# Scientific Machine Learning

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Josef Ressel Centre for Symbolic Regression Heuristic and Evolutionary Algorithms Laboratory University of Applied Sciences Upper Austria





JOSEF RESSEL CENTER FOR SYMBOLIC REGRESSION



HEURISTIC AND EVOLUTIONARY ALGORITHMS LABORATORY



# Short bio

#### Dipl.-Ing. Dr. Bogdan Burlacu

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# **Education and work**

- 2009 BEng. Systems and Computer Engineering, "Gh. Asachi" Technical Univ. Iași, Romania
- 2008-2011 Software dev, SC Software Development Partnership SRL, Iași, Romania
- 2011-present Research Associate, University of Applied Sciences Upper Austria, https://fh-ooe.at
- 2015-present Senior Researcher, Josef Ressel Centre for Symbolic Regression, https://symreg.at
- $\cdot$  2017 PhD. Computer Science, Johannes Kepler University Linz, Austria
- 2018-present Lecturer, Human Centered Computing, MSc course Data Preprocessing and Analysis

#### **Open-source projects**

HeuristicLab (https://dev.heuristiclab.com) - heuristic and evolutionary optimization framework (C#) Operon (https://github.com/heal-research/operon) - large-scale symbolic regression (C++) Vstat (https://github.com/heal-research/vstat) - numerically stable, SIMD-enabled statistics (C++) Pappus (https://github.com/heal-research/pappus) - interval and affine arithmetic (C++)

https://github.com/heal-researchhttps://github.com/foolnotion

Introduction HEAL, SymReg, SciML

Symbolic Regression Overview

Example: Shape Constraints

Example: Inter-atomic Potentials

# Heuristic and Evolutionary Algorithms Laboratory (HEAL)

# **Research** group

- · Established at FH Upper Austria in 2005
- · 5 professors, 17 research associates
- · interns, students (bachelor, master)

# **Research output**

- > 25 research projects, >6M€ funding
- > 200 publications (peer-reviewed)
- $\cdot$  > 10 dissertations
- $\cdot$  > 60 theses (bachelor and master)

## Scientific and industrial partners

https://heal.heuristiclab.com/partners

# Heuristic and Evolutionary Algorithms Laboratory (HEAL)

# HeuristicLab

- · Interactive development, analysis and application of optimization methods
- Plug-in architecture, distributed computing capabilities

#### Main focus on combinatorial and symbolic regression/classification problems

- (probabilistic) traveling salesman, knapsack, bin packing, vehicle routing, job shop scheduling, orienteering, quadratic assignment, and others
- · symbolic regression and classification

#### Large collection of optimization methods

- metaheuristics (evolutionary, tabu search, simulated annealing, etc.)
- · tree ensemble methods, kernel methods, Gaussian processes, neural networks

# Heuristic and Evolutionary Algorithms Laboratory (HEAL)

# Many interesting optimization problems

- $\cdot$  production scheduling
- · stacking in steel industries or container terminals
- · dynamic warehouse operations
- · cancer diagnosis based on tumor marker data
- · properties of synthetic materials
- predictive maintenance
- · process modeling based on virtual sensors
  - · exhaust gas modeling
  - · blast furnace modeling
  - · foam quality of firefighting vehicles
  - · plasma nitriding
  - $\cdot \;$  granulate homogeneity in plastic recycling machines

#### Close cooperation with domain experts

#### Focus on knowledge discovery, insight into the industrial process

# Josef Ressel Centre for Symbolic Regression (JRZ)

Founded in 2018 as a joint project between the Christian Doppler Research Association, the University of Applied Sciences Upper Austria and three industry partners:



Head of JRZ Prof. Gabriel Kronberger

## Symbolic regression as a technology:

- · Algorithm design: deterministic symbolic regression (as opposed to e.g. stochastic/metaheuristic)
- · Method development: optimize for accuracy and runtime, keep number of parameters low
- · Integration of physical knowledge: shape constraints

# https://symreg.at/

# Josef Ressel Centre for Symbolic Regression (JRZ)

# AVL ್ಲಿ

#### - Development, simulation and testing of powertrain systems

- Virtual sensors and test bench
- Real-time control on control units
- Reduction of test bench and development times



#### - Friction materials, components for friction systems

- Improved friction system development through modeling and simulation
- Model- and data warehousing for Tribological systems
- Automatic validation, shorter development cycles



- optimize the process for stability and optimal throughput
- virtual sensors
- modeling and optimal control

#### What is SciML?

Blend of traditional scientific mechanistic modeling with machine learning methodologies.

Mechanistic (traditional) modeling: differential equations (by and large)

Machine learning: (deep) neural nets, kernel methods, tree ensemble methods, symbolic regression, etc.

#### Main challenges

Complex applications: complex and multi-scale dynamics, data are sparse and expensive to acquire High consequence: decisions can have severe outcomes, need for explainable models Technically challenging: numerical difficulties, computing gradients, running code in HPC environments **Focus shift** from *prediction* to *understanding*:

- · extracting insights from data requires interpretable models
- $\cdot \;$  models should incorporate physical laws, constraints and other scientific domain knowledge
- · physically meaningful behavior and parameters (e.g. Planck's constant, Avogadro's constant)
- · robustness and the ability to quantify uncertainty are required for scientific rigour

"The path from good science to good engineering relies on conducting reproducible simulations that quantitatively explain phenomena, and then being able to document how far those results can be trusted." – Erik van der Giessen et al 2020 Modelling Simul. Mater. Sci. Eng. 28 043001, https://doi.org/10.1088/1361-651X/ab7150

# Scientific Machine Learning



Agrawal and Choudari, Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science, APL Mater. 4, 053208 (2016), https://doi.org/10.1063/1.4946894

SciML Foundations

Machine Learning for Advanced Scientific Computing Research

|   | <b>Domain-aware</b><br>leveraging & respecting<br>scientific domain knowledge | physical principles & symmetries<br>physics-informed priors<br>structure-exploiting models<br>:  |
|---|---|--|
| d | Interpretable<br>explainable & understandable results                         | model selection<br>exploiting structure in high-dim data<br>uncertainty quantification + ML<br>i |
|   | Robust<br>stable, well-posed &<br>reliable formulations                       | probabilistic modeling in ML<br>quantifying well-posedness<br>reliable hyperparameter estimation |

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# **Scientific Machine Learning**

SciML Capabilities

Machine Learning for Advanced Scientific Computing Research

| Nata-Intoneivo |     |      |    |      |    |
|----------------|-----|------|----|------|----|
|                | ive | ensi | mt | -a-1 | D. |
|                |     |      |    |      |    |

scientific inference & data analysis

ML methods for multimodal data in situ data analysis with ML ML to optimally guide data acquisition

ML-enhanced modeling & sim

ML-hybrid algorithms and models for better scientific computing tools

#### Intelligent automation & decision support

automated decision support, adaptivity, resilience, control

exploration of decision space with ML ML-based resource mgt & control optimal decisions for complex systems

ML parameter tuning

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# **Scientific Machine Learning**



Arrieta et. al, Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI, Information Fusion 58, 2020, https://doi.org/10.1016/j.inffus.2019.12.012



Mishin, Machine-learning interatomic potentials for materials science,

https://doi.org/10.1016/j.actamat.2021.116980

Finding a symbolic expression that matches data from an unknown function.

Core challenge in physics and engineering (in principle, NP-hard: Lu et al. 2016 https://doi.org/10.1155/2016/1021378)

An optimization algorithm would have to explore a very large, combinatorial search space:

- · Discrete in model structure, continuous in model parameters
- $\cdot \;$  Growing exponentially with the length of the expression

# Symbolic Regression

Let  $\mathcal{P}$  be a primitive set (e.g. +, -,  $\times$ ,  $\div$ , exp, sin, etc.) and  $S_{\mathcal{P}}$  the syntactic search space defined by it.

Let  $\Phi$  be the space of possible expressions and their parameters, defined as the set of all tuples  $(E, \theta)$ where  $E \in S_{\mathcal{P}}$  is a symbolic expression and  $\theta \in \mathbb{R}^p$  is a vector of coefficients for E.

We call a tuple  $(E, \theta)$  a symbolic expression model  $M_{E,\theta} \in \Phi$ .

Let  $G : \Phi \times \mathbb{R}^{n \times m} \to \mathbb{R}^n$  be a function that evaluates model  $M_{E,\theta} \in \Phi$  on some training data **X** (with corresponding dependent target **y**) and outputs a prediction  $\hat{\mathbf{y}} \in \mathbb{R}^n$ .

The overall goal of symbolic regression is to find the optimal model

$$M_{opt} = \underset{M_{E,\theta} \in \Phi}{\operatorname{arg\,min}} \frac{1}{2} ||G(M_{E,\theta}, \mathbf{X}) - \mathbf{y}||^{2}$$

Overarching objective: good extrapolation behavior on unknown (out-of-domain) data.

#### Strategies to search model space $\Phi$ :

- · Evolutionary: genetic programming, grammatical evolution (guided metaheuristic)
- · Generative-enumerative: production rules from a grammar (guided heuristic)
- · Hybrid: AI Feynman, DeepSR, EQL, PNN-SR (mixed heuristic)

## Strategies to optimize model coefficients $\theta$ :

- $\cdot$  non-linear least squares
- · variable projection (if least squares problem is separable)
- · stochastic hill climbing
- metaheuristics e.g. CMA-ES

# Algorithm

· Exact, deterministic, correct, finite number of steps, well understood, proven complexity bounds.

# Heuristic

- · Derived from experience or from empirical evicence
- · Hard to study from a theoretical standpoint
- $\cdot \;$  Usually no guarantees about optimality or complexity bounds
- · Useful practical solving tools, producing good results (not necessarily optimal) in a short amount of time

### **Interlude: Heuristics and Metaheuristics**

#### HEURISTICS FOR INTEGER PROGRAMMING USING SURROGATE CONSTRAINTS

Fred Glover, University of Colorado

#### ABSTRACT

This paper proposes a class of surrogate constraint heuristics for obtaining approximate, near optimal solutions to integer programming groblems. These heuristics are based on a simple framework that illuminates the character of several earlier heuristic proposals and provides a variety of new alternatives. The paper also proposes additional heuristics that can be used either to supplement the surrogate constraint procedures or to provide independent solution strategies. Preliminary computational results are reported for applying one of these alternatives to a class of nontinear generalized set covering problems involving approximately 100 constraints and 300-500 integer variables. The solutions obtained by the tated procedure had objective function values twice as good as values obtained by standard approaches (e.g., reducing the best objective function values of other methods from 85 to 400 on the average. Total solution time for the tested procedure ranged from ten to twenty seconds on the COC 6660.

#### INTRODUCTION

Heuristic solution methods for integer programming have maintained a noticeably separate existence from algorithms. Algorithms have long constituted the more respectable side of the family, assuring an optimal solution in a finite number of steps. Methods that merely claim to be clever, and do not boast an entourage of supporting theorems and proofs, are accorded a lower status. <u>Algorithms are concerted in analytic</u> purity in the high citadels of academic research, heuristics are midwifed by expediency in the dark corners of the practitionner's lair.

Recently, however, there has been a growing recognition that the algorithms are not always successful, and that their heuristic cousins deserve a chance to prove their mettle. Parily this comes from an emerging awareness that algorithms and heuristics are not as different as once supposed - algorithms, after all, are merely fastidious heuristics in which epsilons and deltas abide by the dictates of mathematical etiquette. It may even be said that algorithms exhibit a somewhat compulsive aspect, being denied the freedom that would allow an occasional inconsistency or an exception to ultimate convergence. (Unfortunately, ultimate convergence sometimes acquires a relicious significance; it seems not to happen in this world.)

#### Metaheuristic

Iterative master process that guides and modifies the operations of subordinate heuristics.

- · combines different concepts for *exploring* and *exploiting* the search space
- · uses learning strategies in order to structure information
- · may manipulate a complete or incomplete solution or set of solutions at each iteration
- subordinate heuristics may be high or low level procedures, or simple local search, or just a construction method

May be inspired from natural behaviors, emergent phenomena, etc.

May push the analogy too far https://github.com/fcampelo/EC-bestiary

# Symbolic Regression

y = 2x + 5

- · Abstract syntax trees typically used for representation
- Easy to manipulate
- Fast evaluation and amenable to autodiff (e.g. using duals  $a + b\epsilon$ ,  $\epsilon^2 = 0$ )
- $\cdot\,$  Can be compiled to machine code (LLVM, asmjit), CUDA/openCL kernels
- · Straightforward to transform (algebraic rules/identities) or prune
- · Derivatives can be computed symbolically
- $\cdot$  Coefficients tunable with non-linear least squares (e.g. leaf nodes 2, 5)

#### **Genetic Programming**

- · Simulates the process of natural evolution ("survival of the fittest")
- $\cdot~$  Stochastic search guided by heuristics and a cost ("fitness") function
- · Relies on genetic operators: selection, crossover, mutation
- · Very general: no need for *a priori* knowledge, can find model structure and coefficients

# Extensions

- · Memetic approaches (+ local optimization: gradient-based, trust region etc.)
- · Parallel/distributed approaches: island models, parallel tempering
- · Multi-objective strategies (Pareto-based, decomposition-based)

# Caveats

- · Non-deterministic
- $\cdot~$  Can produce overly complex expressions
- $\cdot \;$  Tradeoff between parsimony and accuracy

# Symbolic Regression

## **Genetic Programming**



#### Deep learning and other approaches

- PINNs: "physics-informed NN" eqn. learners, PDE solvers (https://doi.org/10.1038/s41598-021-92278-w)
- Al-Feynman: divide and conquer, heuristic approach (https://arxiv.org/abs/2006.10782)
- DeepSR: RNN + risk seeking policy gradients (https://arxiv.org/abs/1912.04871)
- EQL: equation learning network (http://proceedings.mlr.press/v80/sahoo18a.html)
- PNNs: parsimonious neural networks (https://www.nature.com/articles/s41598-021-92278-w)

#### Motivation

- · black box nature of deep learning hinders explainability and new scientific discovery
- $\cdot\,$  critical need to tackle "knowledge integration" in the deep learning pipeline
- · knowledge integration can be: feature engineering, network architecture design, regularization, etc.

# Approach

- $\cdot\,$  encode model equations (e.g. PDEs) as part of the network itself
- · taking into acount the physics of the problem
- · loss function includes PDE residuals as well as terms for initial and boundary conditions



Kim et al. 2021 https://doi.org/10.1007/s12206-021-0342-5



Kim et al. 2021 https://doi.org/10.1007/s12206-021-0342-5

# AI Feynman (Udrescu et al. 2020)



- $\cdot\;$  Collection of heuristics for discovering physical laws
- · AST represented as a graph
- Recursive application of solvers and problem decomposition heuristics
- Exploits neural networks, graph modularity, hypothesis testing, normalizing flows

# **AI Feynman**



https://cbmm.mit.edu/publications/ai-feynman-20-pareto-optimal-symbolic-regression-exploiting-graph-modularity

# Al Feynman

|    | Equation   | Symmetries |
|----|--|------------|
| 1  | $\delta = -5.41 + 4.9 \frac{\alpha - \beta + \gamma/\chi}{3\chi}$  | TC         |
| 2  | $\chi = 0.23 + 14.2 \frac{\alpha + \beta}{3\gamma}^{3\gamma}$  | TS         |
| 3  | $\beta = 213.80940889 (1 - e^{-0.54723748542\alpha})$  |            |
| 4  | $\delta = 6.87 + 11\sqrt{\alpha\beta\gamma}$   | Р          |
| 5  | $V = \left[ R_1^{-1} + R_2^{-1} + R_3^{-1} + R_4^{-1} \right]^{-1} I_0 \cos \omega t  \text{(Parallel resistors)}$   | PGSM       |
| 6  | $I_0 = \frac{V_0}{\sqrt{R^2 + (\omega L - \frac{1}{\omega C})^2}}  (\text{RLC circuit })$  | MG         |
| 7  | $I = \frac{\sqrt{V_0 \cos \omega t}}{\sqrt{R^2 + (\omega L - \frac{1}{\omega C})^2}}  \text{(RLC circuit)}$  | MG         |
| 8  | $V_2 = \left(\frac{R_2}{R_1 + R_2} - \frac{R_x}{R_x + R_3}\right) V_1$ (Wheatstone bridge)   | SGMA       |
| 9  | $v = c \frac{(v_1 + v_2 + v_3)/c + v_1 v_2 v_3/c^3}{1 + (v_1 v_2 + v_1 v_3 + v_2 v_3)/c^2} $ (Velocity addition)   | AG         |
| 10 | $v = c \frac{(v_1 + v_2 + v_3 + v_4)/c + (v_2 v_3 v_4 + v_1 v_3 v_4 + v_1 v_2 v_4 + v_1 v_2 v_3)/c^3}{1 + (v_1 v_2 + v_1 v_3 + v_1 v_4 + v_2 v_3 + v_2 v_4 + v_3 v_4)/c^2 + v_1 v_2 v_3 v_4/c^4} $ (Velocity addition) | GA         |
| 11 | $z = (x^4 + y^4)^{1/4}$ (L <sub>4</sub> -norm)   | AC         |
| 12 | $w = xyz - z\sqrt{1 - x^2}\sqrt{1 - y^2} - y\sqrt{1 - x^2}\sqrt{1 - z^2} - x\sqrt{1 - y^2}\sqrt{1 - z^2}$  | GA         |
| 13 | $z = \frac{xy + \sqrt{1 - x^2 - y^2 + x^2 y^2}}{y\sqrt{1 - x^2} - x\sqrt{1 - y^2}}$  | А          |
| 14 | $z = y\sqrt{1-x^2} + x\sqrt{1-y^2}$  | А          |
| 15 | $z = xy - \sqrt{1 - x^2}\sqrt{1 - y^2}$  | А          |
| 16 | $r = \frac{a}{\cot(\alpha/2) + \cot(\beta/2)}$ (Incircle)  | GMAC       |

https://cbmm.mit.edu/publications/ai-feynman-20-pareto-optimal-symbolic-regression-exploitinggraph-modularity

# Approach

- use a large model (neural network) to search the space of small models (symbolic expressions)
- $\cdot$  exploits background knowledge about the form of the expressions
- · generates mathematical expressions using a recurrent neural network (RNN)
- $\cdot\;$  the RNN is trained via a risk-seeking policy gradient
- · AST represented as sequence of tokens (preorder)
- · AST generated sequentially using sampling from RNN-generated token distribution + constraints
- · tree coefficients further optimized with nonlinear least squares (BFGS)

# **Reward function**

$$\begin{split} R(\tau) &= \frac{1}{1 + \text{NRMSE}} \quad (\text{"squashed" NRMSE} \\ \text{NRMSE} &= \frac{1}{\sigma_y} \sqrt{\frac{1}{n} \sum_{i=1}^n \left(y_i - f(X_i)\right)^2} \end{split}$$

# **Deep Symbolic Regression**



Algorithm 1 Deep symbolic regression with risk-seeking policy gradient

input learning rate  $\alpha$ ; entropy coefficient  $\lambda_{\mathcal{H}}$ ; risk factor  $\varepsilon$ ; batch size N; reward function R output Best fitting expression  $\tau^*$ 

- 1: Initialize RNN with parameters  $\theta$ , defining distribution over expressions  $p(\cdot|\theta)$
- 2: repeat

3:  $\mathcal{T} \leftarrow \{\tau^{(i)} \sim p(\cdot|\theta)\}_{i=1}^N$  $\mathcal{T} \leftarrow \{\text{OptimizeConstants}(\tau^{(i)}, R)\}_{i=1}^{N}$ 4:  $\mathcal{R} \leftarrow \{R(\tau^{(i)})\}_{i=1}^N$ 5:  $R_{\varepsilon} \leftarrow (1-\varepsilon)$ -quantile of  $\mathcal{R}$ 6:  $\mathcal{T} \leftarrow \{\tau^{(i)} : R(\tau^{(i)}) > R_c\}$ 7:  $\mathcal{R} \leftarrow \{R(\tau^{(i)}) : R(\tau^{(i)}) > R_{\varepsilon}\}$ 8.  $\hat{q}_1 \leftarrow \text{ReduceMean}((\mathcal{R} - R_{\varepsilon})\nabla_{\theta} \log p(\mathcal{T}|\theta))$ 9:  $\hat{q}_2 \leftarrow \text{ReduceMean}(\lambda_{\mathcal{H}} \nabla_{\theta} \mathcal{H}(\mathcal{T}|\theta))$ 10:  $\theta \leftarrow \theta + \alpha (\hat{q}_1 + \hat{q}_2)$ 11: if max  $\mathcal{R} > R(\tau^*)$  then  $\tau^* \leftarrow \tau^{(\arg \max \mathcal{R})}$ 12: 13: return  $\tau^*$ 

▷ Sample N expressions (Alg. 2 in Appendix A)
▷ Optimize constants w.r.t. reward function
▷ Compute rewards
▷ Compute reward threshold
▷ Select subset of expressions above threshold
▷ Select corresponding subset of rewards
▷))
▷ Compute risk-seeking policy gradient
▷ Compute entropy gradient
▷ Apply gradients
▷ Update best expression

Table 1: Recovery rate comparison of DSR and five baselines on the Nguyen symbolic regression benchmark suite. A bold value represents statistical significance ( $p < 10^{-3}$ ) across all benchmarks.

| Benchmark | Expression                                  | DSR   | PQT   | VPG   | GP    | Eureqa | Wolfram |
|-----------|---|-------|-------|-------|-------|--------|---------|
| Nguyen-1  | $x^3 + x^2 + x$                             | 100%  | 100%  | 96%   | 100%  | 100%   | 100%    |
| Nguyen-2  | $x^4 + x^3 + x^2 + x$                       | 100%  | 99%   | 47%   | 97%   | 100%   | 100%    |
| Nguyen-3  | $x^5 + x^4 + x^3 + x^2 + x$                 | 100%  | 86%   | 4%    | 100%  | 95%    | 100%    |
| Nguyen-4  | $x^{6} + x^{5} + x^{4} + x^{3} + x^{2} + x$ | 100%  | 93%   | 1%    | 100%  | 70%    | 100%    |
| Nguyen-5  | $\sin(x^2)\cos(x) - 1$                      | 72%   | 73%   | 5%    | 45%   | 73%    | 2%      |
| Nguyen-6  | $\sin(x) + \sin(x + x^2)$                   | 100%  | 98%   | 100%  | 91%   | 100%   | 1%      |
| Nguyen-7  | $\log(x+1) + \log(x^2+1)$                   | 35%   | 41%   | 3%    | 0%    | 85%    | 0%      |
| Nguyen-8  | $\sqrt{x}$                                  | 96%   | 21%   | 5%    | 5%    | 0%     | 71%     |
| Nguyen-9  | $\sin(x) + \sin(y^2)$                       | 100%  | 100%  | 100%  | 100%  | 100%   | _       |
| Nguyen-10 | $2\sin(x)\cos(y)$                           | 100%  | 91%   | 99%   | 76%   | 64%    | _       |
| Nguyen-11 | $x^y$                                       | 100%  | 100%  | 100%  | 7%    | 100%   | _       |
| Nguyen-12 | $x^4 - x^3 + \tfrac{1}{2}y^2 - y$           | 0%    | 0%    | 0%    | 0%    | 0%     | -       |
|           | Average                                     | 83.6% | 75.2% | 46.7% | 60.1% | 73.9%  | -       |

# Approach

- · fully connected feed forward network structure
- $\cdot\,$  nodes/neurons include base functions (e.g.  $+,-,\times,\div,\sin,\cos,$  etc)
- · compositions of base functions are generated across network layers
- $\cdot\;$  able to learn relatively simple formula, able to control cart-pendulum system

# **Regularized division**

- $\cdot\,\,$  division introduces poles with abrupt changes in convexity and diverging function values
- real systems are assumed to be unable to generate data at the pole itself (because natural quantities do not diverge)
- $\cdot$  therefore a single branch of the hyperbola 1/b, b > 0 suffices as a basis function
- $\cdot \;$  regularized division only used in the output layer

$$h^{\theta}(a,b) = \begin{cases} \frac{a}{b} & \text{ if } b > \theta \\ 0 & \text{ otherwise} \end{cases}$$

# Equation Learner (Sahoo et al. 2018)



- · trained by stochastic gradient descent (mini batches + Adam)
- · Lasso-like loss function (fully differentiable in its free parameters)
- $\cdot \,$  penalty term  $P^{\theta}$  for small and negative denominators

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} ||f(x_i) - y_i||^2 + \lambda \sum_{i=1}^{L} |W^{(1)}|_1 + P^{\theta}$$

#### Application in Material Science

Learn equations of motion that govern the Hamiltonian dynamics of a particle

Discover melting laws from experimental data

### Approach

- · data obtained generated using molecular dynamics simulations
- · evolutionary optimization of network structure and weights (+ backpropagation)
- · four possible activation functions: linear, relu, tanh, elu
- $\cdot$  search space  $\sim 10^{21}$  possible network structures

# Parsimonious Neural Networks (Desai and Strachan 2021)



Figure 1. Neural network used as the starting point to find the parsimonious neural network as the network that explains the data in the simplest manner possible. The force sub-network is highlighted in orange and is fed into the neural network as a pre-trained model, whose weights are subsequently kept fixed throughout.

#### Desai and Strachan 2021 https://www.nature.com/articles/s41598-021-92278-w

# **Methods Comparison**



La Cava et al, NeurIPS Datasets and Benchmarks 2021, https://arxiv.org/abs/2107.14351

# **Methods Comparison**



La Cava et al, NeurIPS Datasets and Benchmarks 2021, https://arxiv.org/abs/2107.14351

#### Operon (Burlacu et al 2020)

- evolutionary system on top of Ceres (http://ceres-solver.org), Eigen (https://gitlab.com/libeigen/eigen), Taskflow (https://taskflow.github.io/)
- · tree AST as postorder sequence
- · Levenberg-Marquardt coefficient tuning

#### SRBench

## https://github.com/cavalab/srbench

Shape constraints are general concept applicable to different forms of regression analysis. (but not all methods equally amenable)

## Motivation: ensure conformance to physical expectation

- · Boundedness / Non-negativity / non-positivity (function image)
- · Monotonicity (first derivative)
- · Convexity / concavity (second derivative)

# Approach

- · interval arithmetic (pessimistic approach)
- · sampling the input space (optimistic approach)
- hard vs. soft penalties
- · single- vs. multi-objective

# **Example: Shape Constraints**



# **Example: Shape Constraints**



#### **Interval Arithmetic**

- method for calculating output ranges of mathematical expressions
- · rules for computing output intervals of arithmetic and elementary operators
- · intervals represented as  $[a, b] = \{x \in \mathbb{R} | a \leq x \leq b\}$

#### Weakness

Does not track dependencies between operator arguments ("dependency problem")

- $f(x) = x x, x \in [a, b] IA: [a b, b a], actual: [0, 0]$
- ·  $f(x) = x^2 x, x \in [-1, 1] IA: [-1, 2], actual: [-\frac{1}{4}, 2]$

IA tends to overestimate the output range, actual conforming models might get discarded.

# **Example: Shape Constraints**

#### Basic properties of Interval Arithmetic (cf. Warwick Tucker - Validated Numerics, 2011)

- · Interval addition and multiplication are commutative and associative
- · IA is not distributive in general but sub-distributive  $\forall a, b, c \in \mathbb{IR}, a(b + c) \subseteq ab + ac$
- $\cdot$  Monotone functions

If  $f: X \to \mathbb{R}$  is non-decreasing, then  $f(X) = [f(\underline{X}), f(\overline{X})]$ 

· Inclusion isotonicity

 $f: {\rm I} {\mathbb R}^n \to {\rm I} {\mathbb R} \text{ is inclusion isotonic if } \forall x,y \in {\rm I} {\mathbb R}^n, x \subseteq y \implies f(x) \subseteq f(y)$ 

· Interval extension

 $f:\mathbb{IR}^n\to\mathbb{IR} \text{ is an interval extension of }g:\mathbb{R}^n\to\mathbb{R} \text{ if }\forall x\in\mathbb{R}^n,g(x)=g(x)$ 

# Fundamental theorem of Interval Analysis

If  $f : \mathbb{IR}^n \to \mathbb{IR}$  is inclusion isotonic and an interval extension then  $g(x) \subseteq f(x), \forall x \in \mathbb{IR}^n$ .

#### **Basic properties of Interval Arithmetic**

Usually the input space of the model is limited for example to a d-dimensional box

 $\mathcal{S} = [\underline{x_1}, \overline{x_1}] \times [\underline{x_2}, \overline{x_2}] \times ... \times [\underline{x_d}, \overline{x_d}] \subseteq \mathbb{R}^d$ 

#### IA is both inclusion isotonic and an interval extension

Possible to improve its accuracy by discretizing  $\mathcal{S}$  and computing the union of discretized results.

Greedy approaches, branch-and-bound heuristics for more accurate output.

# **Example: Shape Constraints for Symbolic Regression**



W. Tucker - Validated Numerics for Pedestrians, ©2005 European Mathematical Society

Physics textbook equations from the Feynman Symbolic Regression Database (Udrescu and Tegmark 2020, https://doi.org/10.1126/sciadv.aay2631)

| Instance  | Expression  | Instance  | e Input space  | Constraints                  |
|-----------|---|-----------|--|------------------------------|
|           | $\left( \left( \theta \right)^2 \right)$  | I.6.20    | $(\sigma, \theta) \in [13]^2$                              | $([0\infty], 0, -1)$         |
| I.6.20    | $\exp\left(\frac{-\left(\frac{\pi}{\sigma}\right)}{2}\right)\frac{1}{\sqrt{2\pi}\pi}$       | I.9.18    | (x1, y1, z1, m1, m2, G, x2, y2, z2)                        | $([0\infty], -1, -1, -1, 1,$ |
|           | - ) \\2.16  |           | $\in [34]^3 \times [12]^6$                                 | 1, 1, 1, 1, 1)               |
| I.9.18    | $\frac{G m1 m2}{(x^2 - x_1)^2 + (x^2 - x_1)^2 + (x^2 - x_1)^2}$                             | I.30.5    | $(lambd, n, d) \in [15]^2 \times [25]$                     | $([0\infty], 1, -1, -1)$     |
| I.30.5    | $\operatorname{asin}\left(\frac{lambd}{nd}\right)$  | I.32.17   | $(\epsilon, c, Ef, r, \omega, \omega_0) \in [12]^5 \times$ | ([0∞], 1, 1, 1, 1,           |
| I.32.17   | $\frac{1}{2}\epsilon c E f^2 \frac{8\pi r^2}{3} \frac{\omega^4}{(\omega^2 - \omega_0^2)^2}$ |           | [53]   | 1, -1)                       |
| I.41.16   | $\frac{h\omega^3}{\pi^2c^2\left(\exp\left(\frac{h\omega}{\omega}\right)-1\right)}$          | I.41.16   | $(\omega, T, h, kb, c) \in [15]^5$                         | ([0∞], 0, 1, −1,             |
|           | $n c \left( \exp\left(\frac{kbT}{kbT}\right)^{-1} \right)$                                  |           |  | 1, -1)                       |
| I.48.20   | $\frac{mc}{\sqrt{1-p^2}}$   | I.48.20   | $(m, v, c) \in [15] \times [12] \times [320]$              | $([0\infty], 1, 1, 1)$       |
|           | $\sqrt{1-\frac{1}{c^2}}$  | II.35.21  | $(n_{rho}, mom, B, kb, T) \in [15]^5$                      | $([0\infty], 1, 1, 1,$       |
| II.35.21  | $n_{rho}mom \tanh\left(\frac{momB}{kbT}\right)$   |           |  | -1, -1)                      |
| III 9 52  | $\frac{p_d Eft}{\sin\left(\frac{(\omega-\omega_0)t}{\omega_0}\right)^2}$                    | III.9.52  | $(p_d, Ef, t, h, \omega, \omega_0)$                        | ([0∞], 1, 1, 0, −1,          |
|           | $h \frac{1}{\sqrt{2}}$  |           | $\in [13]^4 \times [15]^2$                                 | 0,0)                         |
| 111.10.19 | $mom\sqrt{Bx^2 + By^2 + Bz^2}$  | III.10.19 | $(mom, Bx, By, Bz) \in [15]^4$                             | $([0\infty], 1, 1, 1, 1)$    |

# Example: Shape Constraints

## Recent work by us (idea much older!)

- · G. Kronberger, C. Haider, M. Kommenda, B. Burlacu (FH OÖ / JRZ)
- F. O. de Franca (CMCC, HAL, Federal Univ. of ABC, Santo Andre, Brazil)
- **Kronberger et al.** Shape-constrained Symbolic Regression Improving Extrapolation with Prior Knowledge, Evolutionary Computation, Oct '21 https://arxiv.org/abs/2103.15624v1

# **Methods comparison**

- $\cdot\,$  test setting included varying levels of Gaussian noise over the training data
- comparison between evolutionary metaheuristics, polynomial regression, auto-sklearn (Feurer et al. 2015) with/without shape constraints

# Results

- · it's complicated! :)
- · shape constraints ensure conforming models, but not necessarily better generalization (test error)
- $\cdot \;$  however, shape-constrained models perform better on noisy data

#### Numerical simulations needed to investigate new materials and their properties.

#### Molecular Dynamics (MD) and Monte Carlo simulations

- Need a realistic model of inter-atomic interactions, represented usually by interaction potentials.
- · Only realistic interaction models are able to produce quantitatively reliable outputs

#### Modeling interatomic potentials

- Empirical / classical approach: very fast, simple analytical formulas, not very accurate
- Quantum: density functional theory (DFT) and others, very accurate, very slow  $O(N^3)$ ... $O(N^4)$
- Machine learning: use data generated by quantum methods, generate surrogate potentials

# **Potential Energy Surfaces (PES)**

Play a pivotal role in (large-scale) particle simulations

Describe the relation between atomic positions and their potential energy

### Very computationally expensive

ML methods recently emerged as a means to model PES at lower computational cost



source: https://en.wikipedia.org/wiki/Potential\_energy\_surface

# **Potential Energy Surfaces (PES)**



Learn the relationship between chemical structure and potential energy.

### **General requirements**

- · general applicability and absence of ad-hoc approximations (potentials that are transferable)
- · accuracy comparable to first-principles methods (including high-order many-body effects)
- $\cdot$  very high efficiency to enable large simulations
- $\cdot \;$  the ability to describe chemical reactions and arbitrary atomic configurations
- $\cdot \;$  the ability to be automatically constructed and systematically improved
- the ability to provide physical insight

Currently available potentials are far from satisfying all the needs

# **Machine-learning Potentials**



Mishin 2021, https://doi.org/10.1016/j.actamat.2021.116980

Traditional (left): based on physical understanding, simple functional form, highly approximate
ML-based (middle): regression based on structural parameters that capture the 3N-D configuration space
Physics-informed ML (right): local structural parameters mapped to parameters of a physics-based PES

# **Machine-learning Potentials**



#### Capturing and mapping structural parameters = big challenge

Musil et. al, *Physics-Inspired Structural Representations for Molecules and Materials*, Chem Rev. 2021 Aug 25, https://doi.org/10.1021/acs.chemrev.100021

# **Machine-learning Potentials**

# Many approaches

- neural networks (most popular)
- · polynomial fitting
- · moment tensor potentials (linear combination of polynomial basis functions)
- · Gaussian processes
- · spectral neighbour analysis
- $\cdot \,$  support vector machines
- interpolating moving least squares
- · symbolic regression

# **Ongoing issues**

- · Generality and transferability (often too system-specific)
- $\cdot$  Conceptual problems related to incorporating rotational, translational and permutational invariance
- · Model complexity and explainability
- · Training data requirements

# "Black-box" methods

- $\cdot\,\,$  almost zero capability of including physical information into the functional forms
- $\cdot \;$  must exclusively rely on the physics-inspired features considered in atomic descriptors
- $\cdot \,$  increased mathematical and computational complexity of resulting interaction models
- · requires large amounts of training data

# "White-box" methods

- emerging as an alternative for ML-based potentials (https://doi.org/10.1063/1.5126336)
- $\cdot\,\,$  provides researchers with analytic equations, which expectably would have better interpretability
- $\cdot \;$  more amenable to the integration of physical knowledge
- $\cdot \;$  not requiring a priori knowledge or predefined functional forms
- $\cdot~$  explicit representation that can be interpreted by domain experts
- $\cdot \,$  smaller number of parameters and better efficiency

# Training data

- · training data available from DFT simulations
- $\cdot\,\,$  data consists of simulation snapshots with atomic positions and energy
- usually in special formats (VASP, POSCAR)
- $\cdot~$  each "data row" is a list of coordinates describing the atomic clusters and an energy value

# Symbolic regression approach

- $\cdot \;$  pairwise atomic distances computed from Cartesian coordinates
- · distances potentially filtered by inner and outer radius parameters
- $\cdot$  functional transformation of the input (distances, forces) followed by  $\sum$

# **Symbolic Regression Potentials**



Hernandez et al., Fast, accurate, and transferable many-body interatomic potentials by symbolic regression, 2019, https://doi.org/10.1038/s41524-019-0249-1

https://gitlab.com/muellergroup/poet

#### Machine learning, critical part of the 4th paradigm of science.

Scientific-ML is an emerging field focusing on applications in computational science. Explainability and interpretability become increasingly important properties of ML models. Existing methods do not quite meet the needs of scientific users. Models should respect or incorporate physical laws. Several hybrid approaches are emerging with the goal of incorporating physical knowledge. Often, ML methods require non-trivial, task-specific modications

SciML methods typically need to run in performance-critical environments.