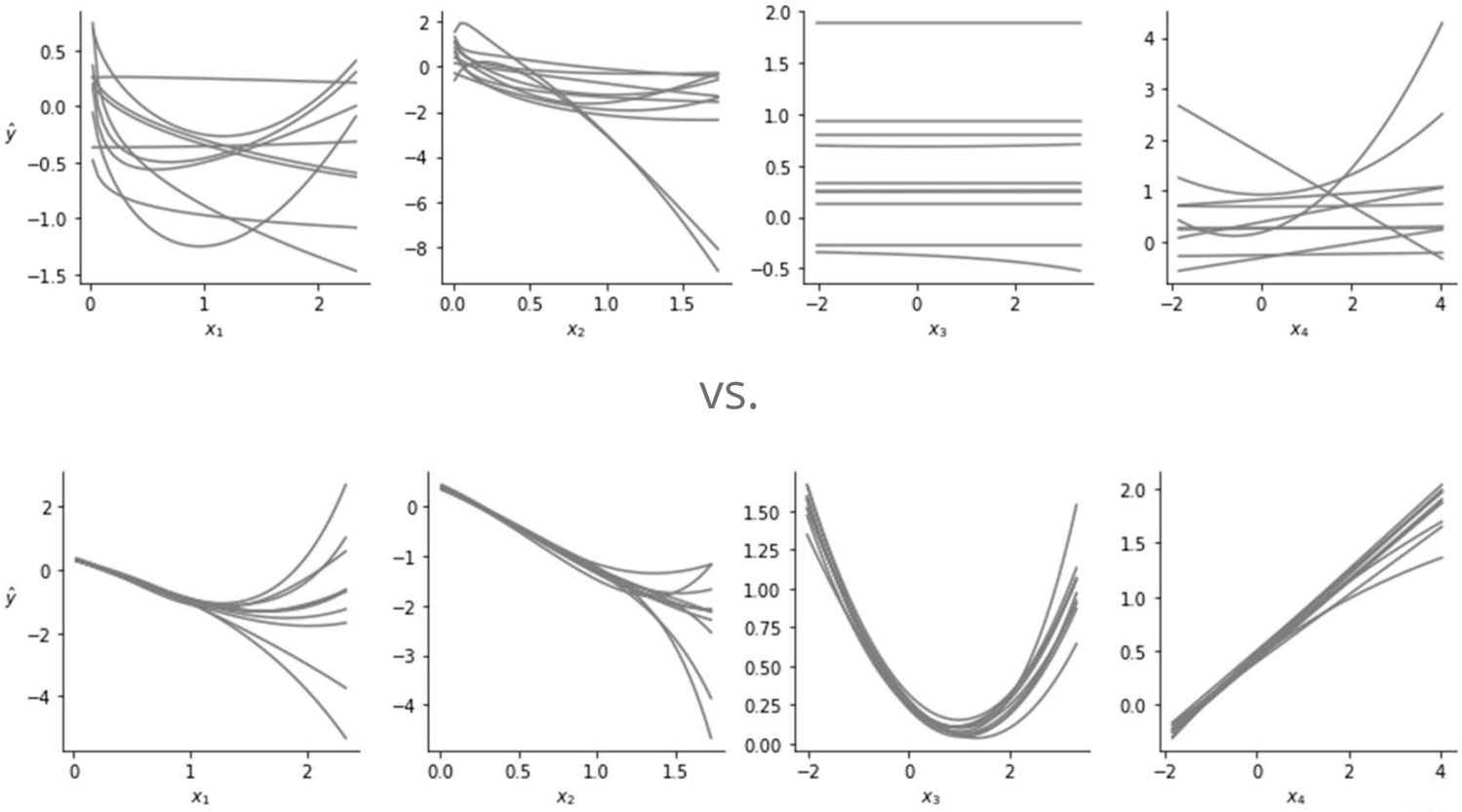

vs.

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Phenotypical Spread

Given:

- $\mathbf{m}$ with k models
- Dataset D with n samples

$$s(\boldsymbol{m}, D) = \frac{1}{n}\sum_{i=0}^{n} \mathrm{IQR}(\{\mathrm{m}_1(D_i) \ \ldots \ m_k(D_i)\})$$

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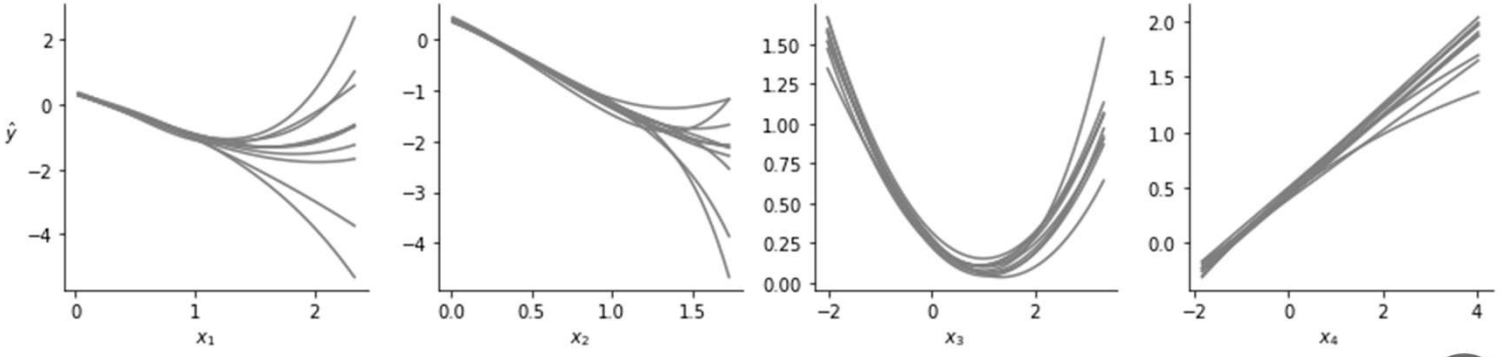

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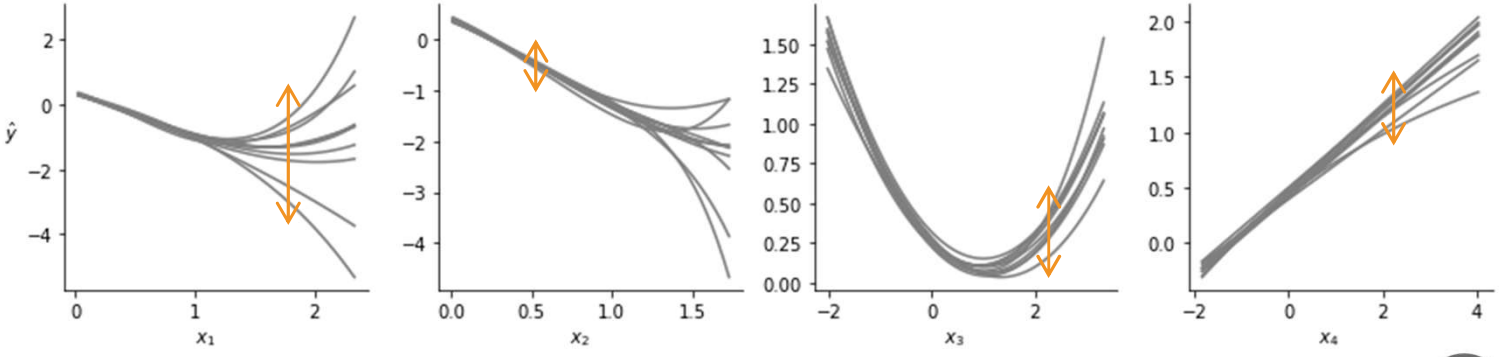

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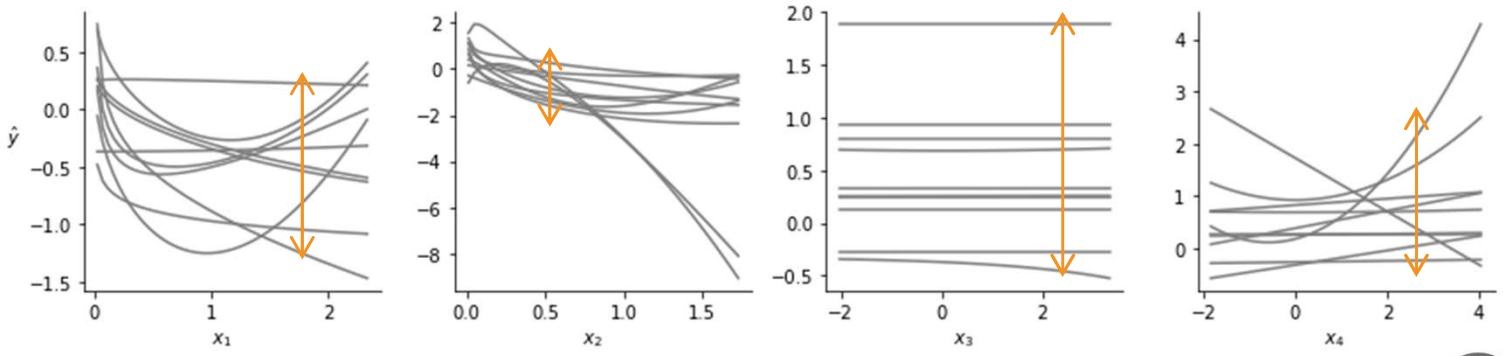
cf. Maarten Keijzer and Vladan Babovic. 2000. Genetic Programming, Ensemble Methods and the Bias/Variance Tradeoff – Introductory Investigations. In *European Conference on Genetic Programming*. Springer, 76–90.



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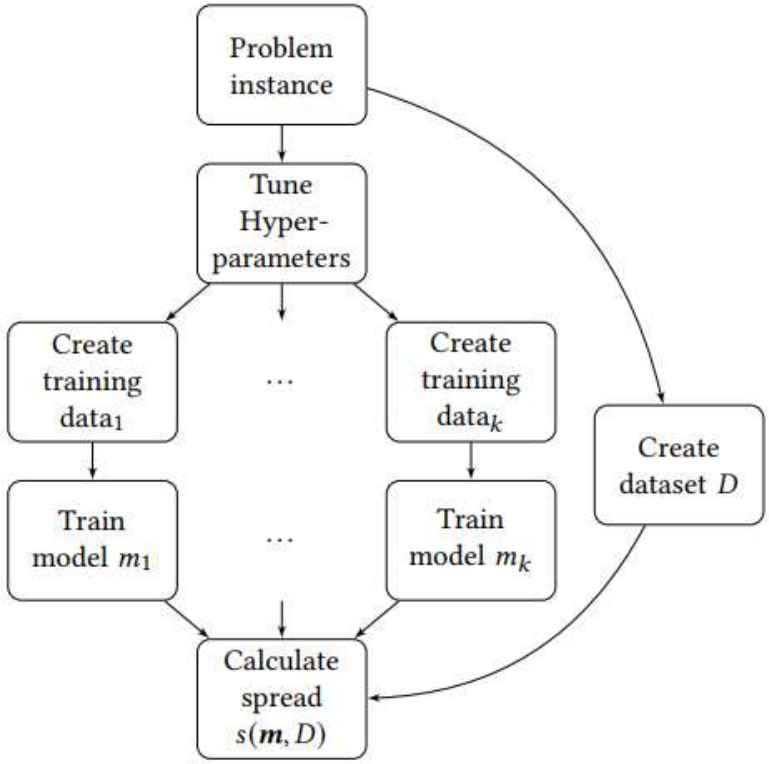
- 96 problem instances
- 5 (non-)evolutionary Algorithms



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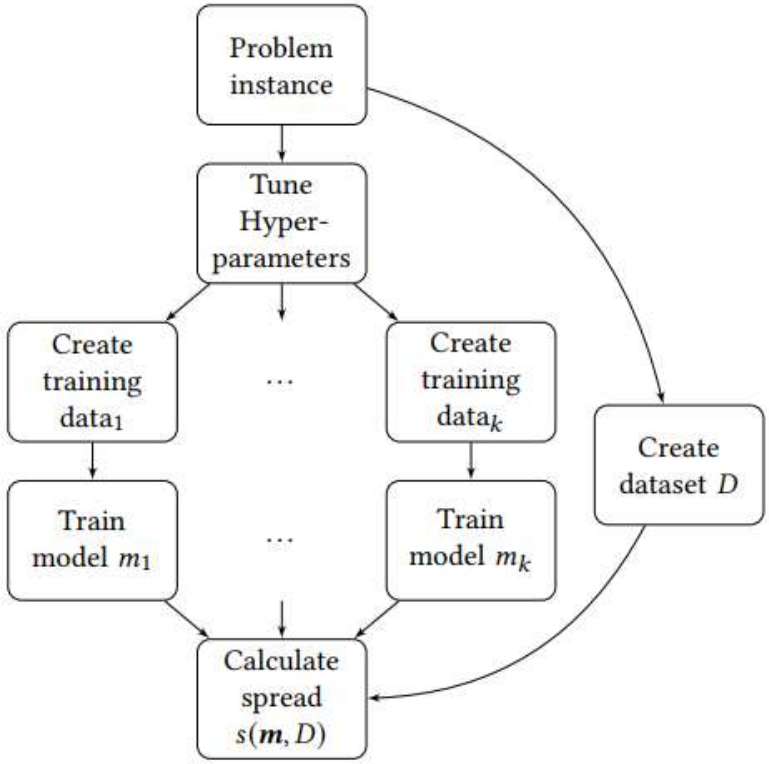
Experimental Setup

- PennML Benchmark Library
  - 32 real world problems
  - 62 Friedman problems

- Algorithms
  - GP
  - GP with local optimization (GP NLS)
  - Linear regression (LR)
  - Polynomial regression (PR)
  - Random forest regression (RF)



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Experimental Setup

- GP and GP NLS
  - max. tree length ∈ {10, 25, 50, 75}
  - population size ∈ {100, 500, 1000}
  - max. generations ∈ {100, 200, 1000}

  cf. Michael Kommenda, Bogdan Burlacu, Gabriel Kronberger and Michael Affenzeller. 2019. Parameter identification for symbolic regression using nonlinear least squares. Genetic Programming and Evolvable Machines (2019), 1–31.
- RF
  - 200 trees
  - $m \in \{0.25, 0.5, 0.75\}$
  - $r \in \{0.1, 0.2, \ldots, 0.7\}$
- PR
  - $\alpha \in \{0, 0.5, 1\}$
  - $\lambda \in \{1 \cdot 10\text{-}7, 2.5 \cdot 10\text{-}7, 5 \cdot 10\text{-}7, 7.5 \cdot 10\text{-}7, 1 \cdot 10\text{-}6, 2.5 \cdot 10\text{-}6 \ldots 7.5 \cdot 10\text{-}2\}$
  - total polynomial degree ∈ {2, 3, 4, 5}. (if > 20 features: max. 3)

GP and GP NLS Settings

Function set	+, -, ×, ÷, x^2, $\sqrt{x}$, exp(x), log(x)
Max. evaluated models	100 000
Selection	Tournament group size 2
Crossover operator	Subtree crossover, 100% probability
Mutation probability	25%
Mutation operator	Change symbol, replace branch, remove branch, single-point
Fitness function	Mean squared error

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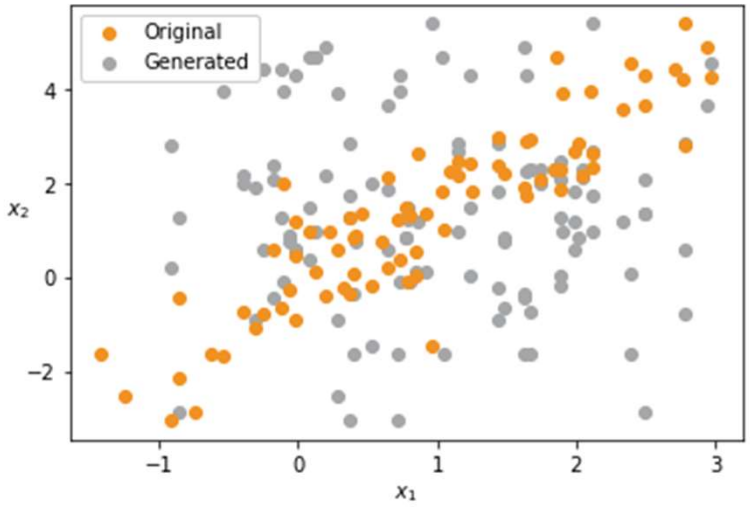
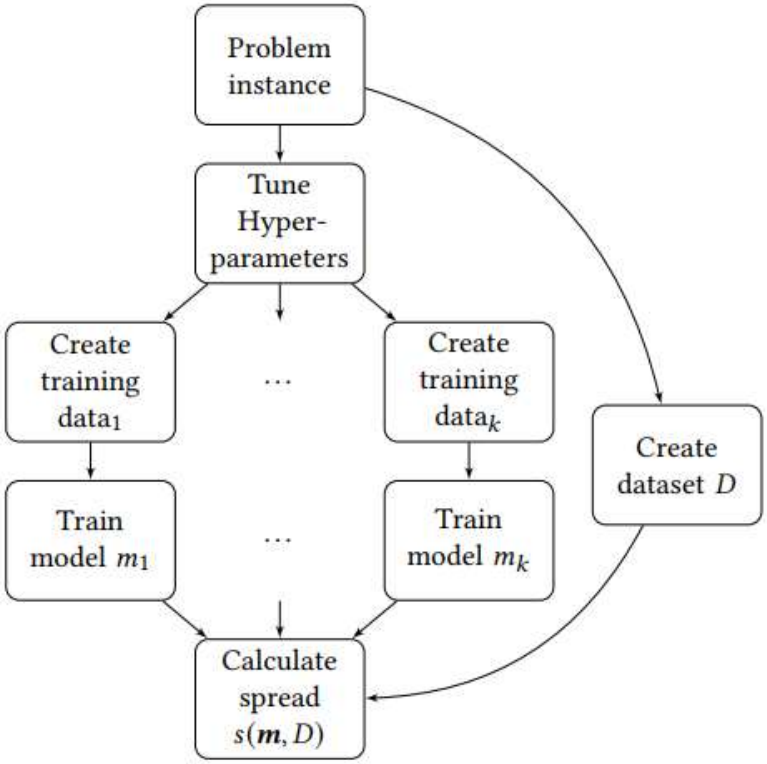
Experimental Setup

- Dataset D generated by sampling from origianl dataset





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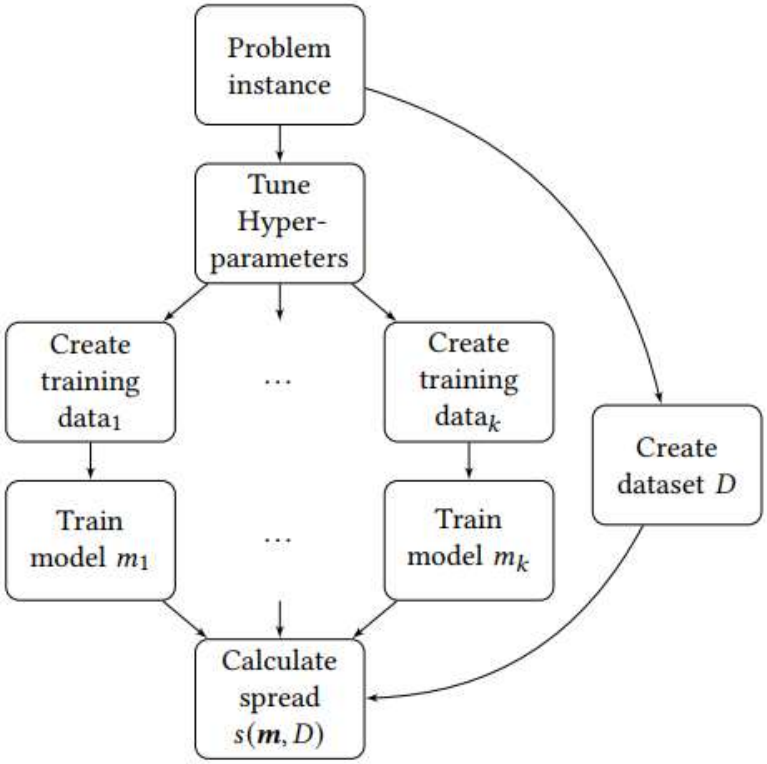
Experimental Setup

Problem	LR	PR	RF	GP	GP NLS
192_vineyard	0,82	0,83	0,67	1.0	1.47
195_auto_price	2058,8	1445,8	751,49	1625,6	2256,4
210_cloud	0,14	0,13	0,15	0,24	0,35
228_elusage	2,62	2,87	3,5	2,15	2,58
...	...	...	...	...	...



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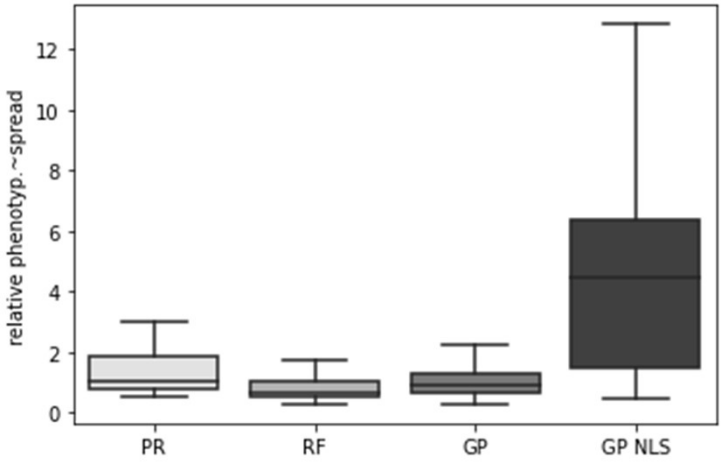
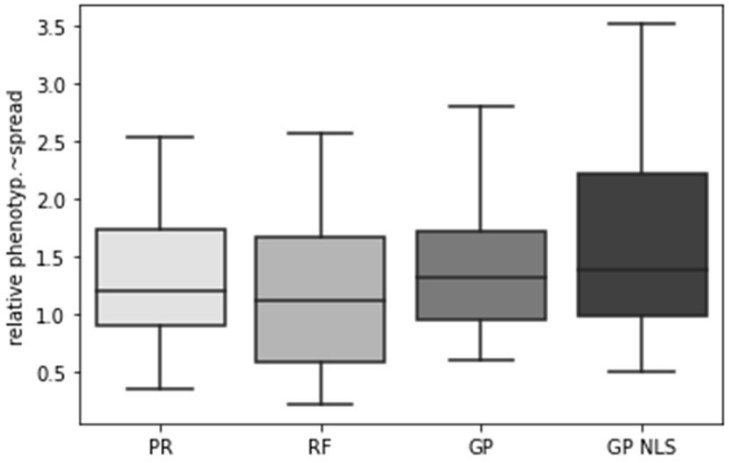
Distribution of Spread

Values per problem instance relative to value of linear regression

Friedman Problems



Real World Problems



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Statistical Significance

- Rank-wise analysis

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Statistical Significance

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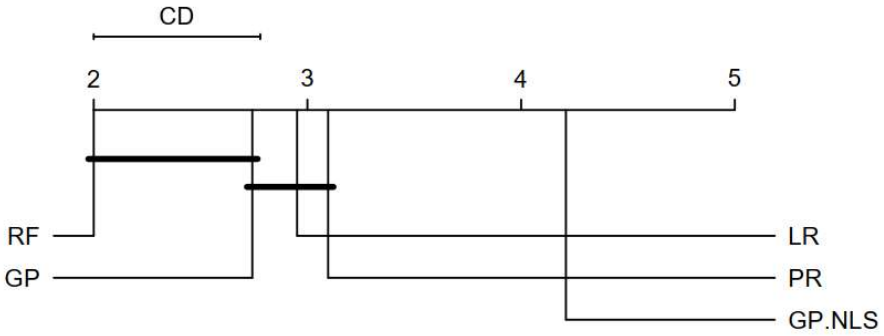
Friedman Problems



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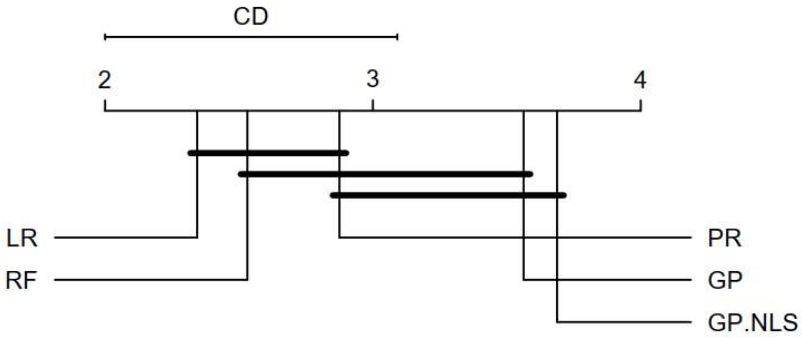

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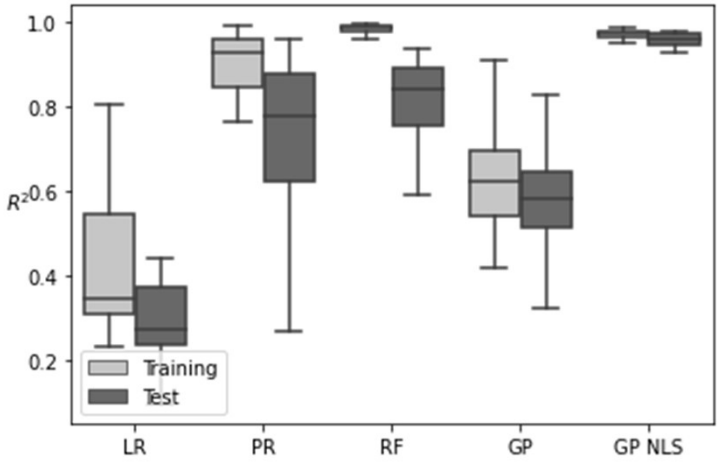
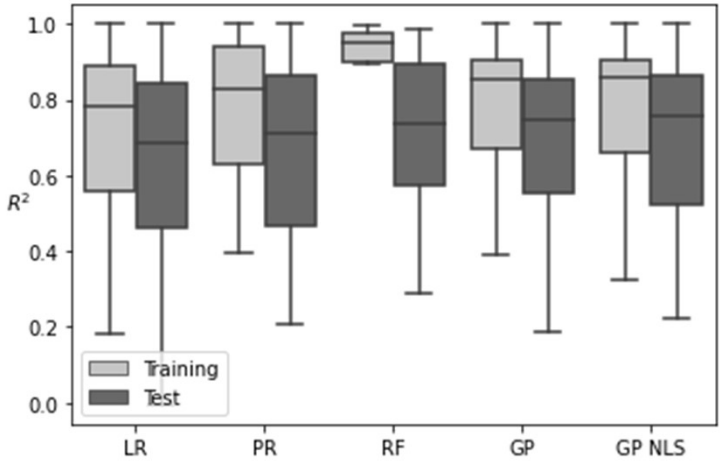
Prediction Error

Median R^2 of all 50 models per Problem

Friedman Problems



Real World Problems



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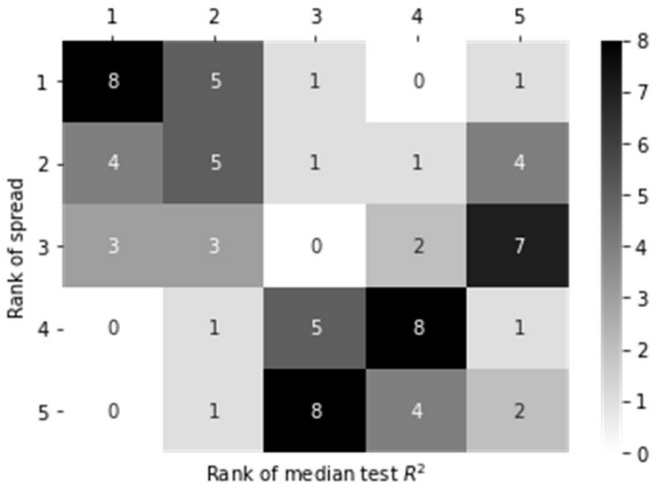
Prediction Error vs. Phenotypical Spread

Rank correlation between prediction error and phenotypical Spread

Friedman Problems
without collinearity



Friedman Problems
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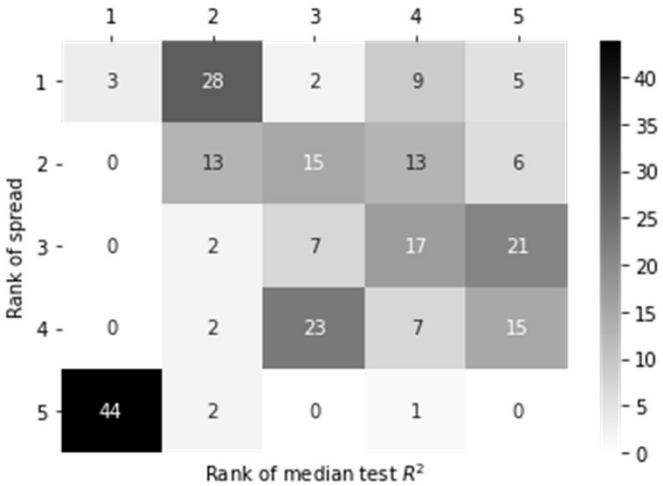
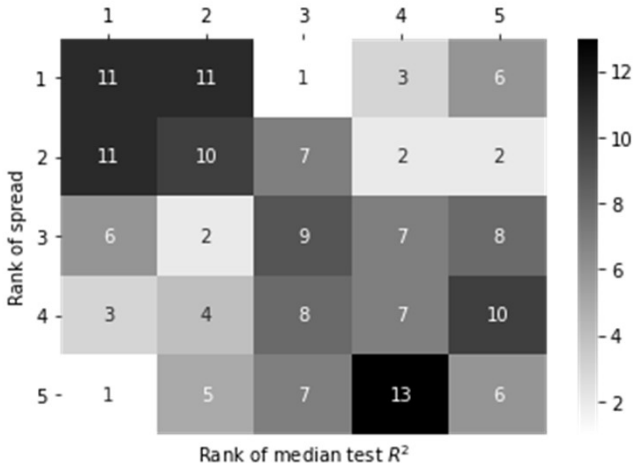


Real World Problems



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Spread in Training and Test

→ Different Calculation of Spread

Sample Index	m_1	m_2	...	m_{50}	IQR Predictions for **Test** instances	IQR Predictions for **Training** instances
1	Train	Train	Test	Train	...	...
2	Train	Test	Train	Train	...	...
3	Test	Test	Train	Test	...	...
4	Train	Train	Train	Train	...	...
...	...	...	...	...	...	...

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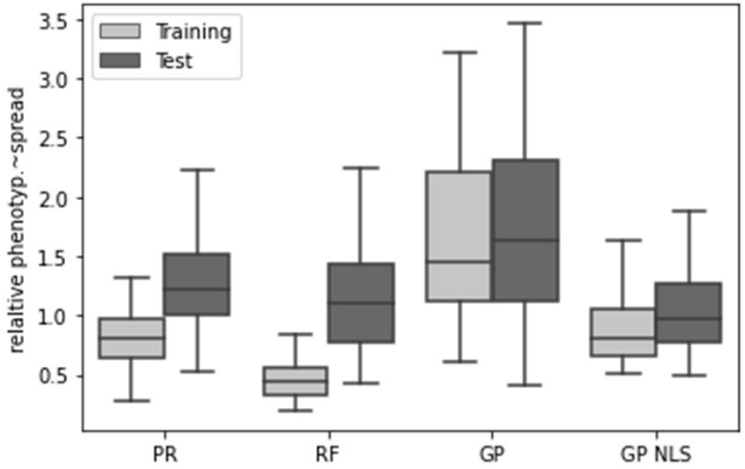
Spread in Training and Test

Friedman Problems



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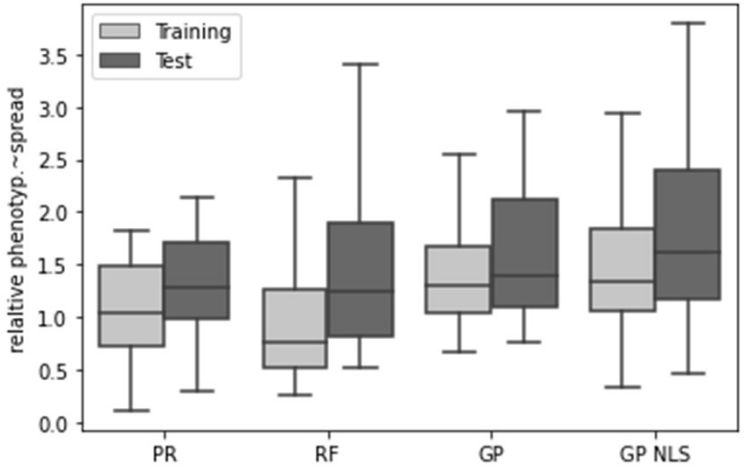

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Conclusion

- Clear differences in modelling accuracy between Friedman and real world Problems
  → High accuracy on Friedman Problems → good results on whole benchmark

- Real world problems and Friedman problems without collinearity:
  Higher accuracy ↔ Lower Spread and vice versa

- Friedman problems with collinearity:
  High accuracy ↔ High Spread
  – Only in extrapolation

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Questions?