

Selection of Polynomial Features by Genetic Algorithms

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[DRAFT July 19, 2013]

Abstract

Many applications require models that have no acceptable linear approximation and many nonlinear models are defined by polynomials. The use of genetic algorithms to find polynomial models is decades old but still poses challenges due to the complexity of the search and different definitions of optimal solution.

This paper describes a two-step method that uses genetic algorithms and linear regression to find empirical polynomial regressions. Experiments on common datasets show that, discounting the training computational effort, this method is quite competitive.

1 Introduction

With notable exceptions (*e.g.* neural networks) machine learning regression techniques are based on linear models. The linearity assumption has many advantages including reduced computational complexity and strong theoretical framework. However nonlinearity is unavoidable in many application scenarios, specially those with phase transitions or feedback loops, so common in ecology, cybernetics, robotics and other areas.

Polynomials, one of the most studied subjects in mathematics, generalize linear functions and define, perhaps, the simplest and most used nonlinear models. Applications include colorimetric calibration [17], explicit formulae for turbulent pipe flows [8], computational linguistics [20] and more recently, analytical techniques for cultural heritage materials [7], liquid epoxy molding process [5], B-spline surface reconstruction [9], product design [6] or forecasting cyanotoxins presence in water reservoirs [10]. This not only illustrates the wide spectrum of applications but, additionally, work in each one of these polynomial models uses, at some point, a genetic algorithm.

Genetic algorithms (GA) where, arguably, one of the hottest topics of research in the recent decades and with good reason since they outline an optimization scheme easy to conceptualize and with very broad application. If a nonlinear (or otherwise) model requires parameterization, GAs provide a simple and often effective approach to search for locally optimal parameters. Research related to genetic algorithms abound and spans from the 1950s seminal work of Nils Aall Barricelli [1] in the Institute for Advanced Study of Princeton to today’s principal area of study for thousands of researchers, covered in hundreds of conferences, workshops and other meetings. Perhaps the key impulse to GAs come from John Holland’s work and his book “Adaptation in Natural and Artificial Systems” [12].

One interesting take on genetic algorithms, named *genetic programming* by John Koza [14], proposed the use of GAs to search the syntactic structure of complex functions. This syntatic structure search is keen to the central ideas of deep learning [3, 2], the subarea of machine learning actually producing the most promising results (*e.g.* [23]). It is also related to the work presented in this paper in the sense that, unlike linear models that have a simple structure, $y = \sum_i \beta_i x_i$, nonlinear (in particular polynomial) models pose an additional “structure” search problem.

The idea of using GAs to find a polynomial regression is not new [16, 26, 25] but still generates original research [11, 4]. In line with that research this work describes a general method to find a polynomial regression of a given dataset. The optimal regression minimises a cost function that accounts for both the root-mean-square error (rmse) and a regularization factor to avoid over-fitting.

It turns out that, discarding the computational cost of training, the polynomial regression method presented here, Genetic Algorithms for Polynomials (GAPOLY), provides a quite competitive regression method. Indeed, it is only systematically out-performed by random forests, an *ensemble* method.

The remainder of this paper is organized as usual: the next section describes the details of our method and is followed by a presentation of some performance results. The last section draws some conclusions and points future research tasks.

2 Genetic Algorithms for Polynomials

This section is dedicated to describe an algorithm to find a polynomial regression from a given dataset. It starts with a brief introduction and description of the algorithm and proceeds into core details as the encoding used to represent individual polynomial instances in the GA populations and the regularization of the cost function.

A usual representation of polynomials is

$$p(x_1, \dots, x_k) = \sum_i \theta_i m_i$$

where each m_i is a monomial, $m_i = \prod_j x_j^{\alpha_{ij}}$, the exponents are non-negative integers, $\alpha_{ij} \in \mathbb{N}_0$, and the coefficients are real valued, $\theta_i \in \mathbb{R}$. For example $p(x_1, x_2, x_3) = 2x_1 + x_2x_3 + \frac{1}{2}x_1^2x_3$ has monomials $m_1 = x_1, m_2 = x_2x_3$ and $m_3 = x_1^2x_3$ coefficients $\theta_1 = 2, \theta_2 = 1$ and $\theta_3 = 1/2$ and exponents $\alpha_{1,1} = 1, \alpha_{2,2} = 1, \alpha_{2,3} = 1, \alpha_{3,1} = 2, \alpha_{3,3} = 1$ and all other $\alpha_{ij} = 0$. The exponents alone are a matrix that defines the monomial structure of the polynomial, $A = [\alpha_{ij}]$. For the example above

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 2 & 0 & 1 \end{bmatrix} \sim \begin{bmatrix} x_1 \\ x_2x_3 \\ x_1^2x_3 \end{bmatrix}$$

where each row defines a monomial and each column represents a variable. Changing the order of the rows doesn't change the polynomial whereas changing the order of the columns corresponds to changing the respective variables.

This representation of polynomials makes the problem of structure search very clear: except for the trivial cases, the number of possible monomials given n variables and a maximum joint degree d grows exponentially with either n or d . But more importantly, the polynomial regression problem can be naturally split into two subproblems:

1. for a given set of monomials m_1, \dots, m_R , find the regression coefficients $\theta_1, \dots, \theta_R$ that minimize the rmse on a given dataset;
2. find the fittest set of monomials, *i.e.* the polynomial that minimizes the rmse on the same dataset;

More precisely, concerning the first problem, let \mathcal{D} be a dataset with N observations of variables Y, X_1, \dots, X_n and $\mathcal{M} = \{m_1, \dots, m_R\}$ a set of R monomial expressions over X_1, \dots, X_n . Define the hypothesis¹

$$h_{\Theta, \mathcal{M}}(x_1, \dots, x_n) = \sum_{j=1}^R \theta_j m_j|_{X_i=x_i, \forall 1 \leq i \leq n}$$

and let the cost

$$J(\Theta; \mathcal{M}, \mathcal{D}) = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(y^{(i)} - h_{\Theta, \mathcal{M}}(x_1^{(i)}, \dots, x_n^{(i)}) \right)^2} \quad (1)$$

¹The expression $m|_{X=x}$ reads “replace all instances of X by x in m ”.

be the usual root-mean-square error (rmse) function. Now the first problem can be stated as:

Given a dataset \mathcal{D} and a set of monomials \mathcal{M} , find parameters Θ that minimize $J(\Theta; \mathcal{M}, \mathcal{D})$.

It turns out that this problem can be solved as a usual linear regression problem by expanding \mathcal{D} with columns that replicate the monomials in \mathcal{M} .

The second problem is treated in the GA setting: Let \mathcal{D} be a dataset as above and \mathcal{P} a set of polynomials. For each polynomial $p \in \mathcal{P}$ let \mathcal{M}_p be the set of monomials in p (without the coefficients) and compute the fitness

$$\phi_p = \min_{\Theta} J(\Theta; \mathcal{M}_p, \mathcal{D})$$

by solving the first problem. With a fitness of every instance, a GA will apply genetic operators (usually mutation and crossover) to evolve the population \mathcal{P} until a reasonable approximation of a local minimum is found.

Algorithm 1 GAPOLY uses linear regression to find monomial coefficients that minimize the rmse over a dataset and GAs to explore the space of polynomials. At exit the rmse of the fittest instance is bounded by ϵ .

```

function GAPOLY( $D, pop_0, \epsilon$ )
   $pop \leftarrow pop_0$ ;  $err \leftarrow 1.0 + \epsilon$ 
  while  $err > \epsilon$  do
     $pop \leftarrow \text{ITERATEGA}(pop)$  ▷ Build next generation
     $pop \leftarrow \text{SORT}(pop, key = \text{LM.RMSE})$  ▷ Sort by rmse of linear regression
     $err \leftarrow \text{RMSE}(\text{FIRST}(pop))$ 
  end while
  return  $\text{FIRST}(pop)$ 
end function

```

Theorem 1. *The composition of GAs with linear regression, as defined in Algorithm 1, converges to a polynomial that is a local minimum of the rmse function, encapsulated in the fitness function J .*

Proof. It follows from the properties of GAs and linear regression. □

Subsection 2.1 details of the encoding of individual polynomial instances as chromosomes and other parameters of the GA implementation used. The regularization of the cost function is discussed in subsection 2.2.

2.1 Polynomial Encoding

The encoding for any polynomial will be as follows:

1. an initial segment detailing which monomials are active (the 1st monomial is always active), this is represented in unary description, i.e., each monomial is identified by a single bit
2. the remaining is split into m sets of bits of equal size, each one representing a monomial
3. each monomial is split into n sets of d size each, i.e., a variable
4. for each variable, the remaining bits give the binary description of the variable degree, i.e., the maximum exponent is given by $2^d - 1$

Let's see an example: consider polynomial $x_1^3x_3 + x_3^7 + x_1x_2$ with $m = 4, n = 3$ and $d = 3$. One possible encoding would be:

110 – 011,000,001 ; 000,000,111 ; 001,001,000 ; 110,010,101

(for reading purposes the semicolons separate monomials, the commas separate variables)

The first three bits inform that the second and third monomials are active while the fourth is not (as said, the first monomial is always active). This last monomial does not enter neither in the polynomial regression nor in the fitness evaluation. However, it acts as a kind of junk DNA, becoming active when, in a future mutation or crossover, the third bit of the entire sequence flips from 0 to 1.

Let's interpret the first monomial description, 011,000,001. It is divided by three since $n = 3$. The first triple 011 is the binary description of the exponent of variable x_1 which is 3, so the first monomial includes x_1^3 . The second triple, 000, means that x_2 is not part of the monomial. The third triple 001 says that variable x_3 has exponent 1, so the first monomial consists of $x_1^3x_3$. All the remaining sets of nine bits are interpreted the same way and we get the previous polynomial.

Notice that all binary descriptions give rise to valid polynomials. Notice however that this is not a bijective mapping. For each polynomial there are multiple representations. For example, $x_1 + x_2$ and $x_2 + x_1$ have different representations. The authors considered that more complex mappings in order to force a one to one mapping would impact negatively in the algorithm performance without giving anything in return.

If the coding consists of entirely zeros, by convention, it describes polynomial x_1 . This has to do with the execution of the polynomial regression that would fail if we interpret it as the zero polynomial. Anyway, for progressive larger binary descriptions, the chances of getting this zero description decrease exponentially, so it does not impact in any meaningful way in the algorithm's performance.

2.2 Cost Function

The polynomial fitness considered so far is based on the ability to predict the test set after the polynomial regression has found the appropriate coefficients θ_i for each one of the polynomial's monomials m_i .

This fitness function tends to prefer more complex polynomials, namely in the number of monomials which provides the regression algorithm for more fitting possibilities. One way to balance this is to provide a regularization term into the fitness function. Our proposal is to include a multiplicative factor into the fitness function proportional to the number of monomials. Thus, the fitness function becomes,

$$J_{fit}(\Theta; D) = \lambda^m \sqrt{\frac{1}{n} \sum_{i=1}^n \left(y^{(i)} - h_{\Theta} \left(x_1^{(i)}, \dots, x_m^{(i)} \right) \right)^2}$$

where m is the number of monomials the polynomial has. A λ greater than one punishes polynomials with more monomials.

Somewhat unexpectedly after some experiences it was found that lower values for λ sometimes provide better, even if marginal, results. Figure 1 shows results for the Abalone dataset with ten runs for each λ , and figure 2 presents regularization results for the Auto-MPG dataset. The following section Experimental Results includes information about these datasets.

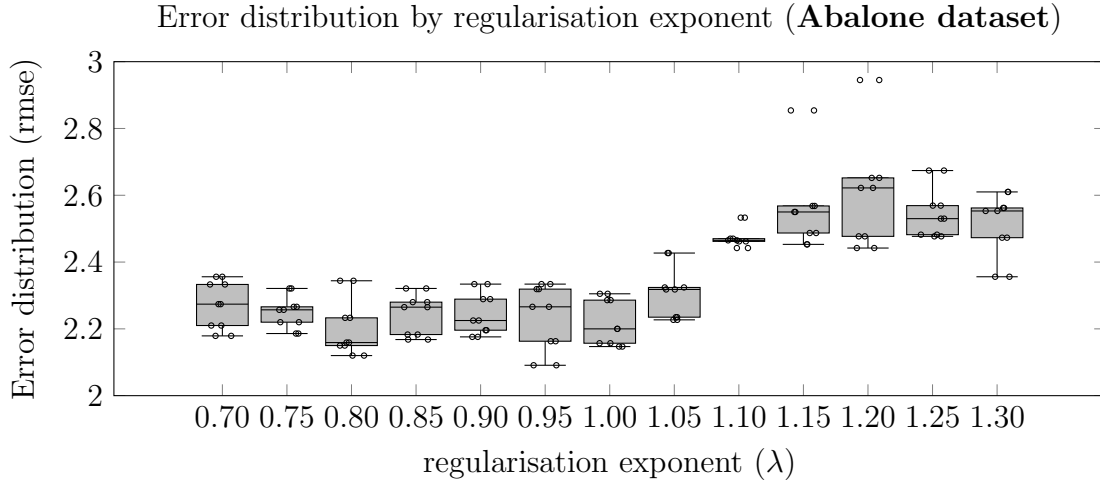


Figure 1: Error distribution by regularisation exponent for the Abalone dataset.

The typical inflection point lies around $\lambda = 0.8$. The following results use the regularisation parameter with this value.

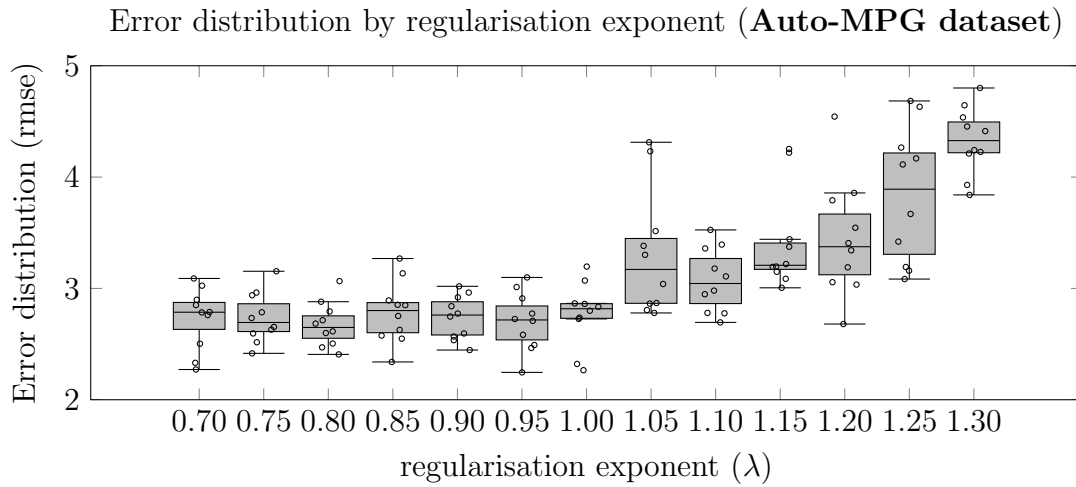


Figure 2: Error distribution by regularisation exponent for the Auto-MPG dataset.

2.3 Genetic Operators

It was used the R package `genalg` [27] for the execution of genetic algorithm. The operators were the standard ones: (a) crossover, i.e., a pair of solutions from the previous generations are combined by splitting and mixing their respective representations, and (b) mutation, changing the values of single bits; the mutation chance applied in the datasets was 5%. There was also elitism between generations, i.e., 20% of the best solutions are kept in the next generation.

3 Experimental Results

- Measured quantities
 - error
 - number of iterations to convergence
 - memory usage
 - F1, ROC, ?
- Selection of datasets and regression algorithms
- Summary Figures and Numeric results

These results were found using R's programming language [19].

To compare this paper’s proposed algorithm we applied the exact same train and test samples using other learning algorithms, namely: Linear Regression, Support Vector Machines [18], Regression Trees [24], Conditional Inference Trees [13, 22, 21] and Random Forests [15]

In order to train and test the performance of GAPOLY it was used several datasets (see below). For each dataset, we selected 70% for training purposes and the remaining observations to make a test set in order to compute the estimated rmse. To achieve more robust results, each dataset were processed 25 times, each one with different samples for the train and test sets. For the datasets with attribute values of different magnitudes, a preliminary scaling was executed. The results below are boxplots for the test set error predictions over these different runs.

Artificial: this is an artificial dataset with four numeric features, x_1, \dots, x_4 , where x_1, x_3 are outcomes from Poisson random variables, and x_2, x_4 from Normal random variables. The dependent variable y is given by expression $x_2x_4^2 + x_1^2x_3 + 5$. The dataset includes 50 observations and, only in this case, there were executed just 10 runs.

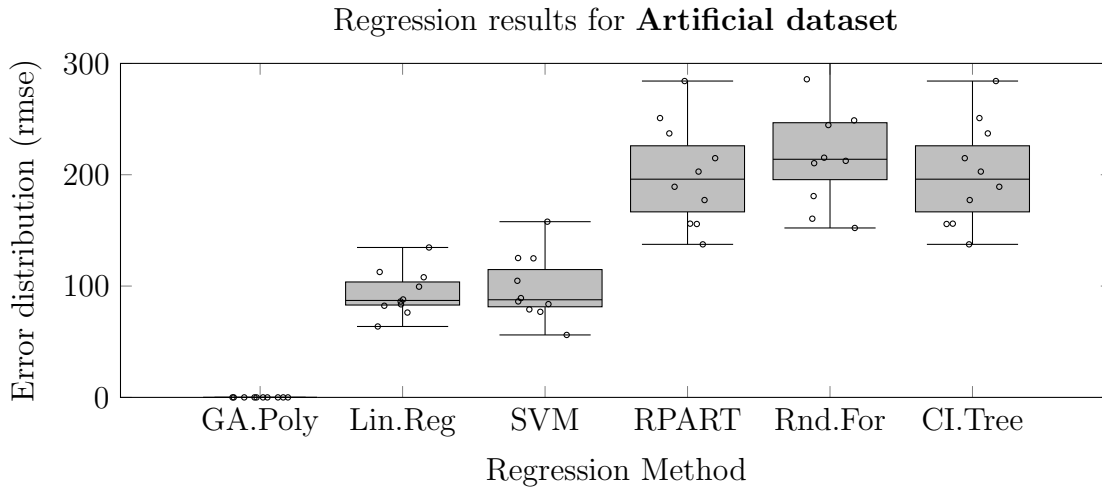


Figure 3: results for Artificial dataset

This dataset was used in order to verify if GAPOLY was able to find the polynomial relation, which the algorithm did (cf. figure 3). In this case, we used a population of 100 solutions with 50 iterations for each run.

In the next datasets, the population has size 250 with 100 iterations for each run.

Housing: This data set concerns the task of predicting housing values in areas of Boston. There are 13 continuous attributes and the dependent variable is the median value of owner-occupied homes in \$1000's². There are 506 observations. Figure 4 presents the results for this dataset.

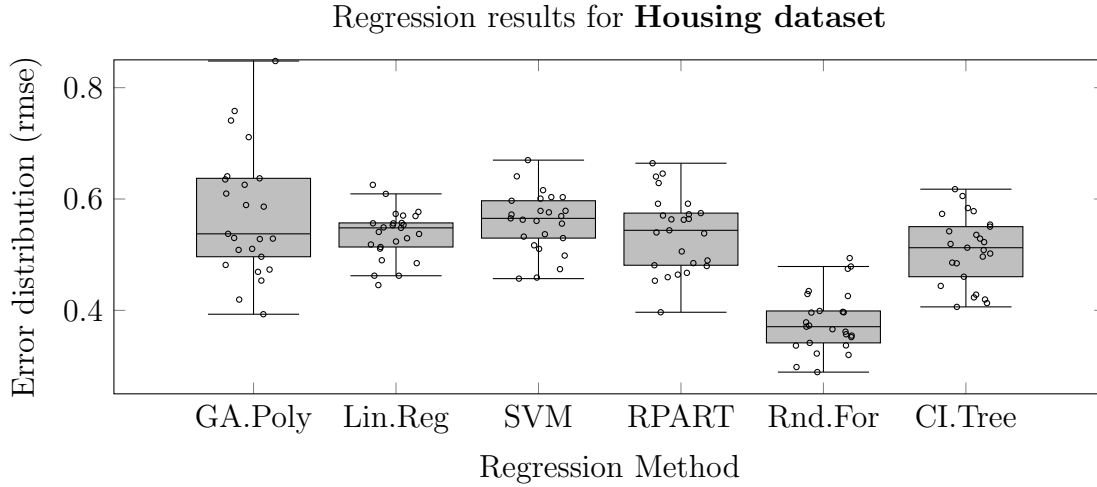


Figure 4: results for Boston Housing dataset

Just as an example of the model the GAPOLY algorithm outputs: in this dataset the best polynomial was the following:

$$y = -0.12x_6x_9^4 + 0.78x_6 - 0.4x_9^2x_{13} + 0.17x_{13}^2 - 0.044$$

where the attributes mean: x_6 , RM average number of rooms per dwelling; x_9 , RAD index of accessibility to radial highways; x_{13} , Lower status of the population.

For comparison if we access the mean decrease in accuracy found by Random Forests, the most important attributes are – in decreasing order – x_{13} , x_6 , x_5 (but x_5 is already considered 4 times less important than x_6). Both algorithms agree in two of their three most important attributes.

Abalone: This dataset can be used to predict the age of a abalone shell using the given 8 numeric attributes concerning several physical measurements. There are 4177 observations. Figure 5 presents the results for this dataset.

Auto-MPG: This dataset is used to predict fuel consumption in miles per gallon, based on two discrete and five continuous attributes. There are 398 observations. Figure 6 presents the results for this dataset.

²This and the remaining regression datasets were selected from Luis Torgo's data repository, <http://www.dcc.fc.up.pt/~ltorgo/Regression/DataSets.html>. Most of these datasets originally come from UCI ML repository, <http://archive.ics.uci.edu/ml/>

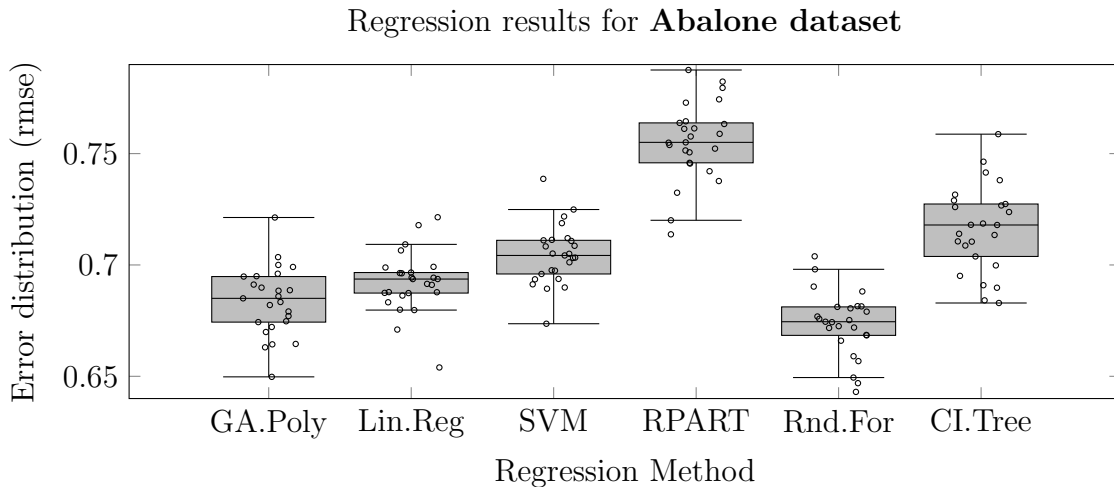


Figure 5: results for Abalone dataset

Kinematics: This dataset is concerned with the realistic simulation of the forward kinematics of an 8 link robot arm. The task is to predict the distance of the end-effector from a target using 8 continuous attributes. There are 8192 observations. Figure 7 presents the results for this dataset.

3.1 Convergence speed

The GA quickly proceeds in the first 50 to 100 generations to reasonable error rates. Then, it proceeds slower achieving best solutions with marginal error reduction. Since the entire learning process takes some time, in the current R implementation³, placing a limit between 50 to 100 generations already achieves good results, relative to higher iteration values. Figure 8 shows a typical error evolution for the dataset Abalone given two different values for λ .

4 Conclusion

The proposed method has competitive results comparing with some well-known regression methods. Only Random Forest outperforms GAPOLY systematically (it also outperforms all the other regression algorithms). One exception – the

³The processing time can probably be speeded by one to two orders in magnitude if the process is implemented in a low level programming language like C++. However, speed optimisation was not the focus of this article

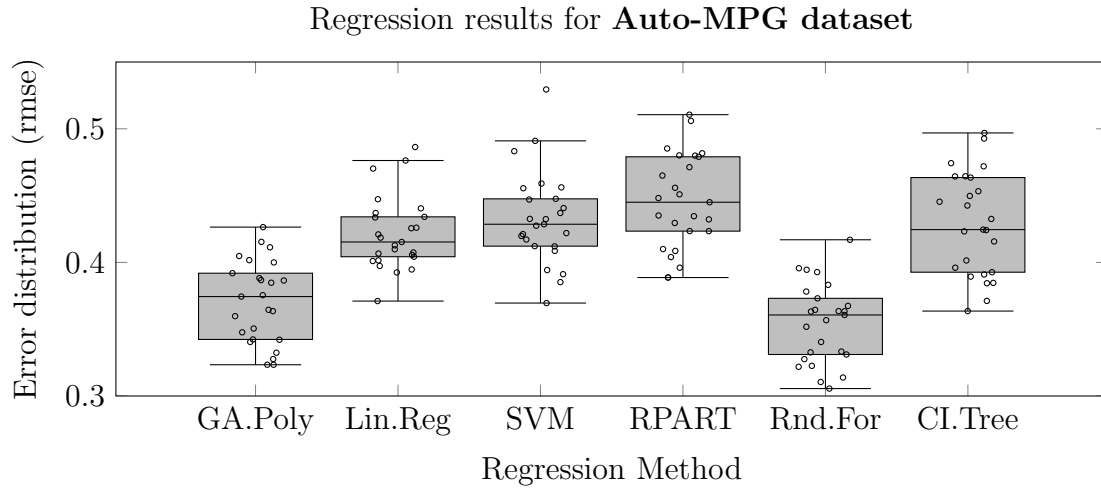


Figure 6: results for Auto-MPG dataset

artificial dataset that uses a straightforward polynomial relation – is the Auto-MPG dataset where GAPOLY has comparable results. This is evidence that applying standard genetic operators for polynomial model searching is a viable tool for regression purposes.

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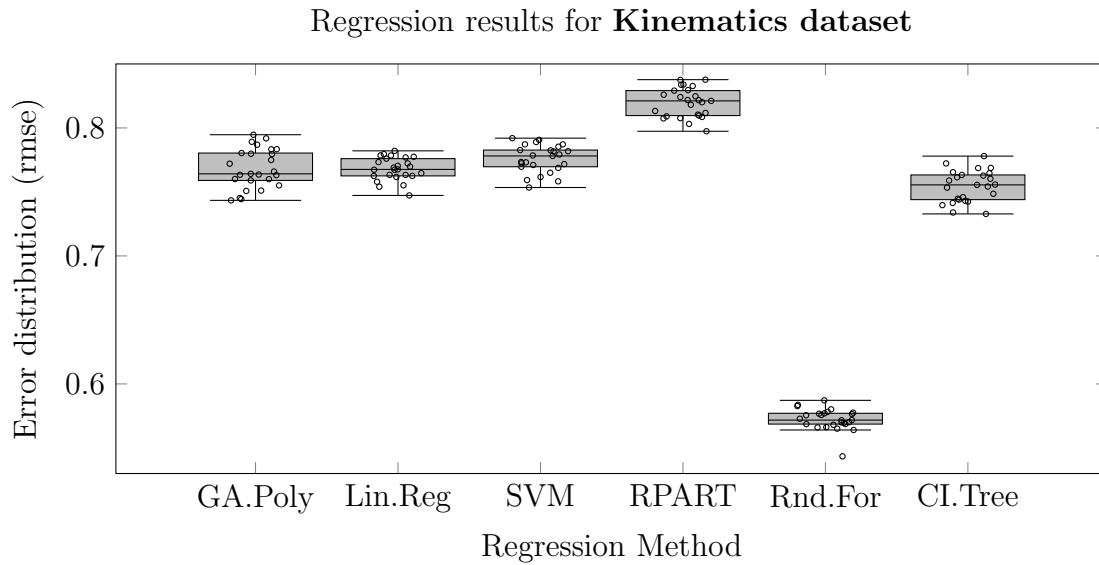


Figure 7: results for Kinematics dataset

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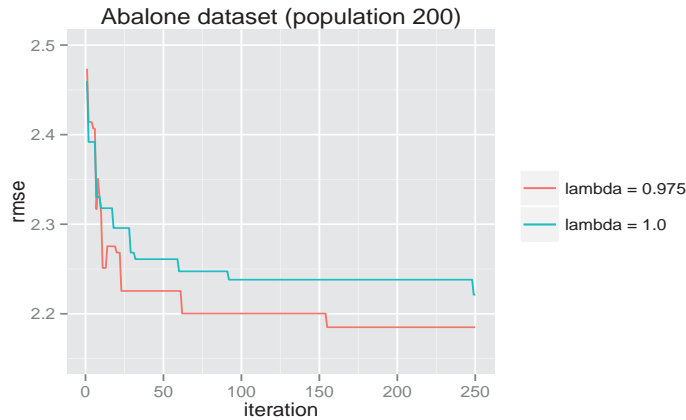


Figure 8: fitness progress for Abalone dataset

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