Vinnytsia National Technical University

STRUCTURAL OPTIMIZATION OF REGRESSION MODELS BASED ON A GENETIC ALGORITHMS

1

Speakers:

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PROBLEM STATEMENT

$$\hat{y} = f\left(x; \theta, s\right)$$

$D = \left\{\left(x_i, y_i\right)\right\}_{i=1}^{N}$ - training sample;

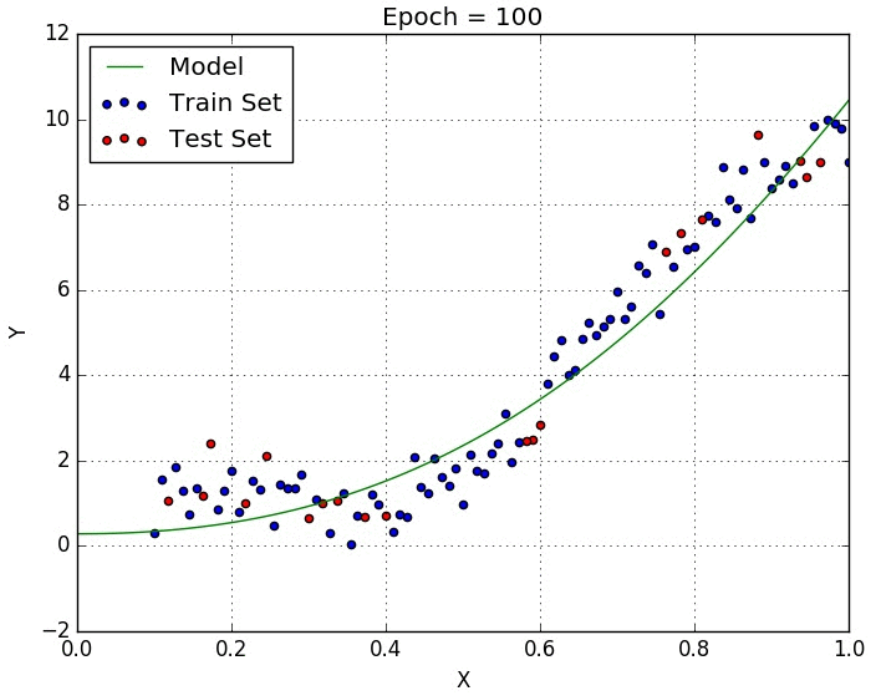
$x_i \in \mathbb{R}^p$ – vector of input features;

$y_i \in \mathbb{R}$ – observed response value;

$f \in F_s$ – class of admissible regression functions;

$\theta \in \Theta(s)$ – vector of model tuning parameters;

$s \in S$ – vector of structural variables that determine the structure of regression model;



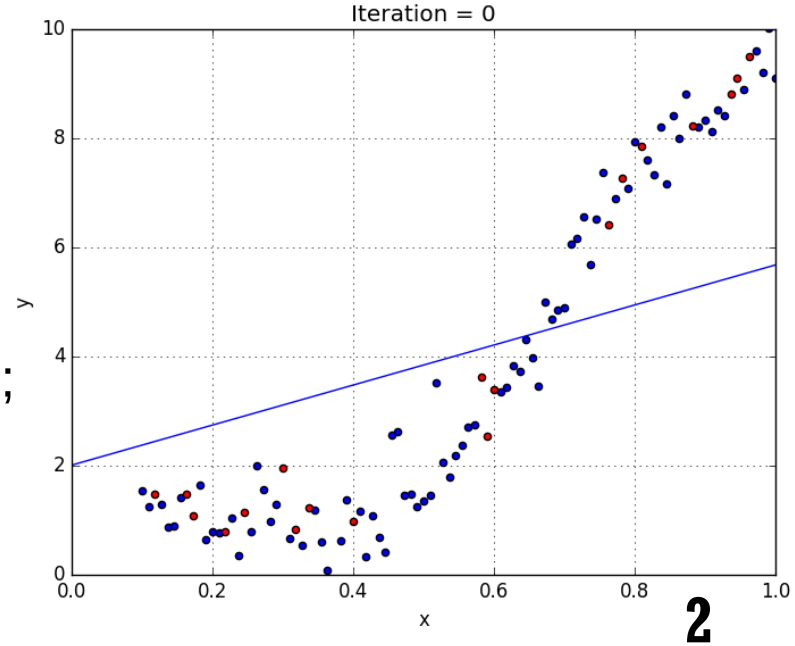
Regression model training task:

$$\frac{1}{N}\sum_{i=1}^{N} L\left(y_i, f\left(x_i; \theta, s\right)\right) + \lambda\Omega\left(\theta, s\right) \to \min_{s \in S} \min_{\theta \in \Theta}$$

$L\left(y_i, f\left(x_i; \theta, s\right)\right) = \left(y_i - f\left(x_i; \theta, s\right)\right)^2$ - mean squared error (MSE) loss;

$\Omega\left(\theta, s\right)$ – regulatory functionality;

λ – regularisation coefficient.



AIM AND OBJECTIVES

- *The aim of this work* is to improve the accuracy of predicting target variable values based on observed data by developing a structural optimization method using evolutionary computation.

Research tasks:

– to develop a genetic algorithm-based optimization method that determines the optimal architecture and type of regression model in high-dimensional feature spaces by sequentially selecting, combining, and varying candidate solution parameters using evolutionary mechanisms.

– to develop an approach for identifying the operational parameters of a genetic algorithm using a benchmark nonlinear function, which will enable the effective detection of the optimal structure of a regression model;

– to assess the effectiveness of established regression model types by applying the developed genetic algorithm-based structural optimization method to benchmark dataset models that represent the descriptive characteristics of real-world systems.

GENETIC ALGORITHM-BASED STRUCTURAL OPTIMIZATION METHOD FOR REGRESSION MODELS

$$c = (s, \theta) \quad (1)$$

s – chromosomes encoding the model structure;

θ – genes directly encoding the regression model parameters.

The chromosome value as a solution for searching the optimal number of the most important features:

$$c \equiv s = (s_1\ s_2\ \ldots\ s_p) \in B^p,\ B = \{0,1\} \quad (2)$$

$$s_j = \begin{cases} 1, \text{if the } j-\text{th feature is selected;} \\ 0, \text{if the } j-\text{th feature is not selected,} \end{cases}$$

Fitness function: $$F(c) = -J(c) = -\left[\frac{1}{N}\sum_{i=1}^{N} L\left(y_i,\ f\left(x_i^{(c)}; \theta^*(c)\right)\right) + \lambda \sum_{j=1}^{p} c_j\right]. \quad (3)$$

$\sum_{j=1}^{p} c_j$ – the number of selected features;

λ – the penalty value for an excessive number of features.

Structural optimization of a regression model is the search for a solution to another fitness function optimization problem:

$$c^* := \arg\max_{c \in \{0,1\}^p} F(c) \quad (4)$$

Population: $$P^{(m)} = \left(c_1^{(m)}, c_2^{(m)}, \ldots, c_M^{(m)}\right) \in C^M = \left(\{0,1\}^P\right)^M \quad (5)$$

m – generation number, M – population size.

GENETIC ALGORITHM FOR STRUCTURAL OPTIMIZATION OF A REGRESSION MODEL

$$P^{(m+1)} = \mathrm{E}\left(P^{(m)}\right) \cup \mathrm{M}\left(\aleph\left(S\left(P^{(m)}\right)\right)\right) \quad (6)$$

$$\mathrm{E}\left(\boldsymbol{P}^{(m)}\right) = \arg\max_{\varepsilon}\left\{F\left(\boldsymbol{c}\right) \mid \boldsymbol{c} \in \boldsymbol{P}^{(m)}\right\} \quad (7)$$

$\varepsilon \in \{1, 2, \ldots, M\}$ - number of elite individuals;

- $\boldsymbol{P}_{sl}^{(m)} = \boldsymbol{S}\left(\boldsymbol{P}^{(m)}\right) = \left\{\boldsymbol{c}_1^{sl}, \boldsymbol{c}_2^{sl}, \ldots, \boldsymbol{c}_M^{sl}\right\}$ - reproduction (selection) operator; (8)

  $\boldsymbol{c}_j^{sl} = \arg\max_{\boldsymbol{c} \in \boldsymbol{T}_j} F(\boldsymbol{c})$ - independent tournament of size τ;

- $\boldsymbol{P}_{cr}^{(m)} = \aleph\left(\boldsymbol{P}_{sl}^{(m)}\right) = \bigcup_{j=1}^{M/2} \aleph\left(\boldsymbol{c}_{2\delta-1}, \boldsymbol{c}_{2\delta}; r_\delta\right)$ - genetic crossover operator; (9)

  $r_\delta \in \{1, 2, \ldots, p-1\}$ - randomly selected crossover point for the δ-th pair of parent chromosomes;

  $\aleph\left(\boldsymbol{c}_{2\delta-1}, \boldsymbol{c}_{2\delta}; r_\delta\right) = \boldsymbol{c}'_{2\delta-1}, \boldsymbol{c}'_{2\delta}$ - two offspring chromosomes are generated according to a given rule.

- $\boldsymbol{P}_{mut}^{(m)} = \mathrm{M}\left(\boldsymbol{P}_{sl}^{(m)}\right) = \left\{\mathrm{M}\left(\boldsymbol{c}_j\right) \mid \boldsymbol{c}_j \in \boldsymbol{P}^{(m)}\right\}$ - genetic mutation operator; (10)

$$\mathrm{M}\left(\boldsymbol{c}_j\right) = \boldsymbol{c}'_j = \left(\boldsymbol{c}'_{1j}, \boldsymbol{c}'_{2j}, \ldots, \boldsymbol{c}'_{ij}\right) \quad \boldsymbol{c}'_{ij} = \begin{cases} 1 - \boldsymbol{c}_{ij}, \text{ with probability } p_{mut}; \\ \boldsymbol{c}_{ij}, \text{ with probability } 1 - p_{mut}. \end{cases}$$

REGRESSION METHODS

LINEAR REGRESSION

$$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + \boldsymbol{b}$$

$\boldsymbol{w}$, $\boldsymbol{b}$ – model parameter vectors

GRADIENT BOOSTING REGRESSION (GBR)

$$f(\boldsymbol{x}) = \sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x})$$

$\alpha_t(\boldsymbol{x})$ – weight coefficient of the t-th decision tree

k-NEAREST NEIGHBORS (kNN)

$$f(\boldsymbol{x}) = \frac{1}{k} \sum_{j \in N_k(\boldsymbol{x})} y_i$$

k – number of nearest points,

$N_k(\boldsymbol{x})$ – k nearest points

RANDOM FOREST (RF)

$$f(\boldsymbol{x}) = \frac{1}{T} \sum_{t=1}^{T} h_t(\boldsymbol{x})$$

T - number of decision trees,

$h_t(x)$ - predicted value from the t-th decision tree

MULTILAYER PERCEPTRON (MLP)

$$f(\boldsymbol{x}) = f_L(\ldots f_2(f_1(\boldsymbol{x})))$$

L - Number of network layers

GENETIC ALGORITHM TUNING

$$y_i = 10\sin\left(\pi x_{i1} x_{i2}\right) + 20\left(x_{i3} - 0,5\right)^2 + 10x_{i4} + 5x_{i5} + \varepsilon_i; \qquad \boldsymbol{X} = \left[x_{ij}\right] \in \mathbb{R}^{N\times p} \qquad (11)$$

$x_{i1}, \ldots, x_{i5}$ - relevant features; $x_{i6}, \ldots, x_{ip}$ - noisy features; ε_i - additive noise;

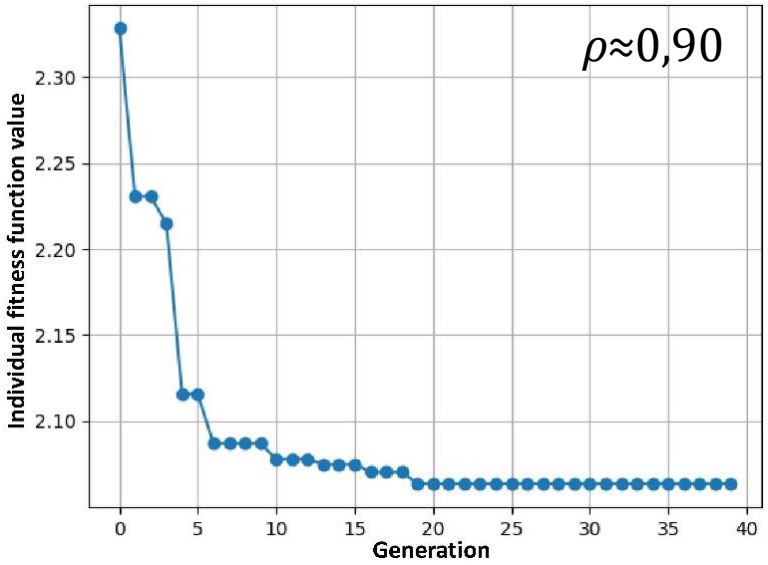
Table 1 - The target variable value based on relevant and noisy features

№	x_1	x_2	x_3	x_4	x_5	x_6	x_{17}	x_{18}	x_{19}	x_{10}	x_{11}	x_{12}	x_{13}	x_{14}	x_{15}	y
0	0,542	0,601	0,558	0,735	0,953	0,854	0,623	0,875	0,320	0,275	0,032	0,242	0,845	0,119	0,774	20,72
1	0,537	0,377	0,939	0,269	0,289	0,597	0,638	0,047	0,152	0,904	0,602	0,677	0,083	0,489	0,697	13,93
2	0,217	0,488	0,488	0,068	0,565	0,702	0,546	0,534	0,401	0,312	0,971	0,608	0,653	0,592	0,048	6,770

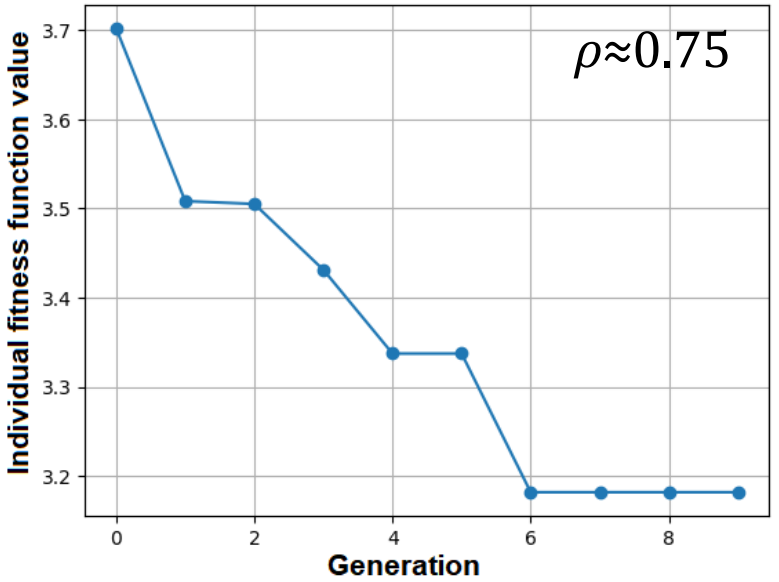
Table 2 - Genetic algorithm parameters for the Friedman-1 dataset

Type of regression model	Population size, M	Crossover/mutation probability, p_{cr}/p_{mut}	Penalty value, λ
kNN	14-50	0,7/0,2	0,01
RF	16-60	0,9/0,1	0,01
GBR	18-40	0,8/0,1	0,04
LR	16-40	0,8/0,2	0,02
MLP	18-40	0,9/0,2	0,01

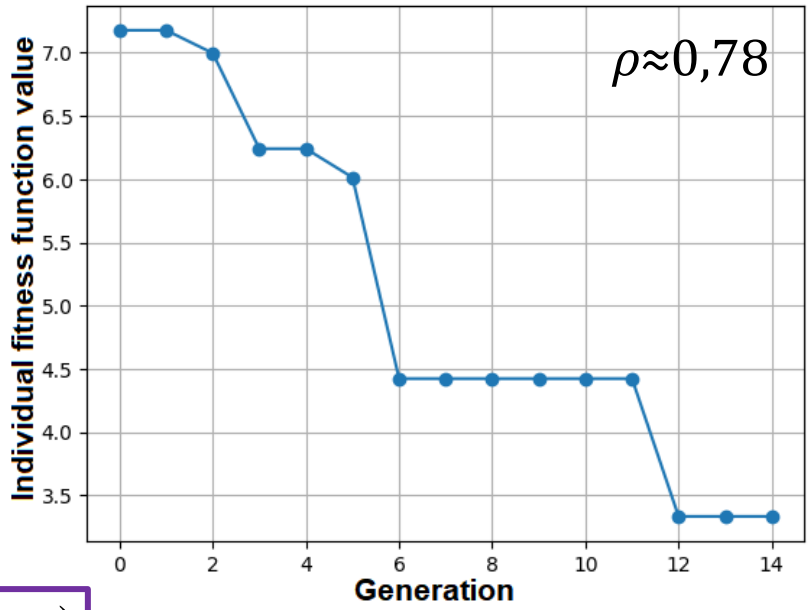
Gradient Boosting Regression



Random Forest

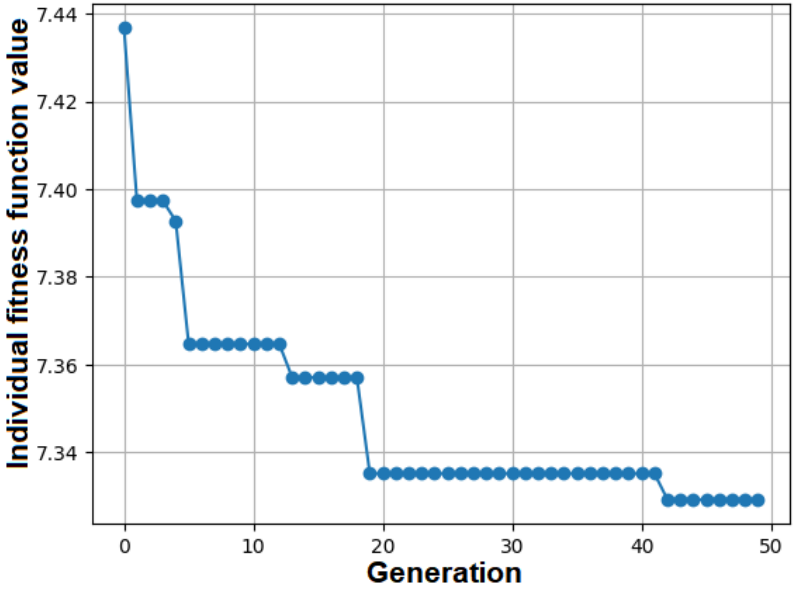


kNN



$$s = (x_1\ x_2\ \dots\ x_{15}) = (111110000000000)$$

Linear regression



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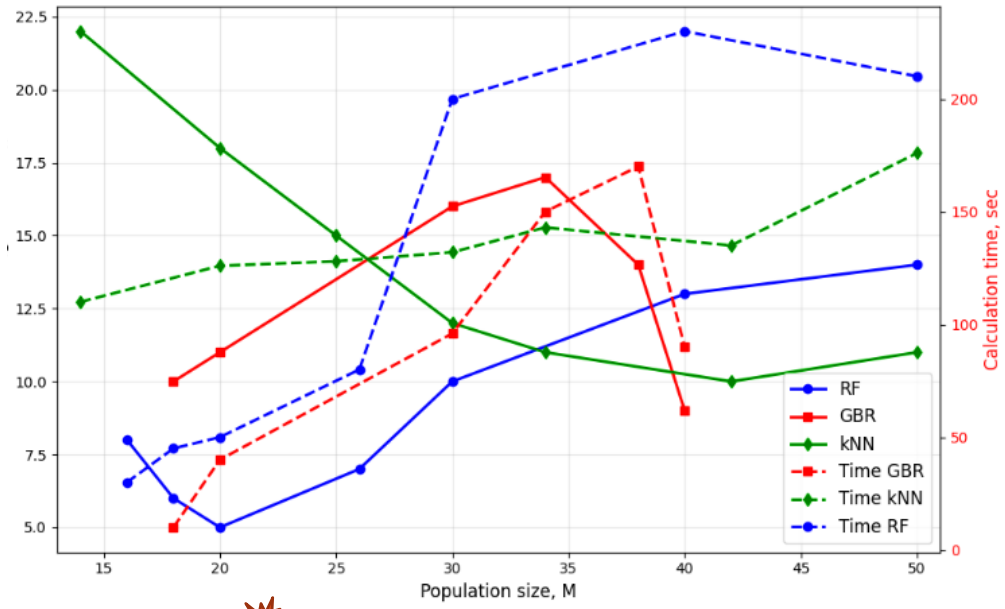
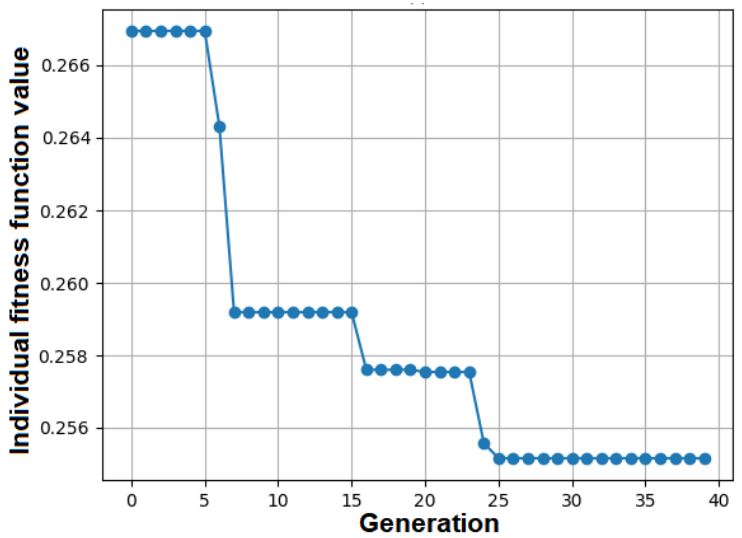


MLP



(111111000100000)

EXPERIMENTAL RESULTS

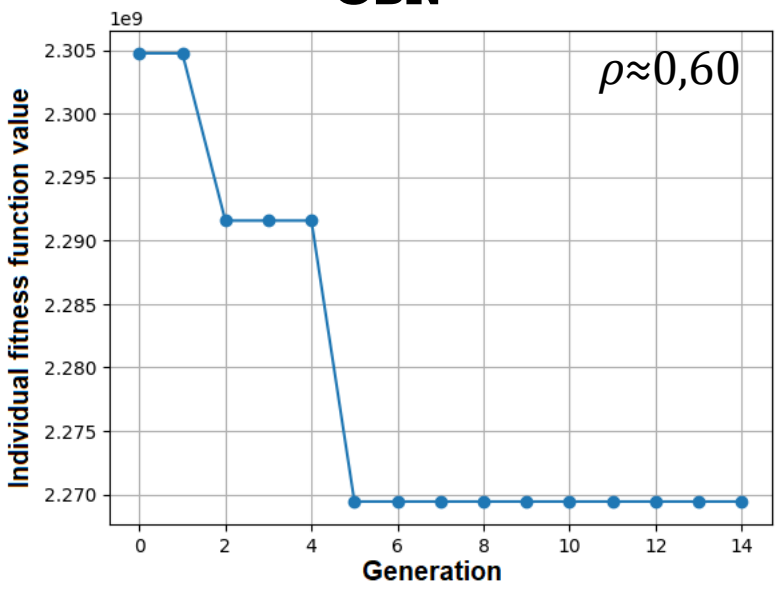
$\rho \approx 0{,}90$

Table 3. Response variable of the California Housing dataset

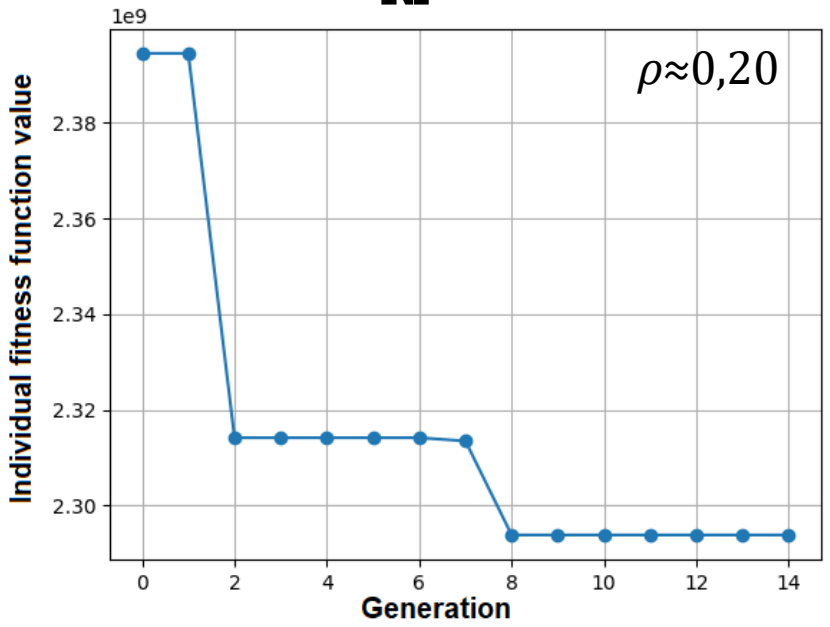
№	Longitude	Latitude	Housing_median_age	Total_ rooms	Total_ bedrooms	Population	Households	Median_income	Median_house_ value
	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	Y
0	-114,31	34,19	15,0	5612,0	1283,0	1015,0	472,0	1,4936	66900,0
1	-114,47	34,40	19,0	7650,0	1901,0	1129,0	463,0	1,8200	80100,0
2	-114,56	33,69	17,0	720,0	174,0	33,0	117,0	1,6509	85700,0

$$\boldsymbol{s} = (x_1\ x_2\ \ldots\ x_8) \equiv (s_1\ s_2\ \ldots\ s_8)$$

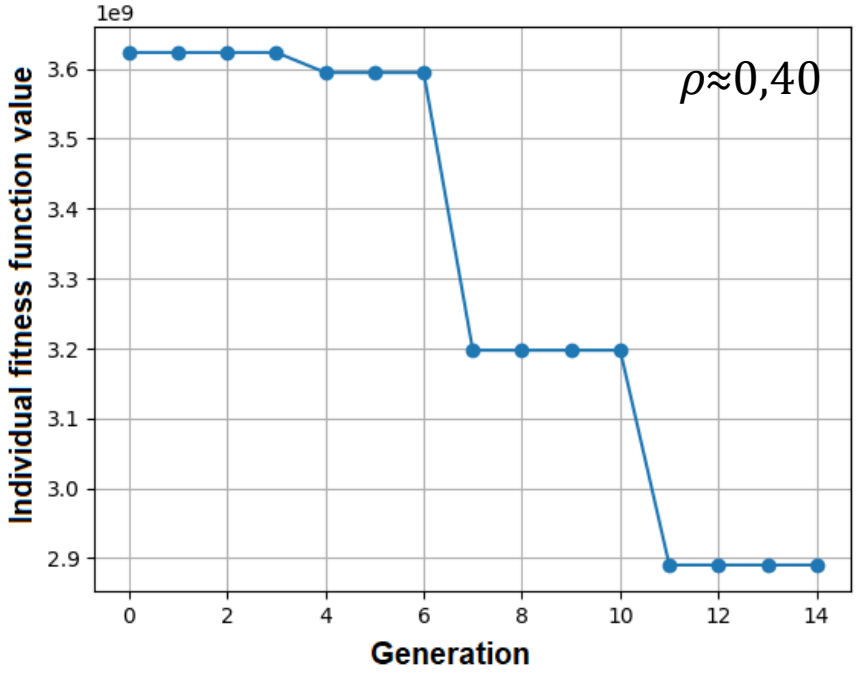
GBR



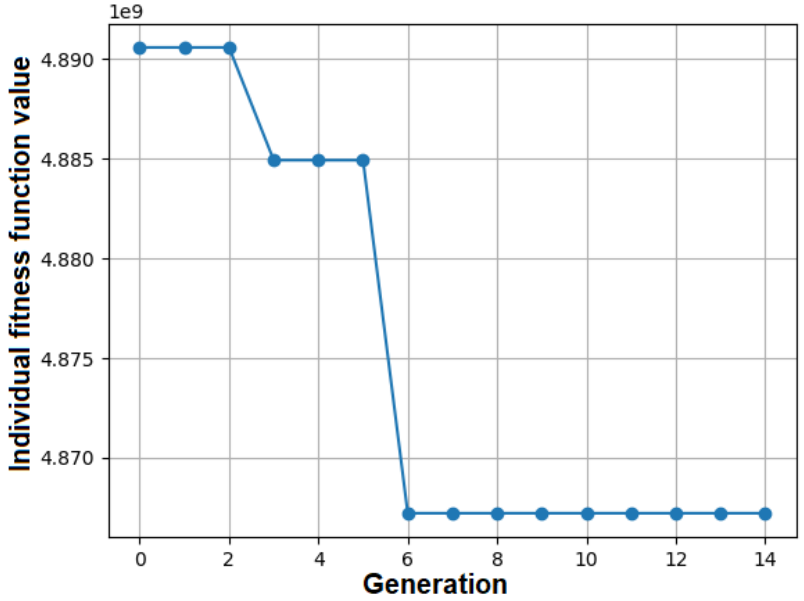
RF



kNN



LR



MLP

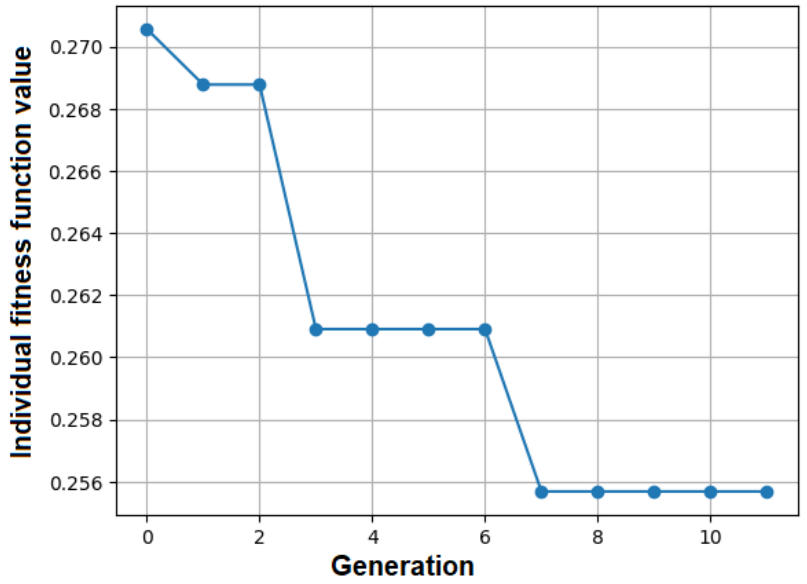
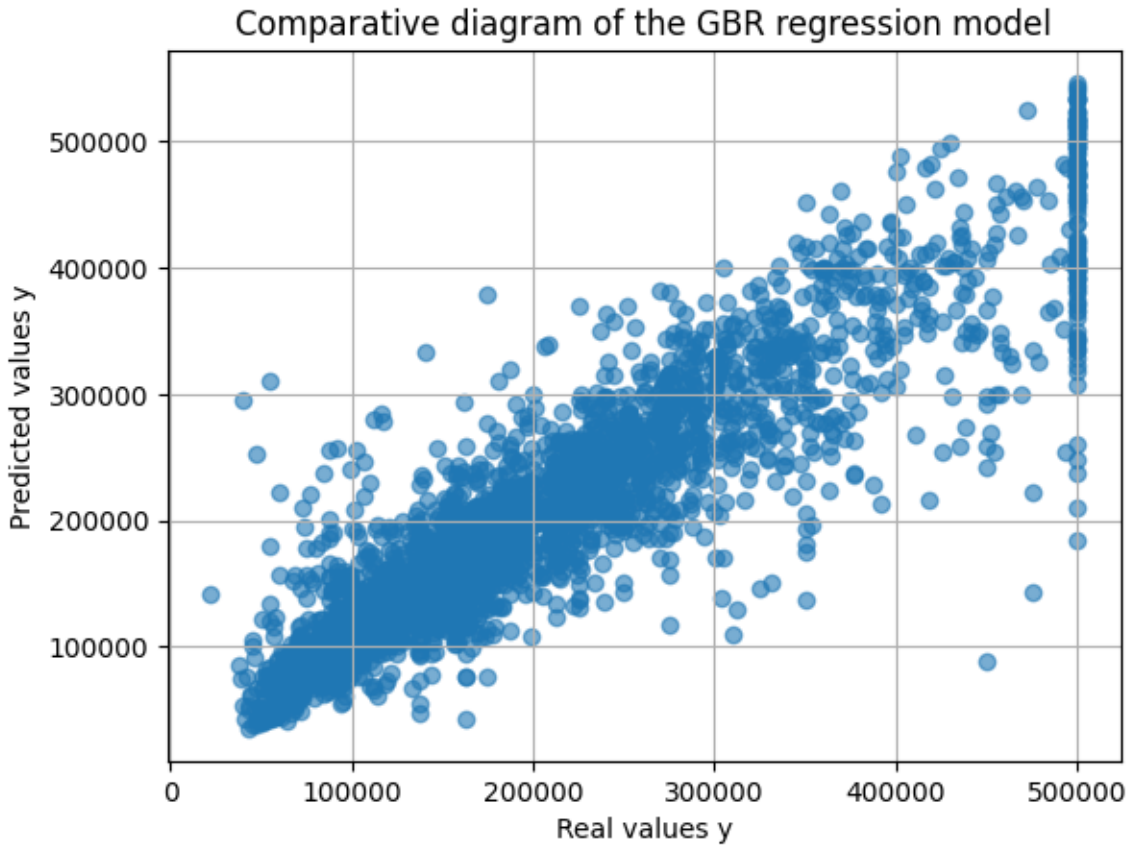


Table 4. Results of regression model structural optimization using a genetic algorithm

Regression Model	Vector of optimal features			Coefficient of determination of the baseline regression model, R^2	Coefficient of determination after structural optimization, R^2		
	Genetic Algorithm	Lasso	Recursive Feature Elimination (RFE)		Genetic Algorithm	Lasso	Recursive Feature Elimination (RFE)
kNN	[1,1,0,0,0,0,0,0]	[1,1,1,1,1,1,1,1]	[1,1,0,0,1,1,0,1]	0,70	0,77	0,70	0,70
RF	[1,1,0,1,0,1,0,1]			0,80	0,82	0,80	0,81
GBR	[1,1,1,1,0,1,0,1]			0,81	0,83	0,81	0,81
LR	[1,1,1,1,1,1,1,1]			0,62	0,62	0,62	0,60
MLP	[1,1,1,1,1,1,1,1]			0,75	0,75	0,75	0,74

REFERENCES

- The paper addresses the solution of an important scientific and practical problem of structural optimization of regression models (SORM) using a genetic algorithm (GA). The application of the GA increased the prediction accuracy of regression models by an average of 5% compared to the use of regularization methods.
- A conditional multi-objective SORM problem is formulated using a two-level minimization of the empirical risk functional on a training dataset for ensemble, local, and globally parametric regression methods. The problem is solved using a genetic algorithm with a fitness function based on a quadratic loss and a feature-number penalty.



- A parameter identification approach for the genetic algorithm based on the nonlinear Friedman-1 function was developed to determine the optimal population size, crossover and mutation probabilities, and the fitness penalty value.
- The testing results demonstrated an average increase in the coefficient of determination of the regression models by $\Delta R^2 = 0.036$, while the number of irrelevant features was reduced by an average of 46% for ensemble and local regression methods based on the genetic algorithm. In addition, the results of the GA iterative computations in SORM exhibited linear-type asymptotic convergence with an empirical coefficient of $\rho \approx 0.90$.

Thank you for your attention!

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