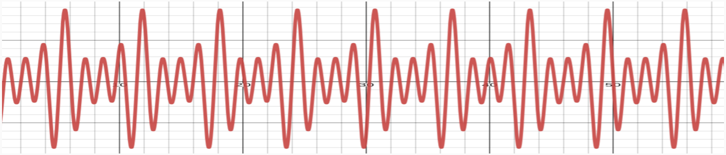
Symbolic Regression



Prof. Fabrício Olivetti de França

Federal University of ABC

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UFABC

Symbolic Regression

Let's keep things linear

Let us frame the linear regression a little bit differently:

$$f(x;\beta) = \beta\phi(x)$$

Now, $\phi(x) \in \mathbb{R}^d \to \mathbb{R}^{d'}$ is a function that **transforms** the original variable space to a different space.

Let's keep things linear

In our previous lectures we have used $\phi(x) = [1; x]$ effectively adding a column of 1s in our dataset.

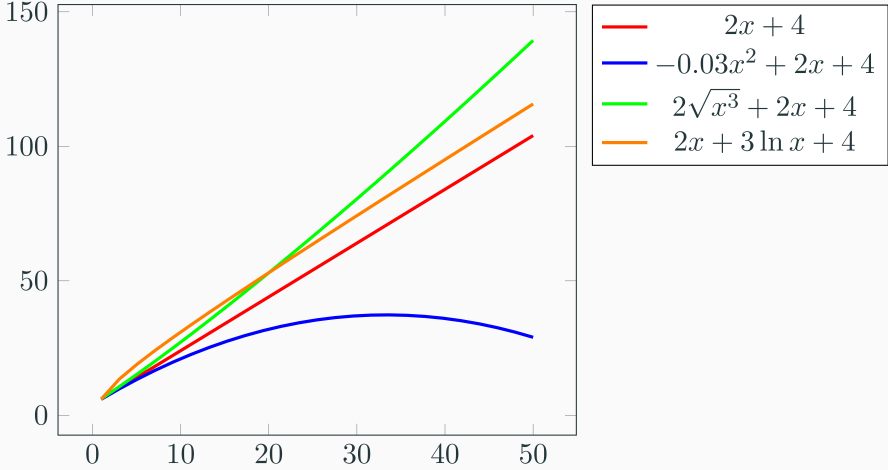
But we are not limited to this simple transformation.

For example, we can have:

$$\phi(x) = [1; x]$$
$$\phi(x) = [1; x; x^2]$$
$$\phi(x) = [1; x; \sqrt{x}]$$
$$\phi(x) = [1; x; \log x; x^2]$$

Let's keep things linear

This will add some nonlinearity to our model without losing the benefit of fitting a linear model.



Let's keep things linear

With this transformation, we now have a hypothesis space composed of all possible transformations:

$$\mathcal{F}_\phi = \left\{ f(\phi(x);\beta) = \beta\phi(x) \mid \beta \in \mathbb{R}^d \right\}$$

$$\mathcal{F} = \left\{ f(\phi(x);\beta) = \beta\phi(x) \mid \phi \in \Phi, \beta \in \mathbb{R}^d_\phi \right\}$$

Let's keep things linear

In the previous example, we were working with one-dimensional predictor. If we have multidimensional x, we can apply the transformations to each one of the predictors or to a subset.

$$\phi(x) = [1; x]$$
$$\phi(x) = [1; x; x_1^2]$$
$$\phi(x) = [1; x; \sqrt{x_1}; x_2^2]$$

Notice that a transformation applied to every predictor will add another d predictors.

Interactions

When making quadratic, cubic, and other polynomial transformations, we often consider the interaction between variables. So, for $d = 2$:

$$\begin{aligned}\phi(x) &= [1; x; x^2] \\ &= [1; x; x_1^2; x_2^2; x_1 x_2]\end{aligned}$$

Notice that by doing so we will have an additional $O(d^2)$ predictors for quadratic predictors and $O(d^3)$ additional predictors for cubic, etc.

Interactions

If we have the interation between two predictors x_1, x_2 modeled as:

$$f(x;\theta) = \beta_1 + \beta_2 x_1 + \beta_3 x_2 + \beta_4 x_1 x_2$$

The effect of x_1 for a fixed value of x_2 would be $\beta_2 + \beta_4 x_2$.

Interactions

The interaction compensates for the influence that one predictor may have for another.

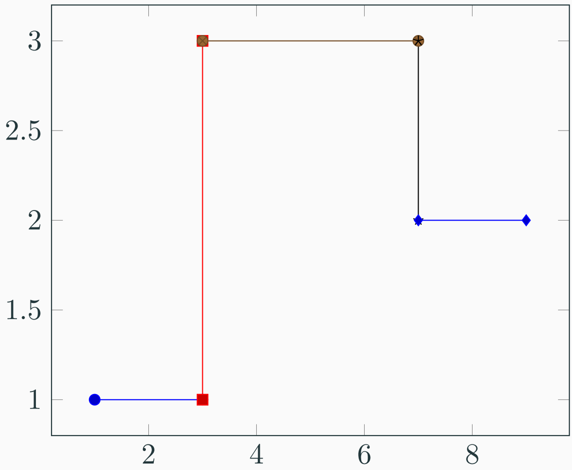
For example, the effect of a treatment to a person may depend of the age of the person

Let's keep things linear

Another feature transformation is the **piecewise predictors**. These are binary predictors that has a value of 1 if x_i is between a certain range, and 0 otherwise.

$$\phi(x) = [\mathbf{1}[l_1 < x \leq u_1]; \mathbf{1}[l_2 < x \leq u_3], \ldots, \mathbf{1}[l_i < x \leq u_i]]$$

Piecewise Predictors



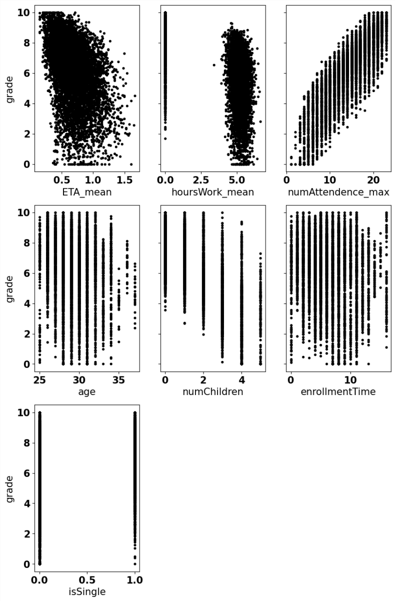
Let’s try some transformations

```
df = pd.read_csv("grade.csv")
xcols = ['ETA_mean', 'hoursWork_mean',
     'numAttendence_max', 'age', 'numChildren',
     'enrollmentTime', 'isSingle']

x, y = df[xcols].values, df.grade.values
x = np.concatenate((np.ones((x.shape[0],1)),x),
           axis=1)
```

Let’s try some transformations

```
_,axs = plt.subplots(3,3, figsize=(10,16), sharey=True)
ix = 0
for i in range(2):
    for j in range(3):
        axs[i,j].plot(df[xcols[ix]].values, df.grade.values,
            '.', color='black')
        axs[i,j].set_xlabel(xcols[ix])
        if j==0:
            axs[i,j].set_ylabel('grade')
        ix = ix+1
axs[2,0].plot(df[xcols[ix]].values, df.grade.values, '.',
          color='black')
```

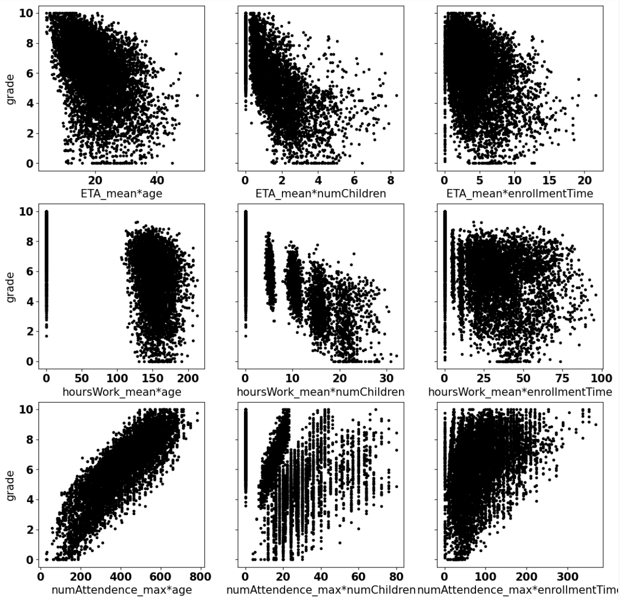
Let’s try some transformations



Let's try some transformations

```
{.python frame=lines framerule=2pt linenos=true
fontsize=\footnotesize
baselinestretch=0.8}t.subplots(3,3,
figsize=(14,14), sharey=True) ix = 0 for i, c1 in
enumerate(xcols[:3]):   for j, c2 in
enumerate(xcols[3:6]):
axs[i,j].plot(df[c1].values*df[c2].values,
df.grade.values,            '.', color='black')
axs[i,j].set_xlabel(f"{c1}*{c2}")
```

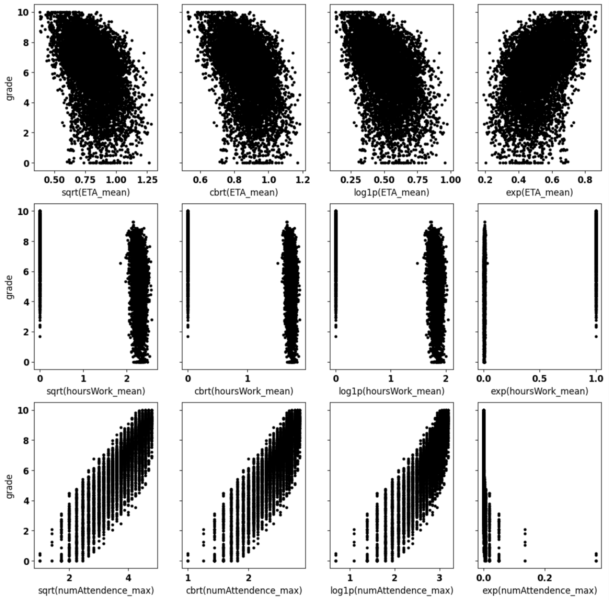
Let's try some transformations



Let’s try some transformations

```
_,axs = plt.subplots(3,4,
   figsize=(14,14), sharey=True)
ix = 0
for i, c1 in enumerate(xcols[:3]):
  for j, (fname,h) in enumerate([('sqrt',np.sqrt),
       ('cbrt', np.cbrt), ('log1p', np.log1p),
       ('exp', lambda x: np.exp(-x))]):
    axs[i,j].plot(h(df[c1].values), df.grade.values,
       '.', color='black')
    axs[i,j].set_xlabel(f"{fname}({c1})")
```

Let’s try some transformations



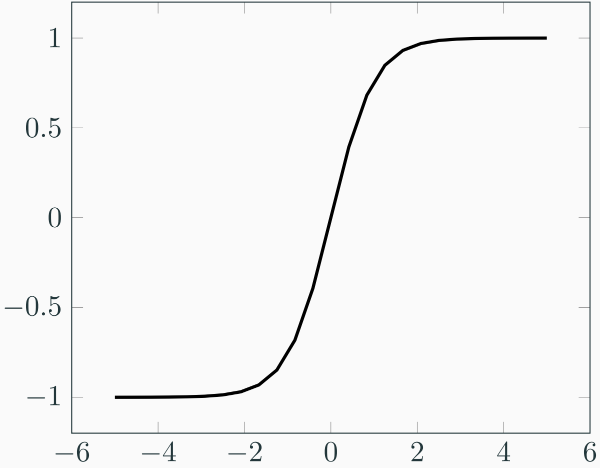
Neural Networks

Neural Networks, specifically feed-forward networks[1], creates a regression model as a chaining of nonlinear functions (called activation) applied to the predictors.

$$
\begin{aligned}
f(x;\theta) = {} & \theta_{13} \tanh(\theta_5 \tanh(\theta_1 x_1 + \theta_2 x_2) + \theta_6 \tan(\theta_3 x_1 + \theta_4 x_2)) \\
& + \theta_{14} \tanh(\theta_{11} \tanh(\theta_7 x_1 + \theta_8 x_2) + \theta_{12} \tan(\theta_9 x_1 + \theta_{10} x_2))
\end{aligned}
$$

[1] Bebis, George, and Michael Georgiopoulos. “Feed-forward neural networks.” Ieee Potentials 13.4 (1994): 27-31.

The $\tanh$ function has the following shape:



If we add a chain of overparameterized $\tanh$, like the previous example, we can shape the function to fit our data:

This overparameterization reduces the Interpretability capabilities of our model. The effect of any of our predictors is unclear.

Gradient Boosting

Another regression model with high accuracy for nonlinear relationship is the **gradient boosting**[2]. The main idea is to iteratively train **weak** models with a modified objective-function at every iteration.

This modified objective-function tries to minimize the current prediction error.

[2] Friedman, Jerome H. "Greedy function approximation: a gradient boosting machine." Annals of statistics (2001): 1189-1232.

Gradient Boosting

This technique starts with a baseline model (F_0 = $\mathcal{E}[y]$) and iteratively creates a new model based on the previous:

$$F_0(x) = \underset{c}{\operatorname{argmin}}\, \mathcal{L}(y; c)$$

$$F_m(x) = F_{m-1}(x) + \underset{h_m \in \mathcal{H}}{\operatorname{argmin}}\, \mathcal{L}(y; F_{m-1}(x) + h_m(x))(x)$$

Gradient Boosting

Since finding h_m that minimizes the objective is infeasible. Instead we specify a base weak learner (i.e., regression tree, linear model) and minimizes the gradient of the current loss function:

$$F_m(x) = F_{m-1}(x) - \gamma \nabla \mathcal{L}(y; F_{m-1}(x))$$

Gradient Boosting

Similar to Neural Networks, Gradient Boosting sacrifices the interpretability to achieve a better accuracy.

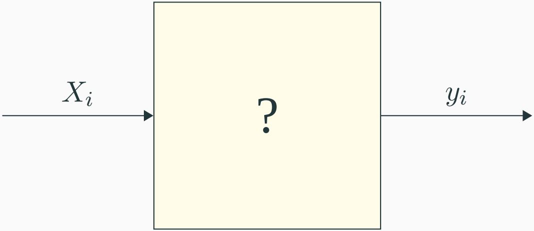
Even though there are some techniques that can measure the **feature importance** for these models, the interpretation is not as straightforward as a linear model (or even a hand-crafted nonlinear model).

These are often called **opaque model** (as oposed to a **transparent model**).

Transparent x Opaque models

Depending on what we want, we have **transparent** and **opaque** models:

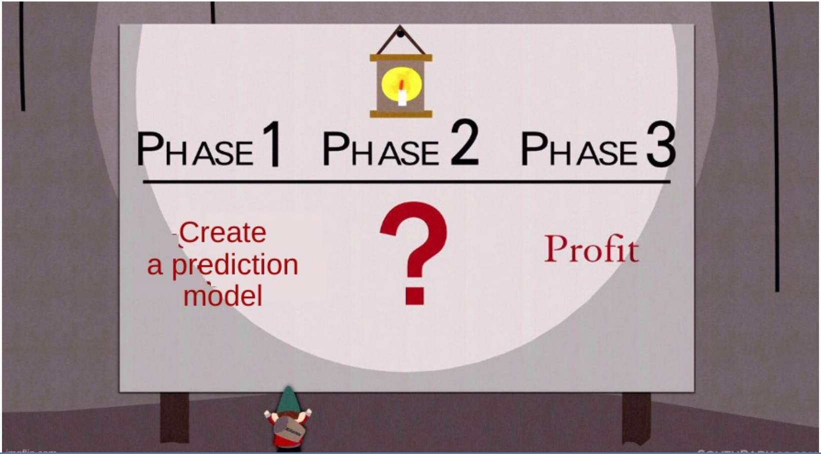
- It is possible to inspect the decision process and the behavior of **transparent** models
- In **opaque** models, this is obscured and external tools are needed to understand its behavior



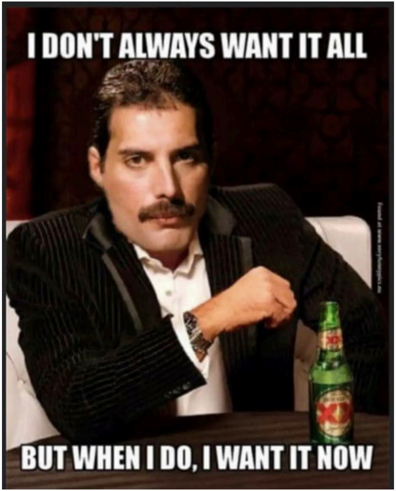
All about prediction

Opaque models (Deep Learning, SVM, Kernel Regression):

- Often associated with a higher predictive power (but not always true).
- If our only concern is prediction, they may be enough.



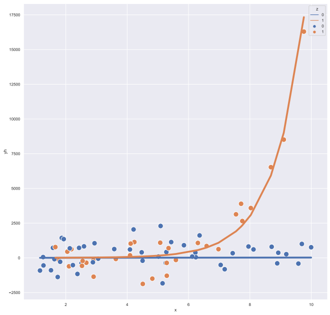
Transparent x Opaque models



If the objective is to study associations, an opaque model may create a barrier to understand the strength of association of a predictor to the outcome.

Symbolic Regression searches for a function form together with the numerical coefficients that best fits the outcome.

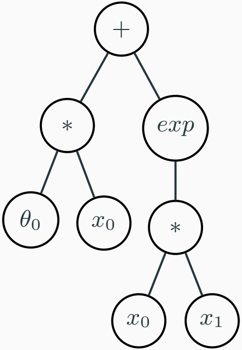
$$f(x, \theta) = \theta_0 x_0 + e^{x_0 x_1}$$



Symbolic Regression

- Genetic Programming is the most common algorithm to search for the expression
- Represents the solution as an expression tree.

$$f(x, \theta) = \theta_0 x_0 + e^{x_0 x_1}$$



Genetic Programming

A very simple search meta-heuristic:

```
gp gens nPop =
  p = initialPopulation nPop
  until (convergence p)
      parents   = select p
      children  = recombine parents
      children' = perturb children
      p         = reproduce p children'
```

Two NP-Hard problems[3]:

- Search for the correct function form $f(x, \theta)$.
- Find the optimal coefficients θ^*.

[3] Virgolin, Marco, and Solon P. Pissis. "Symbolic Regression is NP-hard." arXiv preprint arXiv:2207.01018 (2022).

If we fail into one of them we may discard promising solutions.

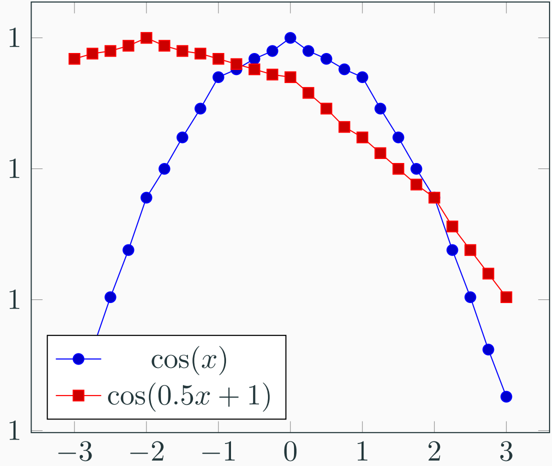


Figure 1: The function $\cos(\theta_1 x + \theta_2)$ may behave differently depending on the choice of θ

Symbolic Regression - GP

Pros:

- It can find the generating function of the studied phenomena.
- Automatically search for interactions, non-linearity and feature selection.

Cons:

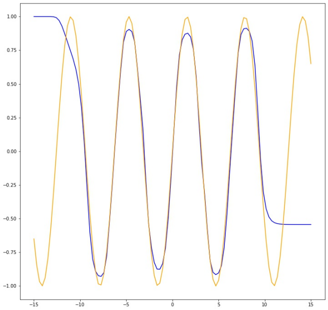
- It can find an obscure function that also fits the studied phenomena.
- The search space can be difficult to navigate.
- Not gradient-based search, it can be slower than opaque models.

Is it worth it?

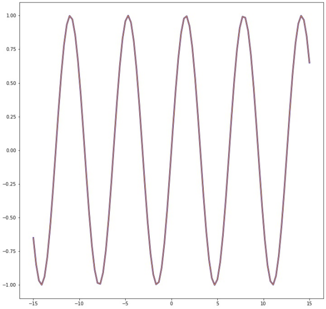
As we can define the primitives, we can choose how *expressive* the model will be.
Consider the $\sin(x)$ function. GP can find the correct model if it contains this function in its primitives.

Is it worth it?

3 layers neural network with sigmoid activation trained on the interval $x \in [-10, 10]$, took 300 seconds and returned this model:



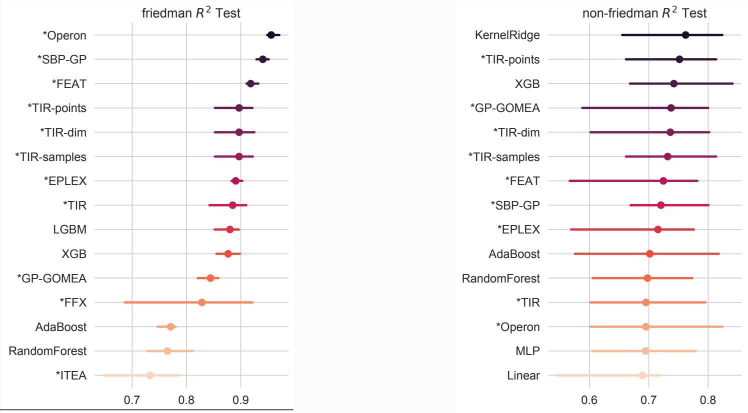
TIR Symbolic Regression model, took 10 seconds and returned this model:



Current State of SR

Is SR competitive?

Benchmark[4] of 22 regression algorithms using 122 benchmark problems, 15 of them are SR algorithms.



[4] La Cava, William, et al. “Contemporary Symbolic Regression Methods and their Relative Performance.” Thirty-fifth Conference on Neural Information Processing Systems Datasets and Benchmarks Track (Round 1). 2021.

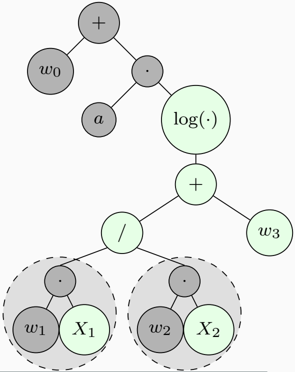
Different approaches

- Many different ideas to improve current results.
- Using nonlinear least squares or ordinary least squares to find θ.
- Constraining the representation.
- Using information theory to improve recombination and perturbation.
- Incorporating multi-objective, diversity control, etc.

Operon C++

Operon C++[5] is a C++ implementation of standard GP and GP with nonlinear least squares for coefficient optimization.

$w_0 + a \cdot \log((w_1 X_1 / w_2 X_2) + w_3)$



- Competitive runtime, good accuracy
- Supports multi-objective optimization, many hyper-parameters to adjust to your liking
- May overparameterize the model

[5] Burlacu, Bogdan, Gabriel Kronberger, and Michael Kommenda. "Operon C++ an efficient genetic programming framework for symbolic regression." Proceedings of the 2020 Genetic and Evolutionary Computation Conference Companion. 2020.

Constraint the generated expressions to the form[6]:

invertible function

$$f_{TIR}(\mathbf{x}, \mathbf{w_p}, \mathbf{w_q}) = g\left(\frac{p(\mathbf{x}, \mathbf{w_p})}{1 + q(\mathbf{x}, \mathbf{w_q})}\right)$$

IT expressions

linear coefficient

$$f_{IT}(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{m} w_j \cdot (f_j \circ r_j)(\mathbf{x})$$

transformation function

interaction function

$$r_j(\mathbf{x}) = \prod_{i=1}^{d} x_i^{k_{ij}}$$

strength of interaction

[6] Fabrício Olivetti de França. 2022. Transformation-interaction-rational representation for symbolic regression. In Proceedings of the Genetic and Evolutionary Computation Conference (GECCO '22). Association for Computing Machinery, New York, NY, USA,

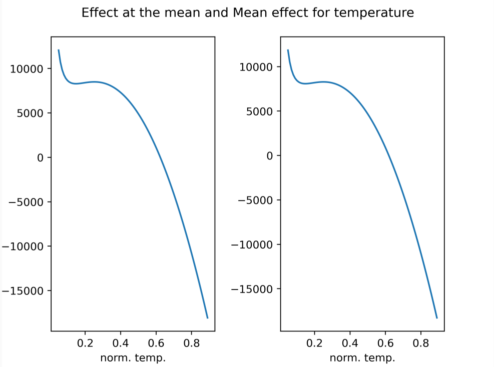
What else?

More benefits to SR

- As a middle ground between opaque and clear model, it can be interpreted
- We can make sure it conforms to our prior-knowledge
- Standard statistical tools can also be applied

Interpreting SR models

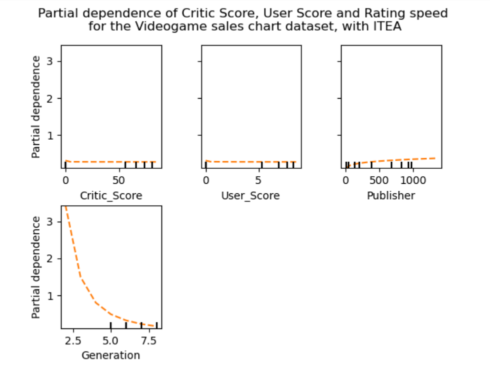
Partial effect at the mean[7] or the mean of the partial effects.



[7] Aldeia, Guilherme Seidyo Imai, and Fabrício Olivetti de França. “Interpretability in symbolic regression: a benchmark of explanatory methods using the Feynman data set.” Genetic Programming and Evolvable Machines (2022): 1-41.

Dataset: Video Game Sales

Or a PDP plot[8] if you want to.

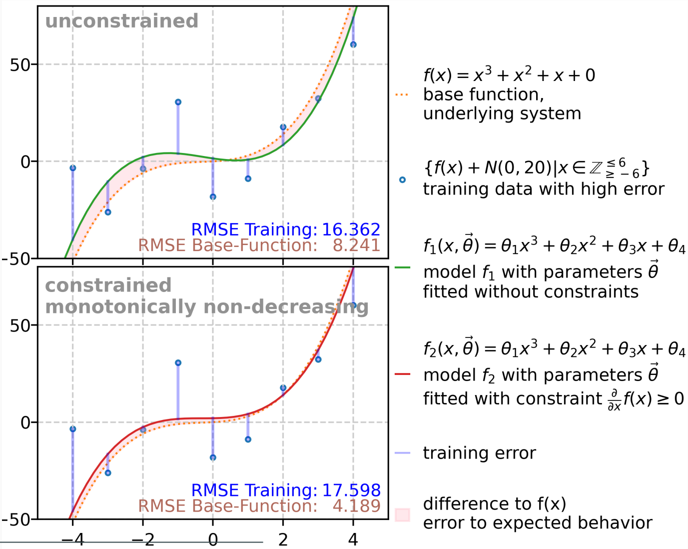


[8] Friedman, Jerome H. "Greedy function approximation: a gradient boosting machine." Annals of statistics (2001): 1189-1232.

Dataset: Video Game Sales - Debug it!

$$
\begin{aligned}
&0.4593106521142636 \\
&+ 0.08 \log(1 + \text{publisher}^3 \text{gen}^{-3}) \\
&- 0.09 \log(1 + \text{critic\_score}^2 \text{user\_score}^3 \text{gen}^3 \text{PC}^3) \\
&+ 0.21 \log(1 + \text{user\_count}^3 \text{gen}^{-3}) \\
&- 1.77 \log(1 + \text{gen})
\end{aligned}
$$

Shape-constraint[9]

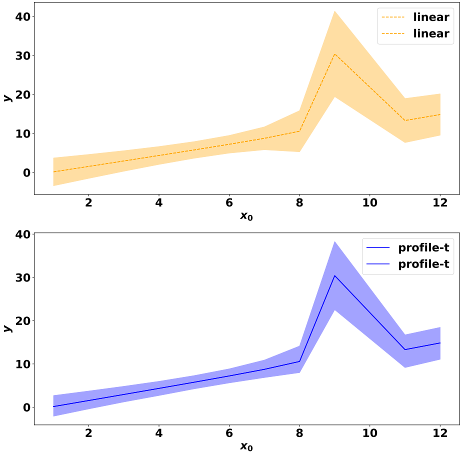


[9] Kronberger, Gabriel, et al. “Shape-Constrained Symbolic Regression—Improving Extrapolation with Prior Knowledge.” Evolutionary Computation 30.1 (2022): 75-98.

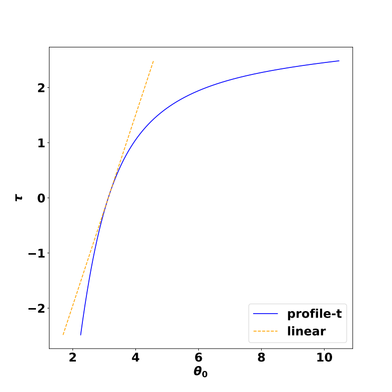
Unlike some opaque models, we can calculate the confidence interval of our parameters and predictions using standard statistical tools:

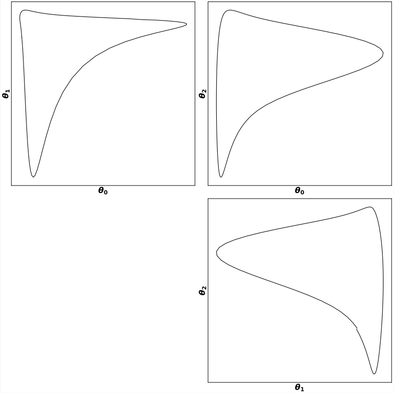
```
SSR 752.76 s^2 28.95
theta   Estimate     Std. Error.   Lower        Upper
0       -1.43e+01    4.29e+00     -2.31e+01    -5.44e+00
1        1.28e+01    2.49e+00      7.67e+00     1.79e+01

Corr. Matrix
[ 1.   -0.97]
[-0.97  1.  ]
```

Prediction intervals:



And many more!

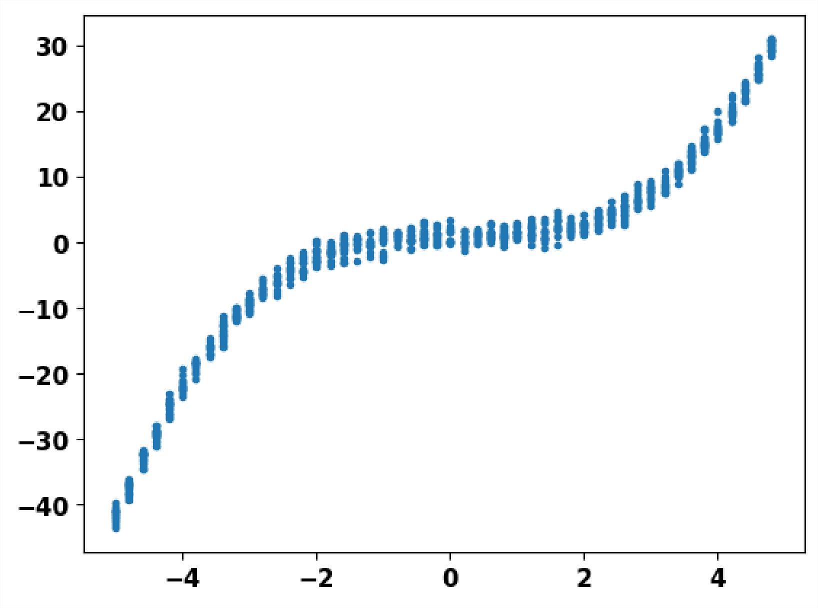




Let’s test it!

```
x = np.repeat(np.arange(-5, 5, 0.2), 15)
y = rng.normal( 0.3*x**3 - 0.2*x**2 + 0.1*x + 1, 1)
plt.plot(x, y, '.')
```

Let’s test it!



Baseline

```
from sklearn.linear_model import LinearRegression

lin = LinearRegression()
lin.fit(x.reshape(-1,1), y)
print("LR: ", lin.score(x.reshape(-1,1), y))
print(f"{lin.coef_}*x")

xpoly = np.vstack([x, x**2, x**3]).T
lin.fit(xpoly,y)
print("Poly: ", lin.score(xpoly, y))
print(f"{lin.coef_}")
```

Baseline

```
LR:  0.8270
Poly:  0.9954
```

Operon

```
from pyoperon.sklearn import SymbolicRegressor
import sympy as sym

reg = SymbolicRegressor()
reg.fit(x.reshape(-1,1),y)
res = [s['objective_values'], s['tree']])
         for s in reg.pareto_front_]

for obj, expr, mdl in res:
  print("Score: ", obj)
  print("Expr: ", reg.get_model_string(expr, 3))
  print("Simplified: ",
       sym.sympify(reg.get_model_string(expr, 3)))
```

Operon

```
Score:  [-0.995512068271637]
Expr:  (1.064 + ((-0.934) * ((((0.106 * X1)
     * ((-0.008) * X1)) * (((-0.908)
     / (((1.019 * X1) - 0.168)
     * (((1.019 * X1) - 0.168) * ((1.019 * X1) - 0.168))))
     - (((1.456 * X1) - ((((1.414 * X1) - 0.486)
     * (0.106 * X1)) * ((-1.207) + (0.106 * X1))))
     / (((-0.390) + (0.232 * X1)) * ((0.232 * X1) + 0.286)
     + (((((1.414 * X1) * ((-2.135) * X1)) + ((-1.207)
     + (0.106 * X1))) - ((-1.915) * X1)) * (0.106 * X1))))
Simplified:  (0.02*X1**8 - 0.03*X1**7 -
            0.01*X1**6 + 0.09*X1**5 - 0.08*X1**4
            - 0.09*X1**3 + 0.06*X1**2 - 0.e-2*X1)/(0.05*X1
            - 0.05*X1**4 - 0.1*X1**3 + 0.05*X1**2 - 0.e-2*
```

Operon

```
reg = SymbolicRegressor(max_length=20,
    allowed_symbols= "add,mul,variable")
```

Operon

```
Score:  [-0.9954367876052856]
Expr:  (1.041 + (0.607 * ((((((0.504 * X1)
        * (0.306 * X1)) * (((-0.430) * X1)
        * ((-0.941) * X1))) + (4.204 * X1))
        * ((-0.002) * X1)) + ((0.179 * X1)
        + ((0.321 * X1) * (((2.229 * X1)
        * (0.693 * X1)) + ((-1.017) * X1))))))))
Simplified:  0.3*X1**3 - 0.2*X1**2 + 0.11*X1 + 1.04
```

Operon

```
reg = SymbolicRegressor(objectives=['r2', 'length'])
```

Operon

```
Score:  [-0.8270264863967896, 5.0]
Simplified:  4.63*X1 - 0.95

Score:  [-0.9850682020187378, 9.0]
Simplified:  0.31*X1**3 - 0.64

Score:  [-0.9953634142875671, 11.0]
Simplified:  X1**2*(0.3*X1 - 0.2) + 1.03

Score:  [-0.9954978227615356, 33.0]
Simplified:  (0.62*X1**6 - 1.85*X1**5 + 1.86*X1**4 + 1.13*X
           - 4.65*X1**2 + 2.46*X1 - 0.31)/(2.07*X1**3
           - 4.81*X1**2 + 2.46*X1 - 0.3)
```

```python
from pyTIR import TIRRegressor

reg = TIRRegressor(100, 100, 0.3, 0.7, (-3, 3),
        transfunctions='Id', alg='MOO')
reg.fit(x.reshape(-1,1), y)
```

```
[0.9937675615949605,20.0]
0.3*x0**3 - 0.2*x0**2 + 0.1*x0 + 1.06

[0.992757244463969,52.0]
(0.3*x0**3 - 0.15*x0**2 + 0.1*x0 + 0.99)/(0.02*x0 + 1.0)
```

```python
from pysr import PySRRegressor

reg = PySRRegressor(binary_operators=["+", "*"],
        unary_operators=[])
reg.fit(x.reshape(-1,1), y)
```

```
x0
4.65*x0
4.64*x0 - 0.95
0.31*x0**3
x0**2*(0.31*x0 - 0.13)
x0**2*(0.3*x0 - 0.2) + 1.03
x0*(x0*(0.3*x0 - 0.2) - 0.89) + x0 + 1.03
```

Terminology learned today

- **nonlinear predictors:** transformed predictors by nonlinear functions.
- **piecewise predictors:** binary predictors describing whether x is inside an interval.
- **transparent models:** models that can be readily interpreted.
- **opaque models:** models that requires adittional tools for interpretation.
- **symbolic regression:** technique that finds for a regression model trying to balance accuracy and simplicity.
- **genetic programming:** algorithm based on evolution that searches for a computer program that solves a problem.

Further reading

- Chapter 3 of Gabriel Kronberger, Bogdan Burlacu, Michael Kommenda, Stephan M. Winkler, Michael Affenzeller. Symbolic Regression. To be plubished.

Next lecture

- Genetic Programming

Acknowledgments