Metaheuristic Search in Mixed Kernel and Spline Truncated Non-parametric Regression

Mustika Hadijati[1], Irwansyah[2], Nurul Fitriyani[1,3], Muhammad Sopian Sauri[4]

***Abstract*—Non-parametric regressions are widely used in data analysis because of their flexibility. Apart from their applicability, it is not easy to find the optimal parameters of the corresponding non-parametric models. This situation is caused by the non-existence of a closed formula of the optimal parameters. In this paper, we propose a metaheuristic approach for optimal parameter search in mixed kernel and truncated spline and kernel regression. Moreover, we provide examples on how to implement the proposed algorithm to both real and simulated datasets. The results indicate that the algorithm yields highly accurate predictions for mixed truncated spline and kernel regression models.**

I. INTRODUCTION

NON-PARAMETRIC regression has been widely used in data analysis because of its flexibility. The non-parametric regression has been widely applied in several real world data analysis, such as the prediction of the water discharge volume in the watersheds in Lombok Island [8], the modeling of the sustainable development goals achievement in East Java [5], the modeling of the population growth rate in West Nusa Tenggara Province [7], and the modeling of the human development index data in East Java [1].

In the non-parametric regression, the regression curve is assumed to be smooth, *i.e.* continuous and differentiable [6], [3]. The two most commonly used nonparametric regression models are the spline and kernel nonparametric regression models. Each of those aforementioned model has its own characteristics corresponding to the relation between its independent and dependent variables. A multivariate non-parametric model generally uses only one approach, such as either truncated splines or kernels. This approach assumed that the relations between each independent variable and the dependent variable are the same for all independent variables. Although, in reality each independent variable can have a different relation pattern to the dependent variable. Several studies have been conducted to provide alternative approaches to obtain better model and predictions. One of those alternatives is by combining more than one non-parametric models for the prediction. Several studies showed that by combining several methods, such as spline and kernel [3], [15], [10], [11], spline, kernel, and Fourier series [1], kernel and Fourier series [2], [13], and so on, give better outcome. These combinations of non-parametric models usually called a mixed non-parametric model. Studies related to mixed nonparametric regression have been done on the combination of spline and kernel estimators and their properties, including models with bi-response [5], multi-response [14], and multivariate variables [15].

In the non-parametric models, the model parameters determine the accuracy of the models. For this reason, it is necessary to determine the optimum values of the parameters to get an accurate non-parametric model. One criterion that can be used to achieve this goal is by minimizing the generalized cross-validation (GCV) value [6], [9]. In most cases, selecting the optimal values of the parameters are computationally expensive. This situation is caused by the non-existence of a closed formula for the optimal parameters and the number of parameters in a model can be very large. In the previous studies, the optimal parameters was found using brute force search [18], [4]. This approach is impossible to use for a model with large number of parameters.

An optimization algorithm, such as metaheuristic search, can be used to overcome this problem and also to make the estimation process more efficient. The studies related to the usage of optimization algorithms in choosing optimal parameters is still not widely explored. Therefore, in this paper, we propose an implementation of metaheuristic search to determine the optimal parameters of mixed kernel and spline truncated regression.

II. MAIN RESULTS

A. Parameter Search Formulation

Given the data $(\mathbf{t}, \mathbf{z}, \mathbf{y}) = (t_{i1}, \ldots, t_{ik}, z_{i1}, \ldots, z_{im}, y_i)_{i=1,2,\ldots,n}$, where $(\mathbf{t}, \mathbf{z})$ is the predictor (independent) variables and $\mathbf{y}$ is the response (dependent) variable. The relationship between $(\mathbf{t}, \mathbf{z})$ and $\mathbf{y}$ is assumed to follow a nonparametric regression model as follows:

$$y_i = \mu\left(t_{i1}, \ldots, t_{ik}, z_{i1}, \ldots, z_{im}\right) + \varepsilon_i \tag{1}$$

for all $i = 1, \ldots, n$. The regression curve $\mu\left(t_{i1}, \ldots, t_{ik}, z_{i1}, \ldots, z_{im}\right)$ is assumed to be unknown and smooth. The random error ε_i is assumed to be independent and is normally distributed with $E(\varepsilon_i) = 0$ and $E(\varepsilon_i^2) = \sigma^2$. In this paper, we assume that the regression

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model is an additive mix between truncated spline and kernel non-parametric regression as follows:

$$\mu\left(t_{i1},\ldots,t_{ik},z_{i1},\ldots,z_{im}\right)=\sum_{r=1}^{k}\hat{\tilde{g}}_r(t_{ir},\tilde{d},\tilde{\alpha})+\sum_{s=1}^{m}\hat{\tilde{h}}_{\beta_s}(z_{is}) \tag{2}$$

where $\tilde{d}$ is the common degree of spline polynomials, $\tilde{\alpha}$ are the knot points for the truncated parts of spline polynomials and $\tilde{\beta}=(\beta_s)_{s=1}^{m}$ are the bandwidths for kernel regression.

In the case of spline-based methods, the resulting patterns typically exhibit piecewise polynomial structures with smooth transitions at the knot points. In contrast, kernel-based methods tend to generate more irregular, locally driven patterns that do not display a clearly defined global structure. Based on these facts, in order to determine whether an independent variable/predictor $\mathbf{x}$ is included as $\mathbf{t}$ or $\mathbf{z}$ in the mixed model 2, use the following steps:

(1) Create a scatter plot between $\mathbf{x}$ and the corresponding response variable
(2) Use the following rules:

(2.1.) If the scatter plot in step (1) exhibit a piece-wise polynomial pattern, then $\mathbf{x}$ will be included as $\mathbf{t}$.
(2.2.) If the scatter plot in step (1) does not exhibit any particular pattern, then $\mathbf{x}$ will be included as $\mathbf{z}$.

For a more detailed description of the aforementioned mixed model, see [15].

Let $f(\mathbf{t},\mathbf{z},\mathbf{y},\tilde{d},\tilde{\alpha},\tilde{\beta})$ be a measure function for the regression model in 2. Some frequently used measure functions include mean squared error (MSE), cross-validation (CV), and generalized cross-validation (GCV). The function $f(\mathbf{t},\mathbf{z},\mathbf{y},\tilde{d},\tilde{\alpha},\tilde{\beta})$ measures how *close* the prediction by the regression model induced by the smoothing parameters $(\tilde{d},\tilde{\alpha},\tilde{\beta})$ to the original data. Therefore, we can formulate a search for the optimal parameters as follows.

Solve

$$\text{Argmin}_{(\tilde{d},\tilde{\alpha},\tilde{\beta})}f(\mathbf{t},\mathbf{z},\mathbf{y},\tilde{d},\tilde{\alpha},\tilde{\beta}) \tag{3}$$

using the Algorithm 1.

Algorithm 1 Find $(\tilde{d},\tilde{\alpha},\tilde{\beta})$ to minimize $f(\mathbf{t},\mathbf{z},\mathbf{y},\tilde{d},\tilde{\alpha},\tilde{\beta})$

Input:
$\mathbf{t}$ = independent variables for spline polynomial
$\mathbf{z}$ = independent variables for kernel regression
$\mathbf{y}$ = dependent variables
n_pop = number of randomly generated initial solutions
$max\_measure$ = fixed upper bound for f
max_iter = number of iterations/process

Initialize:

$pop=(\tilde{d}_i,\tilde{\alpha}_i,\tilde{\beta}_i)_{i=1}^{n\_pop}\leftarrow rand(n\_pop)$ ▷ randomly generated initial solutions
$iteration\leftarrow 0$

while $iteration\leq max\_iter$ or $f>max\_measure$ **do**
$pop\_select\leftarrow selection(pop,f)$ ▷ selection of solutions based on their f value
$pop\_new\leftarrow update\_pop(pop\_select)$ ▷ produce new solutions from the selected solutions
$pop\leftarrow pop\_select\bigcup pop\_new$
$iteration\leftarrow iteration+1$
end while

Here is a description of the parameters and functions in Algorithm 1.

- The parameter n_pop depends on the search method used. For example, if we use simulated annealing, then $n\_pop=1$. If the search algorithms are Particle Swarm Optimization (PSO) and Genetics Algorithm (GA), then $n\_pop>1$.
- There are no close formulas for the values of $max\_measure$ and max_iter. One way to estimate the values is by observation in computational experiments.
- The function `rand(n_pop)` consists of several functions, where each function generates $\tilde{d}$ or $\tilde{\alpha}$ or $\tilde{\beta}$ randomly. So,

$$\begin{aligned} rand(n\_pop) &= rand_{\tilde{d}}(n\_pop,\tilde{d}\_l,\tilde{d}\_u) \\ &\quad\circ rand_{\tilde{\alpha}}(n\_pop,\tilde{\alpha}\_l,\tilde{\alpha}\_u) \\ &\quad\circ rand_{\tilde{\beta}}(n\_pop,\tilde{\beta}\_l,\tilde{\beta}\_u) \end{aligned}$$

and

$$(\tilde{d},\tilde{\alpha},\tilde{\beta})=\left(rand_{\tilde{d}}||rand_{\tilde{\alpha}}||rand_{\tilde{\beta}}\right),$$

with τ_l and τ_u are lower bound and upper bound for the corresponding variable, respectively, where $\tau\in\{\tilde{d},\tilde{\alpha},\tilde{\beta}\}$.
- There are numerous ways to execute the function `selection(pop,f)`. Here are two popular choices:
  a. selection based on the best f value
  b. selection based on the probability, where the probability value is determined by the f value
- The function `update_pop(pop_select)` usually has at least one of the following two functions:
  a. the function `combine`: to combine selected solutions to produce new solutions

b. the function `rand_mut`: to do a random mutation on some of the new solutions

Notice that the function `rand_mut` consists of several functions, where each function performs a random mutation on $\tilde{d}$ or $\tilde{\alpha}$ or $\tilde{\beta}$. So,

$$rand\_mut(pop\_select) = \begin{array}{l} rand\_mut_{\tilde{d}}(n\_pop, p_{\tilde{d}}) \\ \circ\, rand\_mut_{\tilde{\alpha}}(n\_pop, p_{\tilde{\alpha}}) \\ \circ\, rand\_mut_{\tilde{\beta}}(n\_pop, p_{\tilde{\beta}}) \end{array}$$

where p_γ is the mutation probability for the parameter $\gamma \in \{\tilde{d}, \tilde{\alpha}, \tilde{\beta}\}$.

B. Examples

In this part, we give examples on how to apply Algorithm 1 to find optimal parameters of mixed truncated spline and kernel regression. We use two well-known metaheuristic search, genetics algorithm (GA) and particle swarm optimization (PSO), for the regression's optimal parameters search. In this case, there are two kinds of parameters to search, (1) bandwidths for kernel regression, and (2) knot points for spline truncated regression with fixed polynomial degree and number of knot points. The R codes, datasets, and outputs related to these examples are available at https://github.com/iwplus/nonpar-metaheuristic.

One way to measure the optimality of parameters in a mixed non-parametric model is by using generalized cross-validation (GCV). The related GCV function for the model 2 is as follows [15]:

$$GCV\left(\tilde{d}, \tilde{\alpha}, \tilde{\beta}\right) = \frac{n^{-1}\|\left(I - M(\tilde{d}, \tilde{\alpha}, \tilde{\beta})\right)\tilde{y}\|^2}{\left(n^{-1}tr\left(I - M(\tilde{d}, \tilde{\alpha}, \tilde{\beta})\right)\right)^2} \quad (4)$$

with $M(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) = K(\tilde{d}, \tilde{\alpha}) + D(\tilde{\beta})$, where $K(\tilde{d}, \tilde{\alpha})$ is the matrix related to spline truncated approximation with multi-degree $\tilde{d}$ and knot points $\tilde{\alpha}$, and $D(\tilde{\beta})$ is the matrix related to kernel approximation with bandwidths $\tilde{\beta}$. For more details about these matrices, see [15]. In all of our examples, we will use

$$f(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) = GCV(\tilde{d}, \tilde{\alpha}, \tilde{\beta}). \quad (5)$$

1) Datasets descriptions: In order to showcase the performance of our proposed algorithm, we use the following four datasets.

(a) The 2016 percentage data of malnourished children under five years of age in West Nusa Tenggara. We denote this dataset as *A1* data.

(b) A synthetic data with 200 entries, denoted by *M1* data, generated by the following rules:

$$X_1 \sim Uniform(0,1), \quad X_2 \sim Uniform(-1,1),$$

$$\epsilon \sim Normal(0, 0.1^2),$$

$$Y = \sin\left(\tfrac{X_1}{2}\right) + 0.8e^{-X_2^2} + 0.3\cos\left(\tfrac{X_1 X_2}{5}\right) + \epsilon.$$

(c) A synthetic data with 200 entries, denoted by *M2* data, generated by the following rules:

$$X_1 \sim Uniform(0,1), \quad X_2 \sim Uniform(-1,1),$$

$$\epsilon \sim Normal(0, 0.1^2),$$

$$Y = \sin\left(\tfrac{X_1}{2}\right) + 0.8\tfrac{e^{-X_2^2}}{\sqrt{2\pi}} + \epsilon.$$

(d) A synthetic data with 200 entries, denoted by *M3* data, generated by the following rules:

$$X_1, X_3 \sim Uniform(0,1), \quad X_2 \sim Uniform(-1,1),$$

$$\epsilon \sim Normal(0, 0.1^2),$$

$$Y = \sin\left(\tfrac{X_1}{2}\right) + 0.8\tfrac{e^{-X_2^2}}{\sqrt{2\pi}} + 0.3X_3 + \epsilon.$$

Figures 1-4 show the relation patterns between independent variables and the response variable for each data.

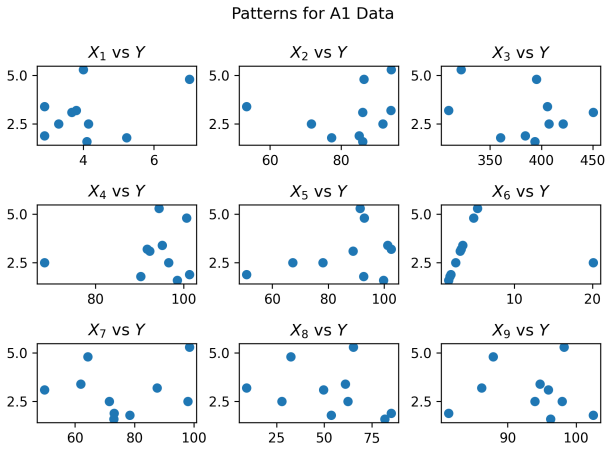

Fig. 1. Scatter plots between each predictor variable to the response variable for A1 data

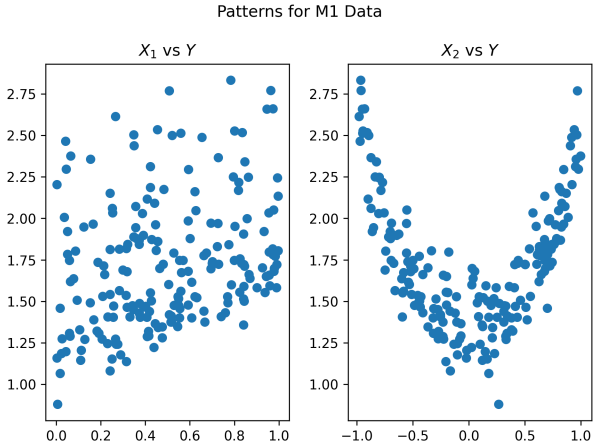

Fig. 2. Scatter plots between each predictor variable to the response variable for M1 data

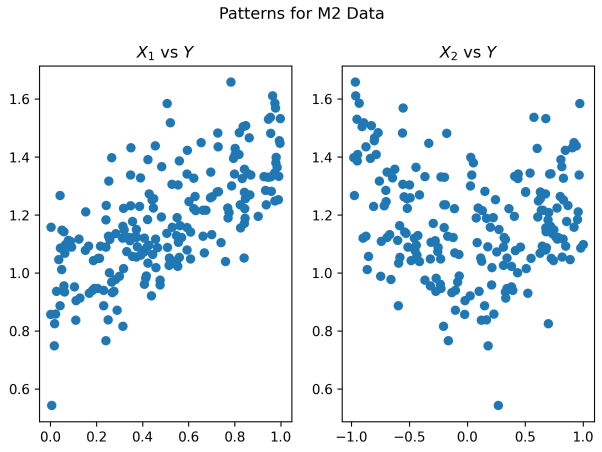

Fig. 3. Scatter plots between each predictor variable to the response variable for M2 data

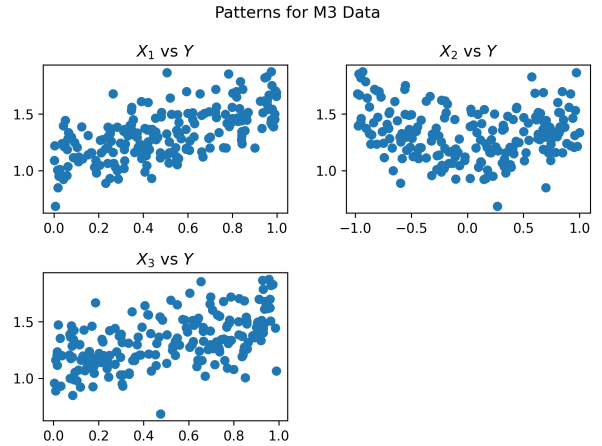

Fig. 4. Scatter plots between each predictor variable to the response variable for M3 data

The patterns summarized on Table I.

Based on, for example, Figure 1, variables X_1, X_2, X_3, X_4, and X_5 appear to follow the characteristics typically associated with the kernel approach, whereas X_6, X_7, X_8, and X_9 exhibit features more consistent with the spline approach. The same classification procedure is applied to datasets *M1*, *M2*, and *M3*.

TABLE I
PATTERNS SUMMARY FOR THE DATASETS A1, M1, M2, AND M3

Dataset	Kernel Pattern	Spline Pattern
A1	X_1, X_2, X_3, X_4, X_5	X_6, X_7, X_8, X_9
M1	X_1	X_2
M2	X_2	X_1
M3	X_2	X_1,X_3

2) Parameters search using genetics algorithm (GA): In order to perform GA search for the optimal parameters, set the following fitness function

$$fitness(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) = \frac{1}{f(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) + 1} \tag{6}$$

where $f(\tilde{d}, \tilde{\alpha}, \tilde{\beta})$ is the GCV function as in equation 5. For simplicity, in this example the multi-degree $\tilde{d}$ and the number of knot points are fixed. Also, each solution candidate represented as a vector $p_i = \left(\tilde{\alpha}_i, \tilde{\beta}_i\right)$ and the solutions population is the set of all p_i. The search objective is to find p_i which maximize $fitness$ function (thus minimize f). In order to complete the GA search, use the following steps:

(a) *Population initialization*: Generate $p_i = \left(\tilde{\alpha}_i, \tilde{\beta}_i\right)$, $i = 1, 2, \ldots, n_{pop}$, at random, such that

$$l_k \leq \tilde{\alpha}_i \leq u_k, l_h \leq \tilde{\beta}_i \leq u_h,$$

where n_{pop} is the number of solutions in the population, l_h and u_h are the vector of lower and upper bounds of bandwidths, respectively, and l_k and u_k are the vectors of minimum and maximum values of corresponding independent variables, respectively.

(b) *Selection*: The selection process follows *rank selection* algorithm. The rank selection consists of the following steps:

(b.1.) Sort the solutions based on their fitness values from smallest to largest

(b.2.) Assign the probability values, $prob_i$, to the solution p_i using the following formula

$$prob_i = \frac{pos_i}{n_{pop}(n_{pop}+1)/2},$$

where pos_i is the position of p_i after the sorting process.

(b.3.) Calculate the cumulative probability, c_i, using the following formula

$$c_i = \begin{cases} prob_i, & \text{if } i = 1 \\ prob_i + c_{i-1}, & \text{otherwise.} \end{cases}$$

(b.4.) Generate a random number r where $r \in [0, 1]$ and find j such that c_j is the smallest cumulative probability values which satisfies $c_j \geq r$. Then, take p_j as a selected solution.

(b.5.) Repeat step (b.4.) until some number of solutions selected

(c) *Crossover*: Let $\tilde{\alpha}_i = (\alpha_{i1}, \ldots, \alpha_{i,n_\alpha n_{knots}})$ and $\tilde{\beta}_i = (\beta_{i1}, \ldots, \beta_{in_\beta})$, where n_α, n_{knots}, and n_β are the number of independent variables related to spline truncated approximation, number of knot points, and the number of independent variables related to kernel approximation, respectively. The crossover between selected solutions p_s and p_t proceeds according to the following steps:

(c.1.) Generate random integers ind_α and ind_β, where $ind_\alpha \in [1, n_\alpha]$ and $ind_\beta \in [1, n_\beta]$.

(c.2.) Derive new solutions using the following formulas

$$O_1 = (\alpha_{s1}, \ldots, \alpha_{s,ind_\alpha - 1}, \alpha_{t,ind_\alpha}, \ldots, \alpha_{t,n_\alpha}, \beta_{s1}, \ldots, \beta_{s,ind_\beta - 1}, \beta_{t,ind_\beta}, \ldots, \beta_{t,n_\beta})$$

$$O_2 = (\alpha_{t1}, \ldots, \alpha_{t,ind_\alpha - 1}, \alpha_{s,ind_\alpha}, \ldots, \alpha_{s,n_\alpha}, \beta_{t1}, \ldots, \beta_{t,ind_\beta - 1}, \beta_{s,ind_\beta}, \ldots, \beta_{s,n_\beta}).$$

(d) *Mutation*: The mutation process on the new solution O_j is as follows:

(d.1.) Generate random integers ind_α and ind_β, where $ind_\alpha \in [1, n_\alpha n_{knots}]$ and $ind_\beta \in [1, n_\beta]$.

(d.2.) Replace α_{j,ind_α} with a random number from the interval $[l_k^{ind_\alpha}, u_k^{ind_\alpha}]$, where l_k^i and u_k^i are the i-th entries of the vectors l_k and u_k, respectively.

(d.3.) Replace β_{j,ind_β} with a random number from the interval $[l_h^{ind_\alpha}, u_h^{ind_\alpha}]$, where l_h^i and u_h^i are the i-th entries of the vectors l_h and u_h, respectively.

(e) Repeat steps (b)-(d) until the maximum iteration reached or the `max_measure` value criterion achieved

For more details on GA, see [17]. Figures 5-8 illustrate the prediction results based on mixed kernel and spline truncated regression with GA search for all datasets.

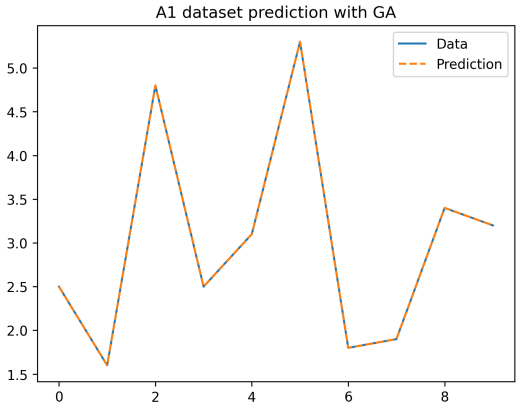

Fig. 5. The A1 dataset prediction with GA search

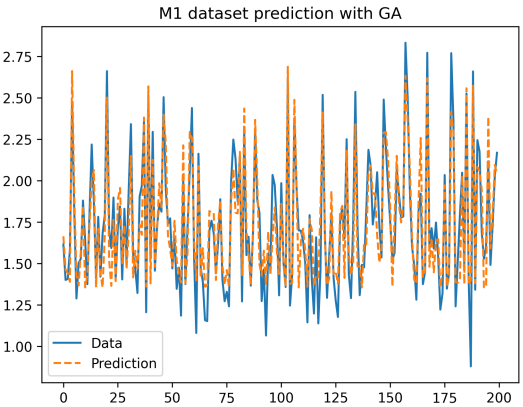

Fig. 6. The M1 dataset prediction with GA search

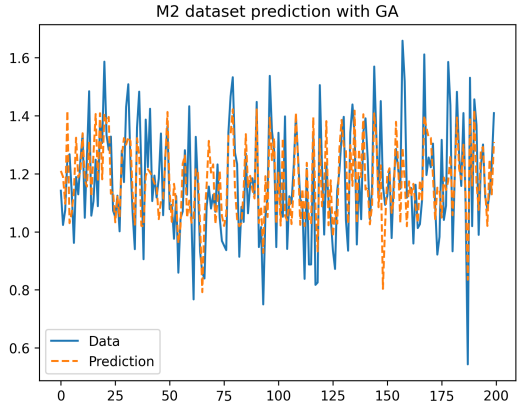

Fig. 7. The M2 dataset prediction with GA search

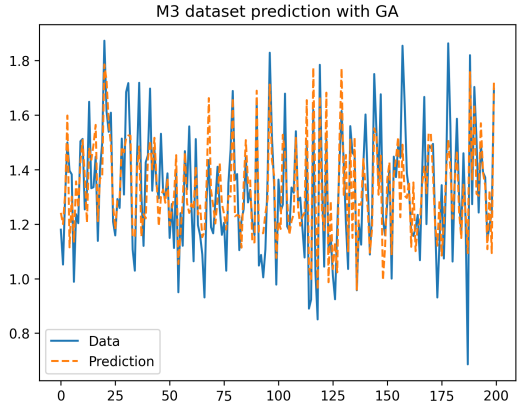

Fig. 8. The M3 dataset prediction with GA search

Table II shows the summary of the performances of GA search for optimal parameters search. The performances are measured by GCV, mean squared error (MSE), and mean average percentage error (MAPE) values. Note that, the A1 dataset prediction with GA search is a refinement of the one in [16].

TABLE II
GA SEARCH PERFORMANCES SUMMARY FOR THE DATASETS A1, M1, M2, AND M3

Dataset	GCV	MSE	MAPE (%)
A1	2.359×10^{-17}	1.67×10^{-20}	2.94×10^{-9}
M1	0.1443786	0.026062	8.11688
M2	0.07065457	0.018231566	9.556029
M3	0.06992612	0.01767	8.3484

3) Parameters search using particle swarm optimization (PSO): In order to perform PSO search for the optimal parameters, set the following fitness function

$$fitness(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) = \frac{1}{f(\tilde{d}, \tilde{\alpha}, \tilde{\beta}) + 1} \tag{7}$$

where $f(\tilde{d}, \tilde{\alpha}, \tilde{\beta})$ is the GCV function as in equation 5. As in GA search setup, in this example the multi-degree $\tilde{d}$ and the number of knot points are fixed. Also, each solution candidate

represented as a vector $p_i = \left(\tilde{\alpha}_i, \tilde{\beta}_i\right)$ and the solutions population is the set of all p_i. The search objective is to find p_i which maximize $fitness$ function (thus minimize f). The PSO search proceeds according the following steps:

(a) *Solution initialization*: Generate $p_i = \left(\tilde{\alpha}_i, \tilde{\beta}_i\right)$, $i = 1, 2, \ldots, n_{pop}$, at random, such that

$$l_k \leq \tilde{\alpha}_i \leq u_k, l_h \leq \tilde{\beta}_i \leq u_h,$$

where n_{pop} is the number of solutions processed in each iteration, l_h and u_h are the vector of lower and upper bounds of bandwidths, respectively, and l_k and u_k are the vectors of minimum and maximum values of corresponding independent variables, respectively.

(b) *Personal best initialization*: Let pb_i be the current personal best for solution p_i. Set $pb_i = p_i$.

(c) *Global best initialization*: Let g be the current global best solution. Find p_j for some $j \in \{1, 2, \ldots, n_{pop}\}$ such that $fitness(p_j) \geq fitness(p_i)$, for all i. Then set $g = p_j$.

(d) *Particle speed initialization*: Let v_i be the particle speed for solution p_i. Set $v_i = (0, 0, \ldots, 0)$.

(e) *Particle speed update*: Update the particle speed using the following equation:

$$v_i = v_i + c_1 \left(pb_i - p_i\right) R_1 + c_2 \left(g - p_i\right) R_2 \quad (8)$$

where c_1 and c_2 are constants such that $0 \leq c_1, c_2 \leq 4$, $R_1 = diag\left(r_1^1, r_2^1, \ldots, r_{n_{pop}}^1\right)$ and $R_2 = diag\left(r_1^2, r_2^2, \ldots, r_{n_{pop}}^2\right)$ with $r_j^k \sim Uniform(0, 1)$.

(f) *Solution update*: Update the solution p_i using the following equation:

$$p_i = p_i + v_i \quad (9)$$

(g) *Update personal and global best*: Use the following steps to update personal and global best:

(g.1.) If $fitness(p_i) \geq fitness(pb_i)$, then set $pb_i = p_i$.
(g.2.) If $fitness(p_i) \geq fitness(g)$, then set $g = p_i$.
(g.3.) Repeat steps (g.1) and (g.2) for all i.

(h) Repeat steps (d)-(g) until the maximum iteration reached or the `max_measure` value criterion achieved

For more details on PSO, see [12]. Figures 9-12 illustrate the prediction results based on mixed kernel and spline truncated regression with PSO search for all datasets.

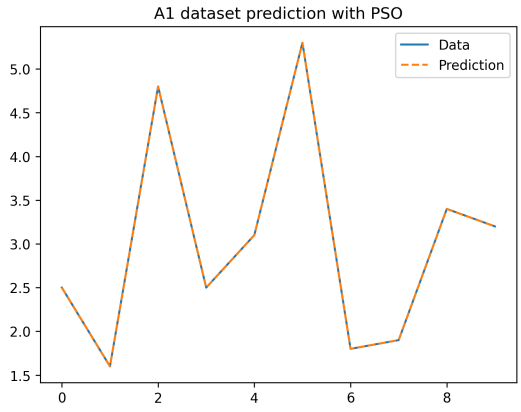

Fig. 9. The A1 dataset prediction with PSO search

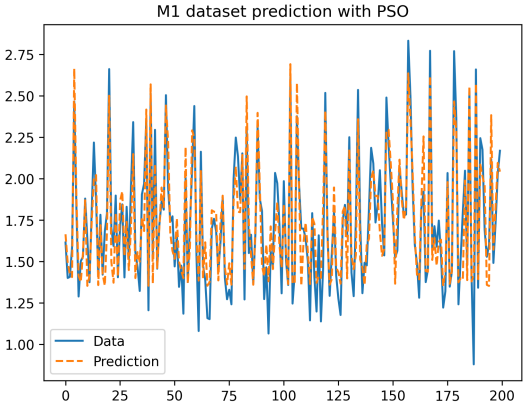

Fig. 10. The M1 dataset prediction with PSO search

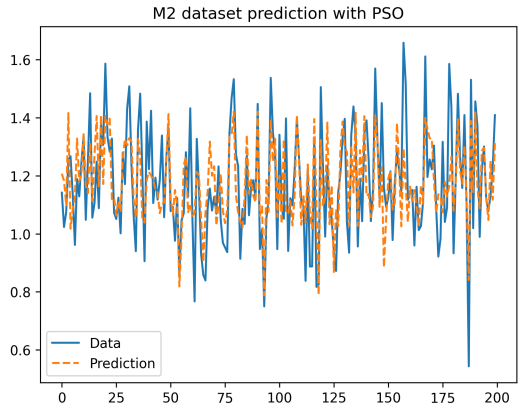

Fig. 11. The M2 dataset prediction with PSO search

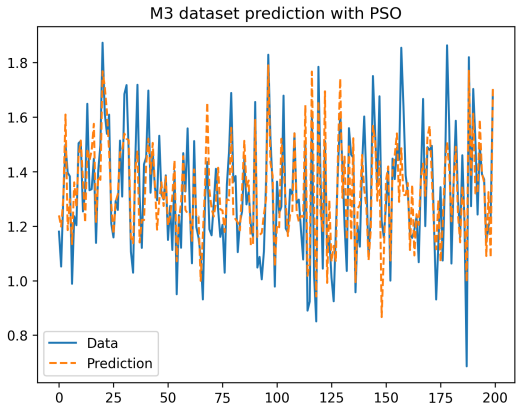

Fig. 12. The M3 dataset prediction with PSO search

Table III shows the summary of the performances of PSO search for optimal parameters search. The performances are measured by GCV, mean squared error (MSE), and mean average percentage error (MAPE) values.

TABLE III
PSO SEARCH PERFORMANCES SUMMARY FOR THE DATASETS A1, M1, M2, AND M3

Dataset	GCV	MSE	MAPE (%)
A1	6.04×10^{-22}	1.32×10^{-25}	1.065×10^{-11}
M1	0.1420934	0.025988	8.0799
M2	0.06799922	0.017978	9.3647
M3	0.06501043	0.017218	8.2632

III. CONCLUSIONS

In this study, we demonstrate that implementing metaheuristic search methods – specifically the genetic algorithm (GA) and particle swarm optimization (PSO) – in mixed truncated spline and kernel regression models yields accurate non-parametric estimates, with MAPE below 10%. This approach can also be adapted for other non-parametric models with minor modifications.

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