A Method for Regularisation of Evolutionary Polynomial Regressions

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Abstract

While many applications require models that have no acceptable linear approximation, the simpler nonlinear models are defined by polynomials. The use of genetic algorithms to find polynomial models from data is known as Evolutionary Polynomial Regression (EPR). This paper introduces Evolutionary Polynomial Regression with Regularisation (EPR^2), an algorithm that extends the EPR method and describes a set of experiences on common datasets that compare both flavours of EPR and other methods including Linear Regression, Regression Trees and Support Vector Regression.

The empiric conclusion of those experiments is that EPR^2 is able to achieve better fitting than other non-ensemble methods and it has shorter computation time than plain EPR.

Keywords: evolutionary polynomial regression, regularisation, feature extraction, dimensionality reduction

1. Introduction

With notable exceptions (*e.g.* neural networks) machine learning regression techniques produce linear models. The linearity assumption has many advantages including reduced computational complexity and strong theoretical framework. However nonlinearity is unavoidable in many application

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scenarios, specially those with phase transitions or feedback loops, so common in engineering, ecology, cybernetics and other areas. The kernel trick in Support Vector Machines (SVM) (Schölkopf et al. (1997); Liang and Lee (2012); Bao et al. (2013)) alleviates this problem by allowing special nonlinear transformations of the feature-space. The condition such transformations must meet is known as the *kernel trick*, $k(x, x') = \langle \varphi(x), \varphi(x') \rangle$, where φ is the feature-space transformation and $\langle \cdot, \cdot \rangle$ denotes inner product. The "trick" consists on computing the kernel $k(x, x')$ while avoiding the computation of the inner product and the transformations $\varphi(x), \varphi(x')$. A special case of polynomial transformation, the *polynomial kernel*, $k(x, x') = \langle x, x' \rangle^d$ is commonly used in regression and classification tasks with SVMs. However general polynomial transformations do not verify the kernel trick.

Polynomials, one of the most studied subjects in mathematics, generalise linear functions and define, perhaps, the simplest and most used nonlinear models. Applications include colorimetric calibration (Mendes and Carvalho, 2005), explicit formulæ for turbulent pipe flows (Davidson et al., 1999), computational linguistics (Sánchez et al., 2009) and more recently analytical techniques for cultural heritage materials (Cséfalvayová et al., 2010), liquid epoxy moulding process (Chan et al., 2011), B-spline surface reconstruction (Gálvez et al., 2012), product design (Chan et al., 2012) or forecasting cyanotoxins presence in water reservoirs (García Nieto et al., 2013). These examples not only illustrate the wide spectrum of applications but, additionally, in each one uses, at some point, a Genetic algorithms (GA).

GAs were, arguably, one of the hottest topics of research in the recent decades and with good reason since they outline an optimisation scheme easy to conceptualise and with very broad application. If a nonlinear (or otherwise) model requires parameterisation, 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 (Barricelli, 1962) 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" (Holland, 1975).

One interesting variation of genetic algorithms, named *genetic programming* by John Koza (Koza, 1992), proposed the use of GAs to search the syntactic structure of complex functions. This syntactic structure search is keen to the central ideas of deep learning (Bengio, 2009; Bengio et al., 2013),

a subarea of machine learning actually producing quite promising results (*e.g.* in Tarlow et al. (2013)). 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 (Maertens et al., 2006; Yu and Lin, 2008; Wu et al., 2009) but still generates original research (Hofwing et al., 2011; Cetisli and Kalkan, 2011). The modern formulation of the use of GA to find polynomial models is known as Evolutionary Polynomial Regression (EPR) and systematisation can be traced back to the work of Davidson, Savic and Walters (Davidson et al. (2003)). Further developments include multi-objective optimisations (Giustolisi and Savic (2009)).

This paper describes an extension of the general EPR method to find a *regularized* polynomial regression of a given dataset. The optimal regression results from a cost function that accounts for both the root-mean-square error (error) and a regularisation factor to avoid over-fitting. Another important change is in the coding mechanism which introduces two new features: (a) inclusion of the linear terms in the polynomial expression, and (b) the activation/deactivation of monoids during evolution to allow the increase/decrease of polynomial expressions.

The next section describes the method's details 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 the description of an algorithm to find a polynomial regression from a given dataset. It starts with a brief introduction and outline of the algorithm and proceeds into core details as the encoding used to represent individual polynomial instances in the GA populations and the regularisation of the cost function.

An usual representation of polynomials is

$$p\left(x_1, \ldots, x_m\right) = \sum_i \theta_i q_i$$

where each q_i is a monomial, $q_i = \prod_j x_j^{\alpha_{ij}}$, 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 $p\left(x_1, x_2, x_3\right) = 2x_1 + x_2x_3 + \frac{1}{2}x_1^2x_3$ has monomials $q_1 = x_1, q_2 = x_2x_3$ and

$q_3 = x_1^2 x_3$, 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 the matrix of monomials is

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 2 & 0 & 1 \end{bmatrix} \sim \begin{bmatrix} x_1 \\ x_2 x_3 \\ x_1^2 x_3 \end{bmatrix}$$

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 $\mathcal{P} = \{q_1, \ldots, q_k\}$, find the regression coefficients $\theta_1, \ldots, \theta_k$ that minimize the error on a given dataset;
2. Find the fittest set of monomials, *i.e.* the polynomial that minimizes the error on the same dataset;

More precisely, concerning the first problem, let $\mathcal{D}$ be a dataset with n observations of variables $Y, X_1, \ldots, X_m$ and $\mathcal{P} = \{q_1, \ldots, q_k\}$ a set of k monomial expressions over $X_1, \ldots, X_m$. Define the hypothesis[1]

$$h_{\Theta,\mathcal{P}}(x_1, \ldots, x_m) = \sum_{j=1}^{k} \theta_j q_j|_{X_i = x_i, \forall 1 \leq i \leq m}$$

and let the cost

$$J_{\text{fit}}(\Theta; \mathcal{P}, \mathcal{D}) = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left(y^{(i)} - h_{\Theta,\mathcal{P}}\left(x_1^{(i)}, \ldots, x_m^{(i)}\right)\right)^2} \quad (1)$$

[1]The expression $q|_{X=x}$ reads "*replace all instances of X by x in q*".

Algorithm 1 Evolutionary Polynomial Regression (EPR) uses linear regression to find monomial coefficients that minimize the error over a dataset and GAs to explore the space of polynomials. The role of the linear regression step is to produce a fitting error that sorts the population. At exit the error of the fittest instance is bounded by ϵ or the maximum number of allowed iterations.

```
function EPR(D, pop_0, ε)
    pop ← pop_0; err ← 1.0 + ε
    while err > ε ∧ ¬LIMIT(iterations) do
        pop ← ITERATEGA(pop)
        pop ← SORT(pop, key = J)    ▷ Sort population by regression error
        err ← J(FIRST(pop))
    end while
    return FIRST(pop)
end function
```

be the usual root-mean-square error (error) function. Now the first problem can be stated as: *Given a dataset $\mathcal{D}$ and a set of monomials $\mathcal{P}$, find parameters Θ that minimize $J_{fit}(\Theta; \mathcal{P}, \mathcal{D})$.*

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 Q a set of polynomials. For each polynomial $p \in Q$ let $\mathcal{P}_p$ be the set of monomials in p (without the coefficients) and compute the fitness

$$\phi_p \quad = \quad \min_{\Theta} J_{\text{fit}}(\Theta; \mathcal{P}_p, \mathcal{D})$$

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 Q until a reasonable approximation of a local minimum is found. Notice that the properties of GAs and linear regression entail that the composition of GAs with linear regression, as defined in Algorithm 1, converges to a polynomial that is a local minimum of the fitness function, encapsulated in the error function J_{fit}.

Subsection 2.1 describes the encoding of individual polynomial instances as chromosomes and other parameters of the utilised GA implementation. The regularisation 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 first monomial is always active), this is represented in unary description, i.e., each monomial is identified by a single bit
2. the remaining bits are split into k sets of equal size, each one representing a monomial
3. each monomial is split into m sets of d size each, *i.e.*, a variable
4. for each variable, the remaining bits are the binary description of the variable degree, *i.e.*, the maximum exponent is given by $2^d - 1$

A short example: consider polynomial $x_1^3 x_3 + x_3^7 + x_1 x_2$ with $k = 4, m = 3$ and $d = 3$. A possible encoding would be (for reading purposes the semicolons separate monomials, the commas separate variables):

```
110 - 011,000,001 ; 000,000,111 ; 001,001,000 ; 110,010,101
```

The first three bits inform that the second and third monomials are active while the fourth is not (the first monomial is always active). This fourth monomial does not enter neither in the polynomial regression nor in the error (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.

Notice that all binary descriptions give rise to valid polynomials. However 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's performance.

In the experiments that led to this article, the tests showed that the inclusion of the linear terms achieved a significant reduction of error rates. So, considering the previous example, the final polynomial would be $x_1^3 x_3 + x_3^7 + x_1 x_2 + x_1 + x_2 + x_3$. The next section discusses this feature.

2.2. Cost Function

The polynomial regression error 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 monomials q_i.

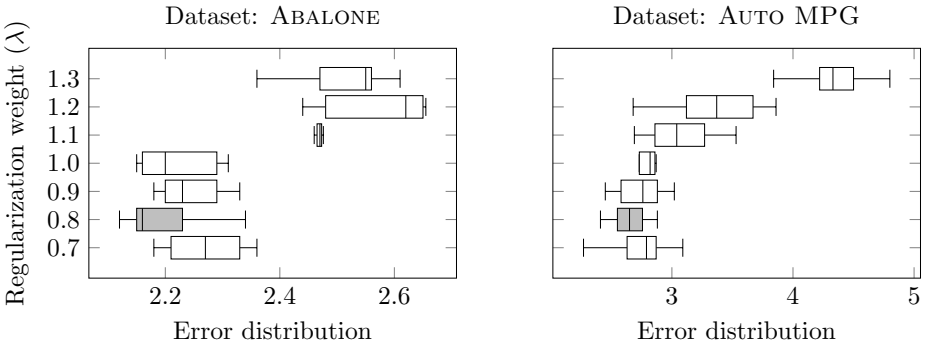

Figure 1: Error distribution by regularisation exponent for the Abalone and Auto MPG datasets. The box plots summarise the error values of 10 runs for each value of λ. The smallest overall error is shown in grey and, in both cases, was achieved with $\lambda = 0.8$.

This error 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 regularisation term into the error function. The article's proposal is to include a multiplicative factor proportional to the number of monomials. Thus, the error from equation 1 defines

$$J_{\text{reg}}\left(\Theta; \mathcal{P}, \mathcal{D}\right) \quad = \quad \lambda^k J_{\text{fit}}\left(\Theta; \mathcal{P}, \mathcal{D}\right) \tag{2}$$

where k is the number of monomials in the polynomial. When $\lambda > 1$ polynomials with more monomials are penalized.

Figure 1 shows regularisation results for the Abalone and Auto MPG datasets with ten runs for each λ (the following section includes information about these datasets). The typical inflection point lies around $\lambda = 0.8$. This somewhat paradoxical result – since regularisation tries to minimize the model's complexity in order to prevent overfitting – is somewhat justified by the inclusion of the linear terms mentioned in the previous section. The linear terms 'pushes' the model to linearity while a regularisation term $\lambda < 1$ tries to add non-linearity terms. Within this tension, the algorithm is able to reduce the overall error, compared to the typical implementation EPR found in the literature.

We'll denote by Evolutionary Polynomial Regression with Regularisation (EPR^2) the proposed extension of the EPR algorithm which includes the regularised cost function together with the new features in polynomial coding.

2.3. Genetic Operators

To perform the genetic algorithm it was used the R package genalg (Willighagen, 2012). 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 survive to the next generation.

3. Experimental Results

The results were found using `R` programming language (R Core Team, 2013)[2]. To compare this paper's proposed algorithm we applied the exact same train and test samples using several well-known learning algorithms for regression, namely: the classic EPR, Linear Regression, Support Vector Machines (Meyer et al., 2012), Regression Trees (Therneau et al., 2013) and Conditional Inference Trees (Hothorn et al., 2006; Strobl et al., 2007, 2008). To achieve better error results, the SVM and Regression Tree algorithms had their parameters tuned.

In order to train and test the performance of EPR[2] several mainstream datasets were used. For each dataset, we selected 70% for training purposes and the remaining observations to make a test set in order to compute the estimated error. 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 box plots for the test set error predictions over these different runs.

ARTIFICIAL this is an artificial dataset with four numeric features, $x_1, \ldots x_4$, 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 $x_2 x_4^2 + x_1^2 x_3 + 5$. The dataset includes $n = 50$ observations.

This dataset was used in order to verify if EPR was able to find the polynomial relation, which the algorithm did (cf. figure 2). The genetic

[2]The datasets and the `R` code used to produce the results and plots in this paper are available online at `https://github.com/jpneto/GenAlgPoly`.

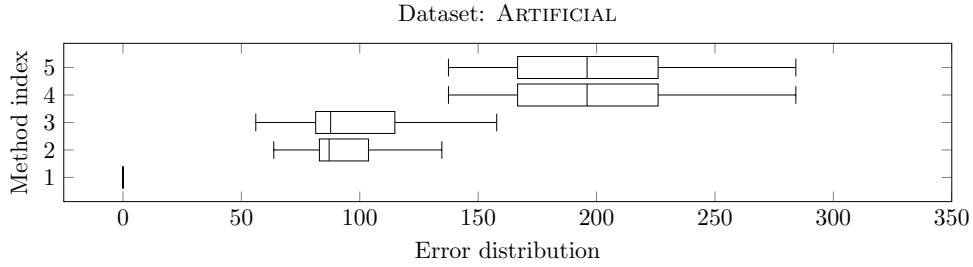

Figure 2: Results for Artificial dataset. As shown, polynomial regression finds the exact polynomial structure that generates the dataset, reducing the test set prediction error to zero. The regression methods depicted are: 1. EPR^2, 2. Linear Regression, 3. SVM, 4. Regression Trees and 5. Conditional Inference Trees

algorithm run with a population of $n = 100$ solutions with 50 iterations for each run.

In the next datasets, the population of the genetic algorithm had size $n = 300$ with 100 iterations for each run. EPR^2 was run with regularisation parameter $lambda = 0.8$.

HOUSING: This data set concerns the task of predicting housing values in areas of Boston. There are $m = 13$ continuous attributes and the dependent variable is the median value of owner-occupied homes in \$1000's. There are $n = 506$ observations.

ABALONE This dataset can be used to predict the age of a abalone shell using the given $m = 8$ numeric attributes concerning several physical measurements. There are $n = 4177$ observations.

AUTO MPG This dataset is used to predict fuel consumption in miles per gallon, based on two discrete and five continuous attributes ($m = 7$). There are $n = 398$ observations.

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 $m = 8$ continuous attributes. There are $n = 8192$ observations.

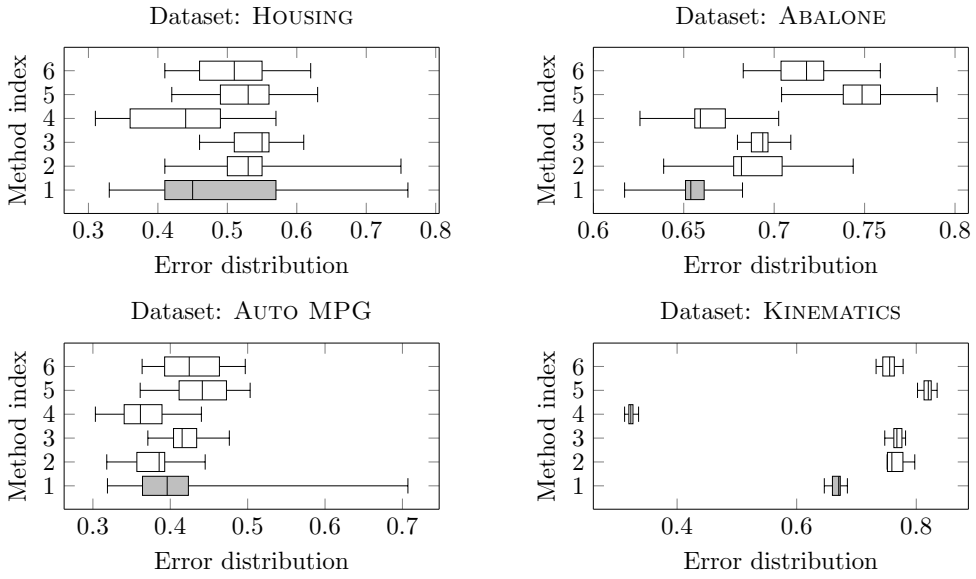

Figure 3: Summary results for different regression methods on the Housing, Abalone, Auto MPG and Kinematics datasets. Random Forests, an ensemble method ("2" in the plots), has the better results. However EPR achieves similar errors in two of the datasets. For the remaining two EPR produces similar errors to the other classic regression methods. The regression methods depicted in these figures are: 1. EPR^2, 2. EPR, 3. Linear Regression, 4. SVM, 5. Regression Trees and 6. Conditional Inference Trees

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 implementation, placing a limit between 50 to 100 generations already achieves good results, relative to higher iteration values. Figure 4 shows a typical error evolution for the dataset Abalone given a regularised version ($\lambda = 0.975$) and a non-regularized ($\lambda = 1.0$).

4. Conclusion and Future Work

[Discutir a localidade do regressor]

Of the regression methods considered, SVM achieved the best results in 3 out of 4 datasets. However, SVM was tuned for each particular dataset while EPR^2 was executed with its parameters preset. Even so, EPR^2 had

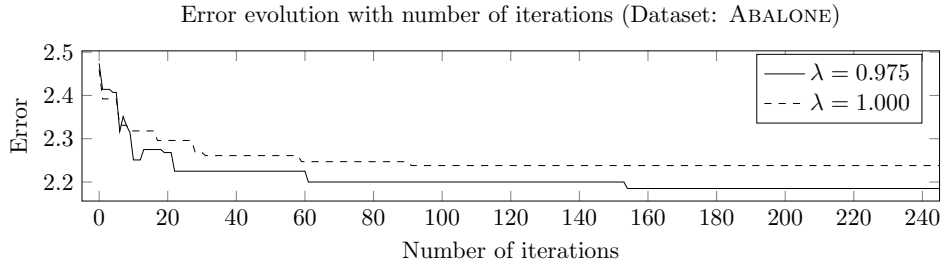

Figure 4: Error progress for Abalone dataset during a single execution of the genetic algorithm. The figure shows the fitness evolution for two different regularisation values. The population for both consisted of 200 polynomials. The error values seem to stabilise around iteration 250.

the best error in the Abalone dataset, and achieved competitive results in the Housing and Auto MPG datasets.

Comparing EPR and EPR^2 – which is the main article's topic – the regularized version achieved much better results at Abalone and especially Kinematics. The Housing improved errors when compared with EPR in a difference in means, resulted in a 95% HDI (Highest Density Interval) equal to [0.001, 0.119] which, while borderline, achieves statistical significance. Only in the Auto MOG dataset EPR achieved better results, even if not that different from EPR^2.

For complexity considerations EPR and EPR^2 demands some processing time. On a quad-core computer, processing the Kinematics dataset (with 8k observations) takes approximately 5 minutes. The processing time can probably be speeded between 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.

A cross-validation procedure can be implemented to refine the appropriate parameter values to achieve better errors. Namely, the regularisation parameter, λ, can be tested with several values, instead of being fixed at 0.8. Other parameters like mutation chance or the amount of elitism could also be tested. However, these type of tests need a low-level, fast implementation of EPR and were not considered.

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The datasets used herein were selected from Luís Torgo's data repository, `http://www.dcc.fc.up.pt/~ltorgo/Regression/DataSets.html`. Most come originally from UCI ML repository, `http://archive.ics.uci.edu/ml/`.

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