Symbolic Regression or:

How I Learned to Worry About my Machine Learning Models

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First there was data...

Huge amount of data can be collected nowadays due to:

- Increase of available storage space
- New techniques for data collection (not necessarily computer related)
- New ways to process large quantity of raw data
... and then the models were created

With such humongous quantity of data, we had to mine some answers from them!

So we’ve created mathematical models that can answer things like:

“This sample belongs to this category, but this does not!”

“These set of samples defines a group”

“Given these variables, the expected response is $x$”
The Good, ...

Linear Regression:

\[ \hat{y} = w \times x + b \]

Clear interpretation: for every \( x_i \), we (de)increase the total value by \( w_i \).

Surprisingly good enough to fit many real world samples

But if the samples present a nonlinear relationship...
... the Bad, ...

\[ \hat{y} = \text{mean}(y) \quad -- \quad \text{regression} \]

\[ \hat{y} = \text{mode}(y) \quad -- \quad \text{classification} \]

Incredibly simple and incredibly low accuracy!
... and the Deep Learning

\[ h_1 = \{ \tanh (w_1 \cdot x) \mid w_1 \leftarrow W_1 \} \]

\[ h_2 = \{ \tanh (w_2 \cdot h_1) \mid w_2 \leftarrow W_2 \} \]

\[ h_3 = \{ \tanh (w_3 \cdot h_2) \mid w_3 \leftarrow W_3 \} \]

\[ \hat{y} = \tanh(w_4 \cdot h_3) \]

It gets the job done! It can fit anything!

But what does the answer mean? Is the data right?
The answer to the life, the universe and everything

42
The answer to the life, the universe and everything

42

BUT WHAT IS THE QUESTION?
Current state of Data Science in a picture

https://www.xkcd.com/1838/
But isn’t science about learning how things work rather getting a numerical result?
A debt situation

A Machine Learning model can help answer:

- This client will pay his debt?
- How much will he owe?
A debt situation

This can support the decision process to whether the bank will lend money or not! And how much!

https://pixabay.com/pt/euro-dinheiro-pagar-empr%C3%A9stimos-427528/
A debt situation

Wouldn’t it be more interesting to understand why a given profile won’t pay back? Is it something the bank can fix? If it can, more money!
And what if the data is wrong?
And thus the answer is wrong?
Judge Dredd

Can a Machine Learning model estimate recurrence of criminal? Can also estimate the number of jail time a judge should give?
The model will be fitted to the current data, the current data will include collected statistics regarding past crimes...

... and judges mistakes, social prejudice, and the Machine will learn that.
The meaning of life

Sometimes the interesting part of the study is to discover what equations govern a given natural process.
Symbolic Regression

Regression model that searches the space of mathematical expressions for one (or more) that:

- Fits the sampled data
- Is simple!
Symbolic Regression

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The Simple Life of a Mathematical Model

How can we measure the simplicity of a Mathematical Equation?

There is no formalization yet! But we all agree that:

- The smaller the better
- Less nonlinearity is simpler
Genetic Programming

Evolving computer programs described as expressions:

\[ \lambda x \rightarrow (3 \times x) + \sin(x) \]
Genetic Programming

Simple steps:

- Combine expressions
- Change expressions
- Select expressions
- Repeat
Combine Expressions

\[ (+ \text{ (3 \times x) + (c \times x))} + (- \text{ (s \times x) - (c \times x)}) \]
Change Expressions

3 * x + x → 3 - x + x
Select Expressions

Sample the expressions with probability proportional to the simplicity and inversely proportional to the fitting error.

Expected to find a good expression sometime in the near future....
The near future

This algorithm usually take hours to fit simple data with just a few variables...days for complex data...and we usually end up with:

\[ 6.379515826309025 \times 10^{-3} + -0.00^{\text{id}}(x_1^{-4.0} \times x_2^{3.0} \times x_3^{1.0}) + -0.00^{\text{id}}(x_1^{-4.0} \times x_2^{3.0} \times x_3^{2.0}) + -0.01^{\text{id}}(x_1^{-4.0} \times x_2^{3.0} \times x_3^{3.0}) + -0.02^{\text{id}}(x_1^{-4.0} \times x_2^{3.0} \times x_3^{4.0}) + 0.01^{\cos}(x_1^{-3.0} \times x_2^{1.0}) + 0.01^{\cos}(x_1^{-3.0} \times x_3^{1.0}) + 0.01^{\cos}(x_1^{-3.0} \times x_2^{1.0}) + 0.01^{\cos}(x_1^{-2.0} \times x_2^{1.0}) + 0.01^{\cos}(x_1^{-2.0} \times x_2^{2.0}) + 0.01^{\cos}(x_1^{-2.0} \times x_2^{2.0} \times x_3^{1.0}) + 0.00^{\tan}(x_1^{-2.0} \times x_2^{2.0} \times x_3^{1.0}) + \ldots \]
Why?
How to improve it?

Many solutions were devised:

- Array-based representation
- Semantic operators that minimize the observable change
- Search space restriction
How to improve it?

Many solutions were devised:

- Array-based representation
- Semantic operators that minimize the observable change
- Search space restriction through representation
Interaction-Transformation

\[ \hat{y} = \sum_{i} w_i \cdot f_i(P_i(x)) \]

\[ P(x) = \prod_{j} x_{j}^{p_{j}} \]
Data Structure: Expression

Poly = [Int] -- coefficients of a polynomial transformation

Term = (Poly, λ) -- the polynomial applied to a function

Expression = {Term} -- a set of terms
What it can and what cannot

\[ f(x) = \log(x^2) + 5\sqrt{|x|} \]

\[ f(x) = \log(x^2 + x) + 5\sqrt{|x|} \] ❌

\[ f(x) = \sin(\cos(\tan(x^2))) \] ❌

\[ f(x) = \log(x^2) + 5\sqrt{|x|} \] ✓
Simple algorithm

Start with linear expression

Repeat:

Generate all interactions

Generate all transformations

Incrementally add terms as long as they reduce mse

Weights \( w \) are adjusted as a linear regression.
Interaction

Poly1 = [1, 1] -- x1 . x2
Poly2 = [0, 2] -- x2^2

Poly1 + Poly2 = [1, 3] -- x1 . x2^3
Poly1 - Poly2 = [1, -1] -- x1 / x2
Transformation

(Poly1, id) → [(Poly1, sin), (Poly1, cos), (Poly1, tan), ... ]
Marathon Time Prediction

Data: recorded the training data of marathoners from Prague.

Km4weeks: total Kms run in the last 4 weeks
Sp4weeks: avg. speed in the last 4 weeks
Marathon time: target variable
Results

**Multi Layer Perceptron:**
- tanh activation
- $50 \times 50 \times 10$ hidden neurons
- MSE: 0.030

**Symbolic Regression:**
- $\hat{y} = 5.14 - 0.24 \sin(\text{speed}) - 0.12 \cdot \text{speed} - 0.08 \cdot \text{km/speed} - 0.07 \cdot \cos(\text{km}) - 0.02 \tan(\text{km} \cdot \text{speed})$
- MSE: 0.029

**Linear Regression:**
- $\hat{y} = 5.76 - 0.17 \cdot \text{speed}$
- MSE: 0.051
Results

Canonical Genetic Programming:

MSE: 0.038
(after half an hour)
Results

Symbolic Regression also found a solution with $\text{MSE} = 0.02$, but with 20 terms (still much simpler than Neural Network).
Some insights

Evidently, \( \text{km} / \text{speed} \) (fourth term) gives us the expected time!

The first part of the expression. Within the speed range, gives us:
Some insights

This might indicate that:

- The best athletes run faster (duh).
- A “middle class” of athletes keep a lower speed, probably to keep it constant.
- The “lower class” tries to increase their speed at the beginning, raising the average speed, but with a penalty by the final half of the marathon.
Final Remarks

Symbolic Regression can be (in the near future) a very competitive approach to advanced model fitting.

The main advantage is the expressiveness of the model that can help us detect biases in the data and understand what the model is doing.
Final Remarks

So far, there is no SR algorithm capable of dealing with high dimensions while competing with Neural Network regarding minimization of error and speed.