Improving Genetic Programming Based Symbolic Regression Using Deterministic Machine Learning

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What is wrong with Genetic Programming Based Symbolic Regression (GP-SR) ?

- Easy to implement, but hard to analyze
- Works well on toy problems but struggles on high dimensional data

Vicious cycle of GP-SR:

- GP-SR effectively performs feature elimination *only when* sufficiently accurate models are evolved
- High dimensionality makes it difficult for GP-SR to evolve sufficiently accurate models!

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Our hypothesis: Hybridize and you shall win

A hybrid genetic programming (GP) and deterministic machine learning (ML) based symbolic regression algorithm out-performs the genetic programming based symbolic regression (GP-SR) algorithm alone

Method:

- Perform feature extraction using a deterministic, fast machine learning algorithm
- Pass the extracted features to GP-SR for model building

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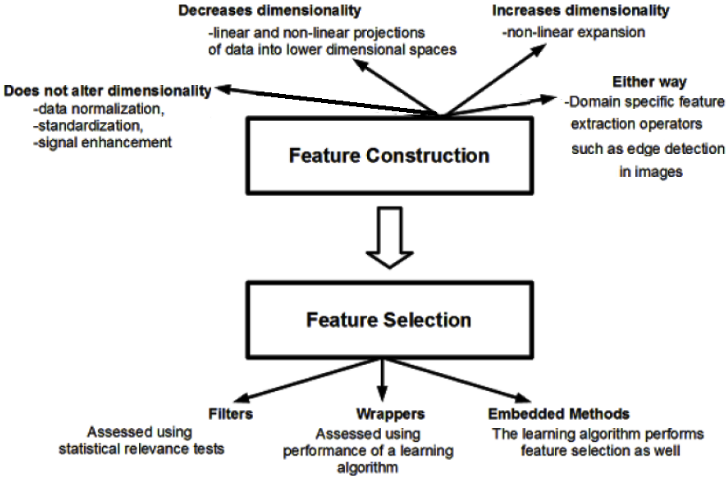
Feature Extraction as a Sequential Process



Feature selection

- Naive way: consider one feature at a time
- Subset Selection
  - *Filters*-independent of the learning algorithm
  - *Wrappers*-assess informativeness based on the performance of the learning algorithm
  - *Embedded Methods*-built in the learning algorithm: decision trees, regularization approach

Regularization for Linear Regression

Given a multivariate dataset $X = \{x_1, x_2, ..., x_N\}$ of observations, the response variable Y is defined as:

$$Y = f(X) = \beta_0 + \sum_{j=1}^{N} \beta_j * x_j$$

$$RSS = min_\beta(\sum_{i=1}^{N} y_i - \beta_0 - \sum_{j=1}^{N} \beta_j * x_{ij})^2$$

Learning algorithm applied to the training data $=>$ overfitting. An additional constraint on the coefficients is imposed in order to tame the coefficients ($\sum_{j=1}^{N} ||\beta_j||_1 \leq t$).

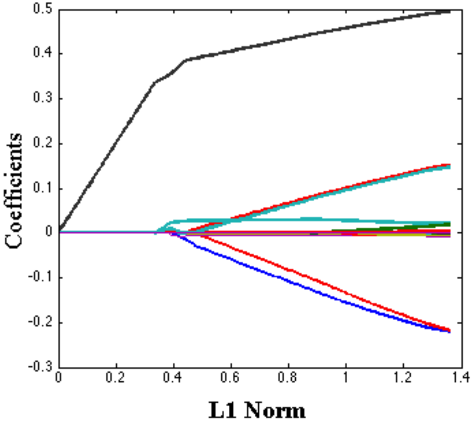
Regularization for Linear Regression cont'd

- LASSO-least absolute shrinkage and selection operator (constraint $l_1$norm)
- Ridge Regression (constraint l_2 norm)
- Elastic Net (hybrid of the two above)

$$Y = f(X) = \beta_0 + \sum_{j=1}^{N} \beta_j * x_j + \lambda_2 ||\beta||_2^2 + \lambda_1 ||\beta||_1$$

λ_1, λ_2 are balanced by a single *mixing* parameter $(0 \leq \alpha \leq 1)$ At the extreme values of α, elastic net behaves like purely lasso or purely ridge regression.

Elastic Net



Adding Nonlinearity-Generalized Linear Models

$$Y = f(X) = \beta_0 + \sum_{j=1}^{N} \beta_j * b_j(X)$$

where $b_j(X)$ are nonlinear basis functions applied to the input variables in order to construct new features.

The Fast Function Extraction: FFX Algorithm

The FFX Idea from McConaghy, 2011

Input $x_1, x_2, x_3, \ldots, x_N$

Stage 1: Feature Construction

Unary and Binary interactions

$\log(x_1)$, $\mathrm{sqrt}(x_1)$ ...

$x_1 * x_2$, $\log(x_1 * x_2)$ ...

Stage 2: Model Building

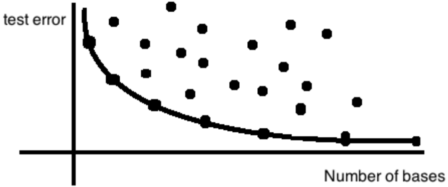
For a set of λs

$y = a1 * x_1 + b$

$y = a1 * x_1 + a2 * x_1 * x_3 + b$

.....

Stage 3: Model Selection

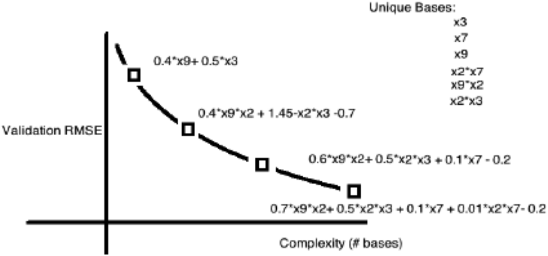


Improving GP-SR using Deterministic Machine Learning

Algorithm 3: The hybrid FFX/GP-SR algorithm

Input: V={v_1,v_2, ..., v_N}
Output: One best model with respect to the validation data error and complexity

```
nonDominatedModels = ffx(trainingDataset)
bases = extractBasisFunctions (nonDominatedModels,
                               validationDataset)
newDataset=createNewDataset(bases)
bestModel = GP-SR(newDataset)
```



Synthetic Benchmark Data Suite Generation

Systemically generated benchmark data suite:

- number of variables : 1-3 , 10 , 25
- order of polynomial: 1 -4
- number of basis functions: 1 -4

- 2500 training, 1250 validation and 1250 test data points
- for each type of polynomial, 30 different datasets

Evaluation Procedure

Experiments

For each dataset :

- FFX runs 1 time
- 30 runs of GP-SR
- 30 runs of FFX/GP-SR

Evaluation Select the model with lowest prediction error on validation set and report:

- prediction error on test set
- similarity to the correct functional form

Algorithm parameters

Parameter	Value
Basis Function Expansion	Exponents : 1 Interactions : Unary, Binary Operators : { }
Elastic Net	α : $\{0, 0.05, 0.1, ..., 1\}$ λ : 100 λ values calculated by glmfit based on α Maximum basis functions allowed : 250
Model Selection	Non-dominated models with respect to validation data error versus number of bases

Default FFX-variant parameters

Algorithm Parameters

Parameter	Value
Representation	GPTIPS Multigene syntax tree Number of genes: 1 Maximum tree depth: 7
Population Size Runtime Budget	500 1 minute
Selection Tournament Size	Lexicographic tournament selection 7
Crossover Operator Crossover Probability	Sub-tree crossover 0.85
Mutation Operator Mutation Probability	Sub-tree mutation 0.1
Reproduction Probability	0.05
Building Blocks	Operators: $\{+, -, *, \mathit{protected}/\}$ Terminal Symbols: $\{x_1, ..., x_N\}$
Fitness	$\frac{1}{N}\sqrt{\sum(y-\hat{y})^2}$
Elitism	Keep 1 best individual

Default GP-SR parameters

Results on 1D data

Example polynomials:

order 1 polynomial:

(1) $y = 0.288 * x_1 + 0.8446$

order 2 polynomials:

(1) $y = 0.14 * x_1^2 + 0.629$

(2) $y = 0.12 * x_1 + 0.03 * x_1^2 + 0.29$

order 3 polynomials:

(1) $y = -0.31 * x_1^3 - 0.11$

(2) $y = 1.35 * x_1^2 - 0.83 * x_1^3 + 0.139$

(3) $y = 0.13 * x_1 + 0.44 * x_1^2 + 0.34 * x_1^3 + 0.39$

order 4 polynomials:

(1) $y = 0.20 * x_1^4 + 0.13$

(2) $y = 0.24 * x_1^3 + 0.23 * x_1^4 + 0.39$

(3) $y = 0.75 * x_1^2 + 0.30 * x_1^3 + 0.35 * x_1^4 + 0.334$

(4) $y = 0.02 * x_1 + 0.13 * x_1^2 + 0.301 * x_1^3 + 0.32 * x_1^4 + 0.91$

Number of times correct form is discovered:

Standalone GP-SR (1 minute)

		Bases			
		1	2	3	4
Order of the Polynomial	1	30	-	-	-
	2	30	29	-	-
	3	30	27	19	-
	4	30	27	11	16

FFX runs with unary (x_i) and binary interactions ($x_i * x_j$) (average run time: 7 seconds)

		Bases			
		1	2	3	4
Order of the Polynomial	1	30	-	-	-
	2	30	30	-	-
	3	0	0	0	-
	4	0	0	0	0

FFX/GP-SR (1 minute GP run on FFX-generated dataset)

		Bases			
		1	2	3	4
Order of the Polynomial	1	30	-	-	-
	2	30	27	-	-
	3	30	26	19	-
	4	30	28	16	17

Correctness of the polynomial form

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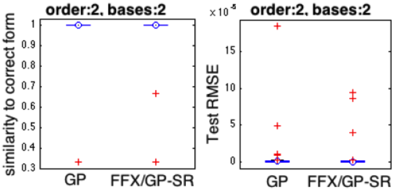
Similarity to correct form & Prediction Accuracy



Wilcoxon Rank Sum Test

Similarity to Correct Form & Prediction accuracy

Results on 2D data

Example polynomials:

order 1 polynomial:

(1) $y = 0.62 * x_2 - 0.854$

order 2 polynomials:

(1) $y = 0.22 * x_1^2 + 0.05$

(2) $y = 0.12 * x_1 - 0.25 * x_1 * x_2 + 0.4$

order 3 polynomials:

(1) $y = 1.67 * x_1^2 * x_2 + 0.46$

(2) $y = 0.17 * x_1 * x_2 + 0.369 * x_2^3 - 0.3$

(3) $y = 0.03 * x_2 - 0.36 * x_1^2 + 0.22 * x_2^3 + 0.42$

order 4 polynomials:

(1) $y = 2.88 * x_1^2 * x_2^2 + 0.15$

(3) $y = 0.4978 * x_1 * x_2^3 - 0.08 * x_1^4 + 0.36$

(3) $y = 2.19 * x_1 * x_2^2 - 0.87 * x_2^3 + 0.87 * x_1^2 * x_2^2 + 0.39$

(4) $y = 0.13 * x_2 - 1.313 * x_1 * x_2 - 0.1 * x_1^3$

$0.4926 * x_1^2 * x_2^2 + 0.19$

Number of times correct form is discovered:

Standalone GP-SR (1 minute)

Order of the Polynomial	Bases 1	2	3	4
1	30	-	-	-
2	30	29	-	-
3	30	22	15	-
4	30	20	10	2

FFX runs on with unary (x_i) and binary interactions ($x_i * x_j$) (average run time: 9 seconds)

Order of the Polynomial	Bases 1	2	3	4
1	30	-	-	-
2	30	16	-	-
3	0	0	0	-
4	0	0	0	0

FFX/GP-SR runs (1 minute GP run on FFX-generated dataset)

Order of the Polynomial	Bases 1	2	3	4
1	30	-	-	-
2	30	30	-	-
3	30	19	14	-
4	30	20	11	3

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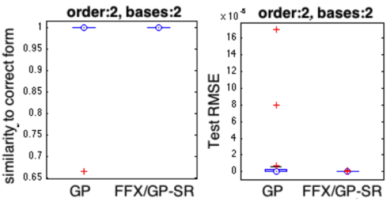

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Similarity to Correct Form & Prediction accuracy

Results on 3D data

Example polynomials:

order 1 polynomial:

$$(1)\quad y = 0.746 * x_3 + 0.8268$$

order 2 polynomials:

$$(1)\quad y = 0.54 * x_3^2 + 0.4$$

$$(2)\quad y = 0.8651 * x_1 - 0.61 * x_2^2 - 0.30$$

order 3 polynomials:

$$(1)\quad y = 0.84 * x_1 * x_2 * x_3 - 0.86$$

$$(2)\quad y = 0.93 * x_1 * x_2 - 0.46 * x_3^3 + 0.88$$

$$(3)\quad y = 0.04 * x_2 - 0.18 * x_2 * x_3 - 0.01 * x_1 * x_2^2 + 0.3$$

order 4 polynomials:

$$(1)\quad y = 0.20 * x_1 * x_2^3 + 0.91$$

$$(2)\quad y = 0.73 * x_1^2 * x_2 - 0.07 * x_1^2 * x_2 * x_3 + 0.39$$

$$(3)\quad y = 1.2 * x_1 * x_2 + 0.68 * x_1^2 * x_2 + 0.48 * x_1^2 * x_2 * x_3 + 0.41$$

$$(4)\quad y = 0.35 * x_3 - 0.32 * x_2 * x_3 - 0.35 * x_1 * x_2^2 - 0.39 * x_3^4 + 0.24$$

Number of times correct form is discovered:

Standalone GP (1 minute)

Order of the Polynomial	Bases 1	Bases 2	Bases 3	Bases 4
1	30	-	-	-
2	30	25	-	-
3	30	25	9	-
4	30	13	12	3

FFX runs with unary (x_i) and binary interactions ($x_i * x_j$) (average run time: 12 seconds)

Order of the Polynomial	Bases 1	Bases 2	Bases 3	Bases 4
1	30	-	-	-
2	29	16	-	-
3	0	0	0	-
4	0	0	0	0

FFX/GP-SR runs (1 minute GP run on FFX-generated dataset)

Order of the Polynomial	Bases 1	Bases 2	Bases 3	Bases 4
1	30	-	-	-
2	30	26	-	-
3	30	28	14	-
4	30	17	12	6

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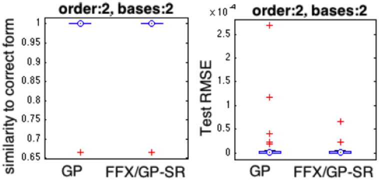
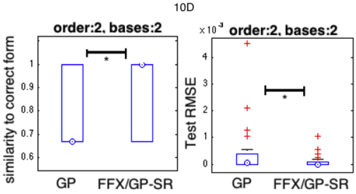


Wilcoxon Rank Sum Test

Similarity to Correct Form & Prediction accuracy

Results on 10D & 25D data (2nd order polynomials)

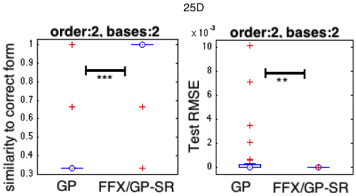


$$y = 0.7 * x_3 - 0.23 * x_9 * x_7 + 0.2$$

where

$$x_i \in x_1, \ldots, x_{10}$$

correctness of polynomial form:
FFX: 10/30, GP-SR: 14/30, FFX/GP-SR: 22/30



$$y = 0.7 * x_3 - 0.23 * x_9 * x_7 + 0.2$$

where

$$x_i \in x_1, \ldots, x_{25}$$

correctness of polynomial form:
FFX: 18/30, GP-SR: 1/30, FFX/GP-SR: 26/30

The hybrid: significantly more similar to the hidden true polynomials & significantly more predictive as dimensionality increases

Discussion

Results show:

- For low dimensional (1 -3) data, GP-SR is competitive with state-of-the-art deterministic ML on our benchmark data suite
- As dimensionality increases (10/25), the hybrid approach wins because hybrid takes advantage of feature extraction provided by the deterministic ML

Therefore, we prove:

- GP-SR is competitive on toy problems, but when dimensionality increases it struggles,
- Hybridize and you shall win!

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Current and Future Work

- Real-world problems: 52 dimensional fMRI dataset (presented at GPTP 2013)
- Other ways of hybridizing the deterministic and GP-based methods for Symbolic Regression
- Comparing all three approaches

Acknowledgments

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Questions ?