Symbolic Regression with Interaction-Transformation

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Topics

1. Goals
2. Interaction-Transformation
3. Experiments
4. Conclusions

Goals

Find the function

Find a function f that minimizes the approximation error:

$$\begin{aligned} \underset{\hat{f}(\mathbf{x})}{\text{minimize}} \quad & \|\epsilon\|^2 \\ \text{subject to} \quad & \hat{f}(\mathbf{x}) = f(\mathbf{x}) + \epsilon. \end{aligned}$$

Simple is better

- Ideally this function should be as simple as possible.
- Conflict of interests:
  - minimize approximation (use universal approximators)
  - maximize simplicity (walk away from generic approximators)

The good...

The Linear Regression:

$$\hat{f}(\mathbf{x}, \mathbf{w}) = \mathbf{w} \cdot \mathbf{x}.$$

- Very simple (and yet useful) model.
- Clear interpretation
- The variables may be non-linear transformation of the original variables.

... the bad...

The mean:

$$\hat{f} = \bar{f}(x)$$

- The average can lie!
- It's just for the sake of the pun

. . . the Deep Learning

A deep chaining of non-linear transformations that just works!

fig

- Universal approximation
- Alien mathematical expression

The best?

Despite its success with error minimization, it raises some questions:

- What does the answer mean?
- What if the data is wrong?

Symbolic Regression

Searches for a function form and the correct parameters.

Hopefully a simple function

Symbolic Regression

Disclaimer: I have large experience with evolutionary algorithms, but limited with Symbolic Regression. I have start studying that last year.

Symbolic Regression

This was my first experience with GP:

$$
\begin{aligned}
6.379515826309025e - 3 + -0.00 * id(x_1^{-}4.0 * x_2^{3}.0 * x_3^{1}.0) \\
+ - 0.00 * id(x_1^{-}4.0 * x_2^{3}.0 * x_3^{2}.0) - 0.01 * id(x_1^{-}4.0 * x_2^{3}.0 * x_3^{3}.0) \\
-0.02 * id(x_1^{-}4.0 * x_2^{3}.0 * x_3^{4}.0) + 0.01 * cos(x_1^{-}3.0 * x_2^{-}1.0) + \\
0.01 * cos(x_1^{-}3.0) + 0.01 * cos(x_1^{-}3.0 * x_3^{1}.0) + 0.01 * cos(x_1^{-}3.0 * x_2^{1}.0) \\
+0.01 * cos(x_1^{-}2.0 * x_2^{-}2.0) - 0.06 * log(x_1^{-}2.0 * x_2^{-}2.0) \\
+0.01 * cos(x_1^{-}2.0 * x_2^{-}1.0) + 0.01 * cos(x_1^{-}2.0 * x_2^{-}1.0 * x_3^{1}.0) \\
+0.01 * cos(x_1^{-}2.0) + 0.01 * cos(x_1^{-}2.0 * x_3^{1}.0) \\
+0.01 * cos(x_1^{-}2.0 * x_3^{2}.0) + 0.01 * cos(x_1^{-}2.0 * x_2^{1}.0) \\
+0.01 * cos(x_1^{-}2.0 * x_2^{1}.0 * x_3^{1}.0) + -0.00 * id(x_1^{-}2.0 * x_2^{2}.0) \\
-0.00 * sin(x_1^{-}2.0 * x_2^{2}.0) + 0.01 * cos(x_1^{-}2.0 * x_2^{2}.0) + \ldots
\end{aligned}
$$

Why?

- Infinite search space
- Redundancy
- Rugged

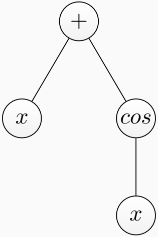
Redundancy

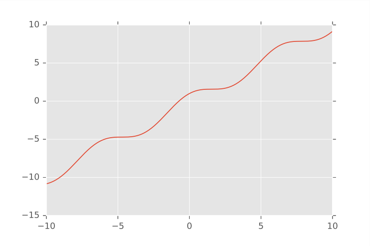
$$f(x) = \frac{x^3}{6} + \frac{x^5}{120} + \frac{x^7}{5040}$$

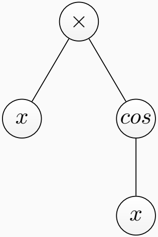
$$f(x) = \frac{16x(\pi - x)}{5\pi^2 - 4x(\pi - x)}$$

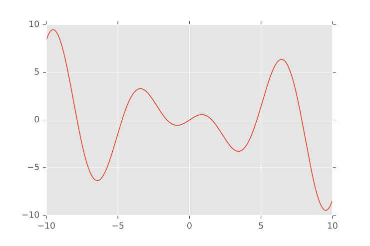
$$\mathbf{f}(\mathbf{x}) = \sin(\mathbf{x}).$$

Rugged space









What I wanted

- A few additive terms (linear regression of transformed variables)
- Each term with as an interaction of a couple of variables
- Maximum of one non-linear function applied to every interaction (no chainings)

Interaction-Transformation

Interaction-Transformation

Constrains the search space to what I want: a **linear combination** of the application of different **transformation functions** on **interactions** of the original variables.

Interaction-Transformation

Essentially, this pattern:

$$\hat{f}(x) = \sum_i w_i \cdot t_i(p_i(x))$$
$$p_i(x) = \prod_{j=1}^{d} x_j^{k_j}$$
$$t_i = \{id, \sin, \cos, \tan, \sqrt{}, \log, \ldots\}$$

Interaction-Transformation

Valid expressions:

- $5.1 \cdot x_1 + 0.2 \cdot x_2$
- $3.5 \sin\left(x_1^2 \cdot x_2\right) + 5 \log\left(x_2^3 / x_1\right)$

Interaction-Transformation

Invalid expressions:

- $\tanh(\tanh(\tanh(w \cdot x)))$
- $\sin(x_1^2 + x_2)/x_3$

Interaction-Transformation

We can control the complexity of the expression by limiting the number of additive terms and the number of interactions:

$$\hat{f}(x) = \sum_{i=1}^{k} w_i \cdot t_i(p_i(x))$$

$$p_i(x) = \prod_{j=1}^{d} x_j^{k_j}$$

$$s.t. |\{k_j \mid k_j \neq 0\}| \leq n$$

Interaction-Transformation

Describing as an Algebraic Data Type can help us generalize to other tasks:

```
IT x        = 0 | Weight (Term x) `add` (IT x)

Term x      = Trans (Inter x)
Trans       = a -> a

Inter x:xs = 1 | x s `mul` Inter xs
```

The meaning of `add` and `mul` can lead us to boolean expressions, decision trees, program synthesis.

SymTree

Simple search heuristic:

```
symtree x leaves | stop      = best leaves
                 | otherwise = symtree x leaves'
  where
    leaves' = [expand leaf | leaf <- leaves]

symtree x [linearRegression x]
```

SymTree

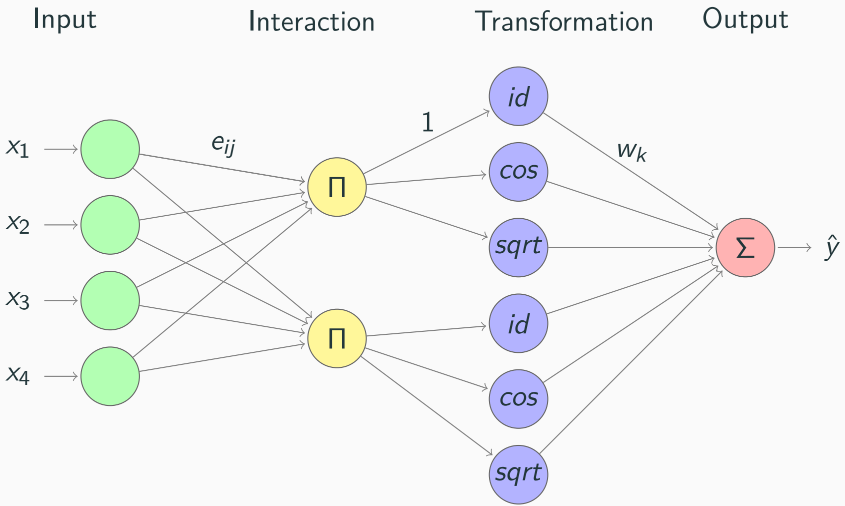
```
expand leaf = expand' leaf terms
  where terms = interaction leaf U transformation leaf

expand' leaf terms = node : expand' leaf leftover
  where (node, leftover) = greedySearch leaf terms
```

IT-ELM

Interaction-Transformation Extreme Learning Machine, it generates lots of random interactions, enumerates the transformations for each interaction and then adjust the weight of the terms using l_0 or l_1 regularization.

IT-ELM


Input
Interaction
Transformation
Output
x_1
x_2
x_3
x_4
e_{ij}
Π
Π
1
id
cos
$sqrt$
id
cos
$sqrt$
w_k
Σ
$\hat{y}$

Experiments

Data sets

Data set	Features	5-Fold / Train-Test
Airfoil	5	5-Fold
Concrete	8	5-Fold
CPU	7	5-Fold
energyCooling	8	5-Fold
energyHeating	8	5-Fold
TowerData	25	5-Fold
wineRed	11	5-Fold
wineWhite	11	5-Fold
yacht	6	5-Fold
Chemical-I	57	Train-Test
F05128-f1	3	Train-Test
F05128-f2	3	Train-Test
Tower	25	Train-Test

Methods

For the sets with folds:

- Each algorithm was run 6 times per fold and the median of the RMSE of the test set is reported
- SymTree was run 1 time per fold (deterministic)

For the sets with train-test split:

- Each algorithm was run 10 times and the median of the RMSE for the test set is reported
- SymTree was run 1 time per data set

Results

For a complete table:

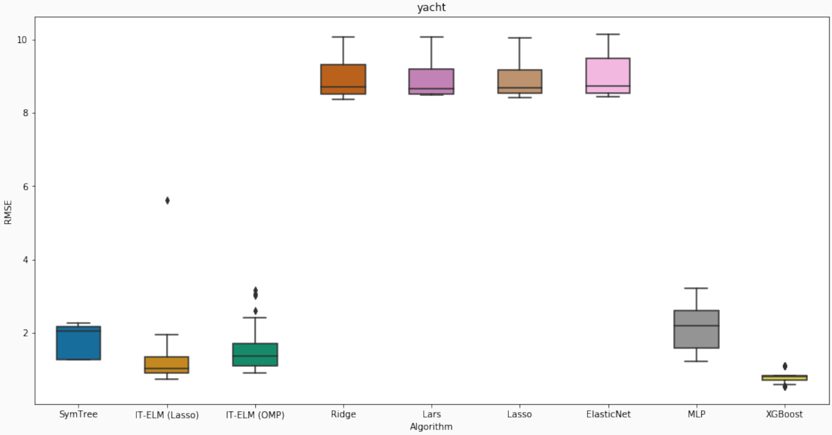
Binder

Cell –> Run All

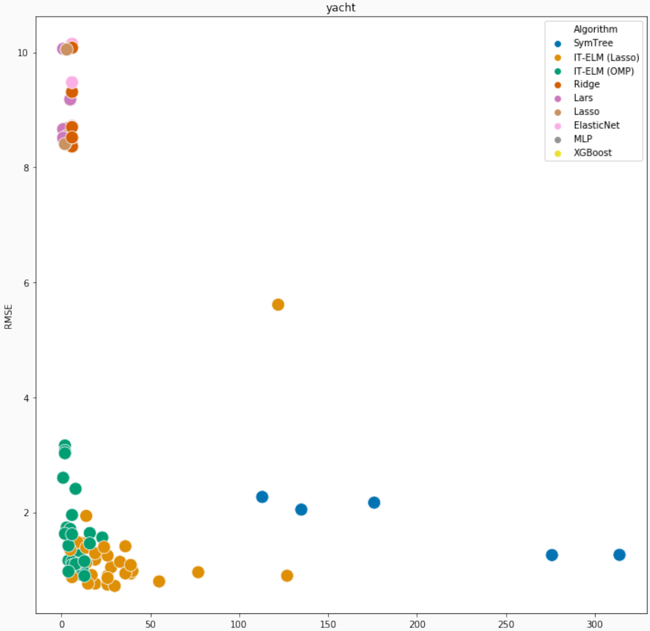
Results

Algorithm	Rank
XGBoost	2
SymTree	3.3
IT-ELM (Lasso)	3.53846
IT-ELM (OMP)	3.84615
MLP	5
Ridge	5.69231
Lars	5.76923
Lasso	6.76923
ElasticNet	7.76923

Results

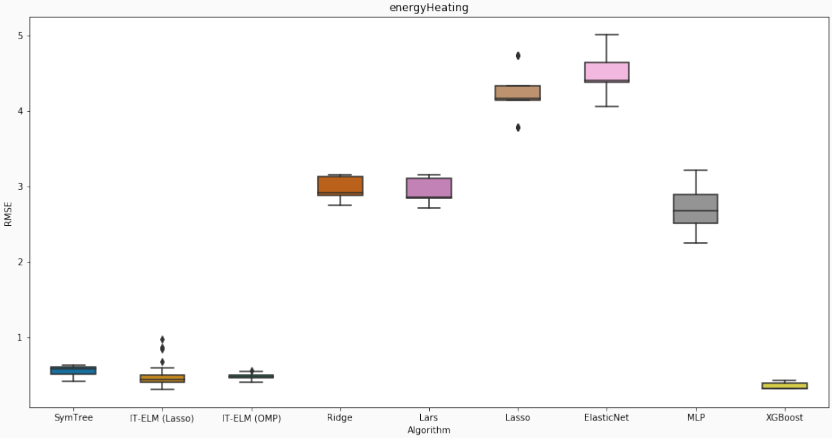

yacht
10
8
6
4
2
RMSE
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost
Algorithm

Results

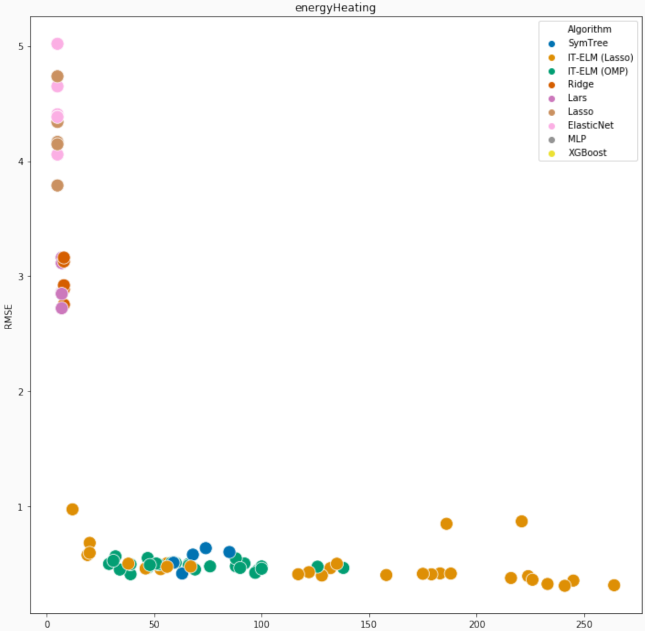


yacht
Algorithm
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost
RMSE
10
8
6
4
2
0
50
100
150
200
250
300

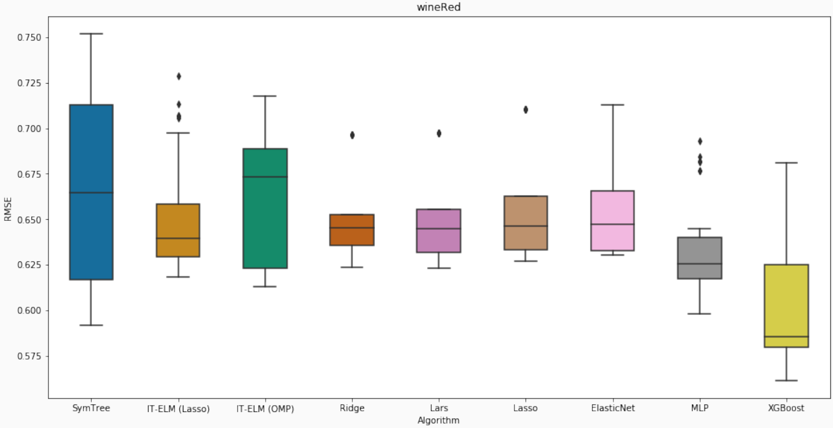
Results


energyHeating
RMSE
5
4
3
2
1
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost
Algorithm

Results

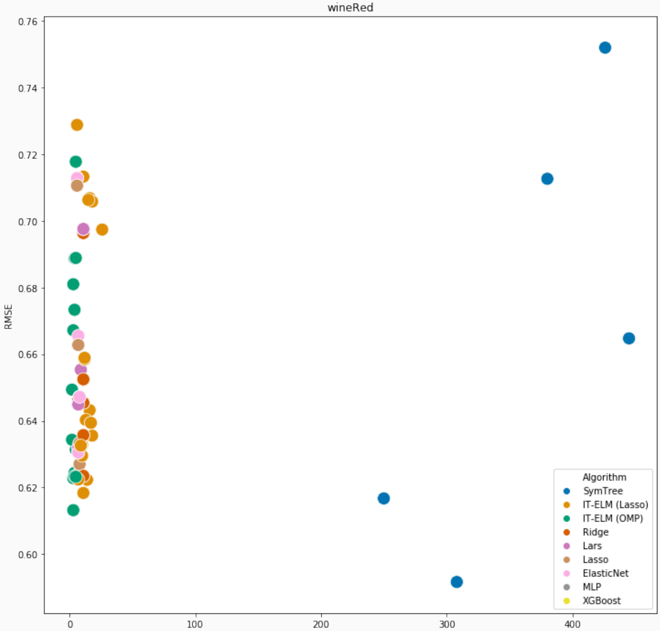

energyHeating
RMSE
5
4
3
2
1
0
50
100
150
200
250
Algorithm
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost

Results



wineRed
0.750
0.725
0.700
0.675
0.650
0.625
0.600
0.575
RMSE
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost
Algorithm

Results


wineRed
RMSE
0.76
0.74
0.72
0.70
0.68
0.66
0.64
0.62
0.60
0
100
200
300
400
Algorithm
SymTree
IT-ELM (Lasso)
IT-ELM (OMP)
Ridge
Lars
Lasso
ElasticNet
MLP
XGBoost

Sample equations

F05128-f1:

$$
\begin{aligned}
-8.3 \times 10^{-3} \log\left(p^2 t^2 v + 1\right) \\
+1 \times 10^{-3} \sin\left(t v^2\right) \\
+3.1 \times 10^{-3} \cos\left(p\right) \\
+8.7 \times 10^{-3} \cos\left(p^2 t v^2\right) \\
-4.06 \cdot 10^{-5} \tan\left(p^2 t^2 v^2\right)
\end{aligned}
$$

Sample equations

CPU:

$$4.9 \times 10^{-4} \cdot \mathit{maxMem}\sqrt{\mathit{repPerf}}$$

Conclusions

Resumo

A representação Interação-Transformação permite definir um espaço de busca de expressões matemáticas simples mas capaz de aproximar diversas bases de dados, sendo competitivo com algoritmos do estado-da-arte de regressão.

Além disso, o algoritmo SymTree é capaz de encontrar uma boa expressão IT com poucas iterações, sendo um algoritmo simples e computacionalmente leve.

Future research

Muitas possibilidades de estudos futuros:

- Generalizar a representação como uma tipo de dado algébrico
- Utilizar essa representação em outros contextos
- Aumentar o espaço de busca permitindo outras expressões simples ainda não compreendidas
- Criar novos algoritmos de busca para esse espaço de busca
- Muitos outros. . .

Try it!

You can try a lightweight version of SymTree at:

https://galdeia.github.io/

It works even on midrange Smartphones!