RMARS: Robustification of Multivariate Adaptive Regression Spline under Polyhedral Uncertainty

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Abstract

Since, with increased volatility and further uncertainties, financial crises translated a high "noise" within data from financial markets and economies into the related models, recent years' events in the financial world have led to radically untrustworthy representations of the future. Hence, robustification started to attract more attention in finance. The presence of noise and data uncertainty raises critical problems to be dealt with on theoretical and computational side. For immunizing against parametric uncertainties, Robust Optimization has gained in great importance as a modeling framework from both a theoretical and a practical point of view. Consequently, we include the existence of uncertainty considering future scenarios into Multivariate Adaptive Regression Spline (MARS) that has an apparent success in modeling real-life data in a variety of application fields, and robustify it through robust optimization proposed to cope with data and resulting model parameter uncertainty. We represent the new Robust MARS (RMARS) in theory and method and apply RMARS on financial market data. We demonstrate its well performance with a simulation study and a numerical experience that refers to basic economic indicators. Results indicate that models from RMARS have much less variability in parameter estimates and in accuracy measures, to the cost of just a slightly lower accuracy than MARS.

Keywords: MARS, Robust Optimization, Polyhedral Uncertainty, RMARS, Finance.

1 Introduction

1.1 The purpose of the study

Multivariate adaptive regression splines (MARS) [1, 2, 3] is a form of non-parametric regression analysis and, in recent years, applied in many fields of science, technology, finance and control design. It is a modern methodology of statistical learning, data mining and estimation theory which is important in both regression and classification. While obtaining a model by this well-known tool MARS, it is supposed that the input data are known exactly. In real life, however, both output and input data include noise. In inverse problems of modeling and data mining, solutions can represent a remarkable sensitivity with respect to perturbations in the parameters which base on the data, and a computed solution can be highly infeasible, suboptimal, or both.

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Therefore, new models have to be developed when optimization results are combined within real-life applications. In our study, we include into MARS the existence of uncertainty considering future scenarios and robustify it through *Robust Optimization* (*RO*) that has been developed by Ben-Tal and Nemirovski [4, 5, 6], and El-Ghaoui et al. [7, 8].

We are interested in the multicriteria tradeoff (antagonism) between ***accuracy*** and ***robustness***. In the line of our research [9, 10, 11, 12], robustness has become, in some sense, an extension of stability or regularity. Stability also means a *small complexity* of the model, or: a *small variance* of the estimation. Our earlier tradeoff between accuracy and regularity [13] aimed at keeping the complexity under some "control"; that was realized and used by us and our coauthors in the form of *Conic MARS* (*CMARS*) in several ways [14, 15, 16]: (*I*) through keeping the discretized integral of first- and second-order partial derivatives of the BFs inside of a "tolerance" or "margin", given by a preselected upper bound, and (*II*) through the model-based approach of modern optimization theory for an integrated approach of the forward and the backward step that constitute the method MARS. Herewith, we could gain from the "power" of integral calculus, and from future advances in calculus, in optimization theory and mathematical programming. We were also prepared to continue making modifications and improvements based on emerging results and principles for discretization schemes.

We underline the core importance of the target of numerical accuracy (precision) as a central goal in of our tradeoff that it establishes together with *regularity* and *robustness*, respectively. Within the CMARS concept and its CQP optimization program, through the "control parameter" which is represented by the upper bound of the complexity term, one can regulate and "tune"the importance that one assigns for the stability (lack of complexity) goal and, by this, for the antagonistic precision target. Furthermore, by CMARS the MARS kind of methods became further "hosted" in optimization, in its theory and its scientific community. Moreover, we even got the promise of gaining from the "power" of RO, which we could introduce and apply through CMARS's robust counterpart, our RCMARS [9, 12].

Through ***RCMARS*** we are also permitted to involve uncertainty in the *input* variables into regression and classification modeling; that uncertainty is typical for real-world challenges, too. In fact, in RCMARS, we have implied uncertainty in both input and output variables. This means that in RCMARS, there is a double way of robustification: (*i*) The regularization (stabilization) in integral form that expresses itself in the involvement of the (squared) first- and second-order partial derivatives of the multivariate basis functions; after discretization of the integrals, we arrive at a *Tikhonov Regularization* (*TR*) problem [17] with first- and second-order complexity terms. This TR problem is turned into a *Conic Quadratic Programming* (*CQP*) problem [13, 15]. (*ii*) The robustification of the output or response variable, with an own uncertainty set. In (*i*), via those first- and second-order terms, we aim at a "flat" model and a one where high "energy" in the model (curvature) is penalized so that we could speak of a "dampened" or "tamed" model, respectively. This also means that in RCMARS, we have, in addition to the robustification, an additional support of the robustification agenda, an "increase" of robustness, whereby that support is of a *fine-tuned* kind of character which is parametric through the bounds of complexity in the CQP program.

In contrast, in our new Robust MARS (***RMARS***), we only have the robustification step (*ii*), whereas the fine-tuning option (*i*) dropped. At the first glance, this seems to be a qualitative

loss. However, RCMARS is leading to a very large computational effort, and parametric studies which are enabled by part (*i*) do even increase those computational costs. It belonged to the main ideas of MARS and CMARS to have (*a*) "*doable*" methods, even with an effect in (*b*) ***variance reduction*** for the estimated model. In this paper, we pay tribute to these important aims (*a*) and (*b*), in the form of our simplified and "*handy*" alternative of RCMARS, called RMARS. By introducing a robustification in MARS, we try to decrease the *estimation variance*. For this aim, we present a simulation study.

1.2 Robust Optimization

Optimization has been a leading methodology in many fields such as engineering, finance and control design, and most applications suppose complete knowledge of the data which are underlying the optimization problem. In other words, it is assumed that to develop a model, the input data are known exactly (fixed). Nevertheless, solutions to optimization problems can represent a significant sensitivity to perturbations in the parameters of the problem. Optimization affected by parameter uncertainty is a focus of the mathematical programming community and a necessity to tackle uncertain data arises to develop models where optimization results are combined within real-world applications [18, 19]. RO is a method to address uncertainty in optimization problems.

The **RO** approach aims to make the optimization model robust, considering constraint violations by solving *robust counterparts* (*RCs*) of these problems in prespecified uncertainty sets for the uncertain parameters. These counterparts are solved for the *worst-case* realization of the uncertain parameters based on uncertainty sets for the random parameters [20]. One has to appropriately determine these sets beforehand; we shall use some control parameters for that purpose.

RO has gained lots of concentration from both a theoretical and a practical point of view as a modeling framework for "immunizing" against parametric uncertainties in mathematical optimization. It is a modeling methodology to model, evaluate and solve optimization problems in which the data are uncertain and only known to belong to some uncertainty set. RO purposes to receive an optimal or near optimal solution that is feasible for each possible realization of the uncertain data [6, 21].

In the following subsection, we introduce with MARS the RO approach which makes the optimization model in MARS robust in view of constraint violations by solving RCs of these problems within uncertainty sets. Although these counterparts are solved for the worst-case realization of those uncertain parameters based on suitably defined uncertainty sets, we shall weaken the concept of "worst case" for reasons of computational complexity. In this study, we work on robustification in terms of *polyhedral uncertainty*. Herewith, we are prepared to cope with not only fixed but also random type of input data; likewise we achieved it with RCMARS [9, 11, 12].

1.3 The significance of uncertainty in finance

Since global economic crisis has caused the necessity for an essential restructuring of the approach to risk and regulation, core elements of a new global financial regulatory-framework have become needed to establish in order to make the financial system more robust and suitable for serving the requirements of the real economy. For this reason, many scientists try to find ways to measure the probability of financial calamities, natural disasters and other catastrophes. They draw attention to the difference between ***known risks*** and ***uncertainty***. The problem is to be thought that most economists and other risk modelers do not separate uncertainty from risk. Economic models suppose that the financial world contain known risks that can be evaluated depend on prior behavior of stock markets and other elements of the monetary system. Nevertheless, there is genuine *uncertainty*, which is the impossibility of knowing exactly what the future keeps even in a probabilistic sense, as well as the *risk* that is the range of probabilities of outcomes pointed out by past events, which may serve as an unreliable guide for the future in an uncertain environment [22, 23, 24]. This means that, the known statistical models may not give trustworthy results.

Uncertainty is one of the characteristic properties in the sector of finance and insurance, as the given data, in both in input and output variables, are affected with "noise" of various kinds, and the scenarios which represent the developments in time, are not deterministic either. In our study, the existence of uncertainty has a strong impact on the way of modeling which, then, becomes the basis of regression and classification and, eventually, of decision making, in our application: financial decision making. In this way, the uncertainty phenomenon enters all parts of the model and its mathematical treatment, and one of the prominent techniques to address this situation is RO. In fact, it refers to *worst-case scenarios*; in our study, we have at hand control parameters in order to regulate the amount of skepticism and optimism or, in other words, *risk-aversion* and *risk-friendliness* in the modeling process. Here, *risk* expresses itself in terms of variance, namely, the estimation variance, as we shall explain. This way of bringing risk into a key role in our reflections is another way of addressing the motivating example of the financial markets, since risk in its various forms is another key phenomenon and criterion in finance. So, in this study, we consider to use RMARS in a financial application as a numerical experience. We want to underline that by all these considerations and measurements, with our robustification we are going much beyond of the concept of regularization which just relates to the output data and the complexity of the modeling functions.

1.4 Scope of the paper

This paper contains six main sections. In Section 1, we introduce into the study, that is, the objectives and outline are represented. Section 2 and Section 3 include theory and approach of MARS and RMARS method, respectively. In Section 4, for a numerical experiment, RMARS applied on a financial dataset for different uncertainty scenarios. Section 5 reveals graphically illustrates and discusses MARS and RMARS results for the simulation performed by us. Finally, a conclusion and future outlook are stated in Section 6.

2 Multivariate Adaptive Regression Spline

MARS introduced by Friedman in 1991 [1] may be presented as an extension of linear models that "automatically" models nonlinearities and interactions. It generates a multivariate-additive (multiplicative) model in a two-stage process which consists of forward and backward stage. In the *forward* stage, MARS finds *basis functions* (*BFs*) that are added to the model by a fast searching algorithm and constructs a possibly large model that overfits the dataset. The process stops when the model reaches the maximum number of BFs. However, this model at the same time contains BFs which contribute most and least to the overall performance. Thus, this forward model is quite complex and includes many incorrect terms. In the *backward* stage, the overfit model is pruned to decrease the complexity while supporting the overall performance with respect to the fit to the data. In that stage, the BFs which contribute smallest to the increase in the residual sum of squares are removed from the model at each stage and, eventually, an optimally estimated model is generated [1, 2].

MARS uses expansions of piecewise linear BFs created by dataset. The BFs, $[x-\varphi)]_+$ and $[x-\varphi]_-$, have the following form [2]:

$$[x-\varphi]_+ = \begin{cases} x-\varphi, & \text{if } x > \varphi \\ 0, & \text{otherwise} \end{cases}, \quad [x-\varphi]_- = \begin{cases} \varphi - x, & \text{if } x < \varphi \\ 0, & \text{otherwise} \end{cases}, \tag{1}$$

where φ is a univariate knot obtained from the dataset. These two functions are called *truncated linear functions*. Each function is piecewise linear, with a knot at the value φ, and both function together are called a reflected pair. The aim is to construct reflected pairs for each input x_j $(j = 1, 2, \ldots, p)$ with p-dimensional knots $\boldsymbol{\varphi}_i = (\varphi_{i,1}, \varphi_{i,2}, \ldots, \varphi_{i,p})^T$ at each observed value x_{ij} $(i = 1, 2, \ldots, N)$. Thus, the collection of BFs is written by a set of S defined as

$$S := \Big\{ \big[x_j - \varphi\big]_+, \big[x_j - \varphi\big]_- \mid \varphi \in \{x_{1,j}, x_{2,j}, \ldots, x_{N,j}\}, j = 1, 2, \ldots, p \Big\}, \tag{2}$$

where N is the number of observations and p is the dimension of the input space. There are $2Np$ BFs if all of the input values are distinct. In *the forward stage* of MARS, the model that fits the data is built by using BFs from the set S and their products. So, the model has the form

$$Y = \beta_0 + \sum_{m=1}^{M} \beta_m T_m(\boldsymbol{x}^m) + \varepsilon, \tag{3}$$

with a vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_p)^T$. Here, ε is uncorrelated random error term that is supposed to have a normal distribution with zero mean and finite variance, M is the set of BFs in the current model. Moreover, $T_m(\boldsymbol{x}^m)$ are BFs from the set S in Eqn. (3) or *multivariate* products of two or more such functions, $\boldsymbol{x}^m$ is a subvector of $\boldsymbol{x}$ that contributes to the the function T_m, and β are the unknown coefficients for the constant 1 $(m = 0)$ or for the mth BF. Given the observations represented by the data $(\boldsymbol{x}_i, y_i)$ $(i = 1, 2, \ldots, N)$, the form of the mth BF is as follows [2]:

$$T_m(\boldsymbol{x}^m) := \prod_{k=1}^{K_m} [s_{km} \cdot (x_{v(k,m)} - \varphi_{km})]_+. \tag{4}$$

Here, K_m is the number of truncated linear functions multiplied in the mth BF, $x_{v(k,m)}$ is the input variable corresponding to the kth truncated linear function in the mth BF, φ_{km} is the knot value corresponding to the variable $x_{v(k,m)}$ and $s_{km} = \pm 1$.

To generate the model, the MARS forward stepwise algorithm starts with the constant function $T_0(\boldsymbol{x}^0) = 1$ to estimate β_0, and all functions in the set S are candidate functions. Possible forms of the BFs $T_m(\boldsymbol{x}^m)$ are 1, x_n, $[x_n - \varphi_i]_+$, $x_n x_l$, $[x_n - \varphi_i]_+ x_l$ and $[x_n - \varphi_i]_+ [x_l - \varphi_j]_+$ [2, 3]. For each BF, input variables cannot be the same in the MARS algorithm. Therefore, the BFs above use different input variables, x_n and x_l, and their knots, φ_i and φ_j. At each stage, all products of a function $T_m(\boldsymbol{x}^m)$ in the model set are regarded as a new BF and this term is added to the model set. That term which produces the largest decrease in the training error contains the following form:

$$\beta_{M+1} T_n(\boldsymbol{x}^n).[x_j - \varphi]_+ + \beta_{M+2} T_n(\boldsymbol{x}^n).[\varphi - x_j]_+.$$

Here, β_{M+1} and β_{M+2} are coefficients and they are determined by least-squares estimation, along with all other M+1 coefficients in the model. Then, the "winning" products are added to the model and the process stops as soon as the model set reaches some present maximum number of terms. At the end of this forward stepwise process, a large model of the form is obtained. This model does typically *overfit* the data, and so a backward deletion procedure is applied.

The *backward stepwise algorithm* removes the terms that contribute the smallest increase in the residual squared error from the model at each stage, and this iterative procedure continues until an optimal number of effective terms are present in the final model [1]. So, an estimated best model $\hat{f}_\alpha$ of each number of terms α is produced at the end of this process. In the MARS model, *generalized cross-validation* (*GCV*) is used to find the optimal number of terms α. It also shows the lack of fit when using MARS. The GCV criterion defined by Friedman [1] is defined as follows:

$$LOF(\hat{f}_\alpha) = GCV(\alpha) := \frac{\sum_{i=1}^{N} (y_i - \hat{f}_\alpha(\boldsymbol{x_i}))^2}{(1 - M(\alpha)/N)^2}; \tag{5}$$

here, $M(\alpha)$ is the effective number of parameters in the model, and N is the number of sample observations, i.e., of the data [2].

3 Robust Multivariate Adaptive Regression Spline

3.1 Robustification of MARS Model

For MARS, the *optimally estimated model* that has the number of M many basis functions is created by backward-stage of Salford MARS [25]. On the other hand, for RMARS, the randomized form of this estimated model is considered to present the relation between the input variables and the response as follows:

$$Y = g(\breve{\boldsymbol{X}}) + \varepsilon, \tag{6}$$

where Y is the random response variable, $\breve{\boldsymbol{X}} = (\breve{X}_1, \breve{X}_2, \ldots, \breve{X}_p)^T$ is a *random* vector of predictor variables, all of them including "noise". Here, the following general model is considered for

each input $\breve{X}_j$:

$$\breve{X}_j = \bar{X} + \mu_j \ \ (j = 1, 2, \ldots, p).$$

To robustify MARS, the RO is applied on the BFs and we suppose that also the input and output variables of our model are all random. Moreover, the random variables $\breve{X}_j$ are assumed to be normally distributed. These provide us uncertainty sets supposed to contain in *confidence intervals* (*CIs*). Therefore, we include a *perturbation* (uncertainty) into the real input data $\breve{\boldsymbol{x}}_i$ in each dimension, and into the output data $\breve{y}_i$. The perturbations of input and output data are represented by CIs.

When taking into consideration that we have p-dimensional input data, any input data vectors $\breve{\boldsymbol{x}}_i = (\breve{x}_{i,1}, \breve{x}_{i,2}, \ldots, \breve{x}_{i,p})^T$ are represented by $\breve{\breve{\boldsymbol{x}}}_i = (\breve{\breve{x}}_{i,1}, \breve{\breve{x}}_{i,2}, \ldots, \breve{\breve{x}}_{i,p})^T$, including the perturbational term $\boldsymbol{\nabla_i} = (\nabla_{i,1}, \nabla_{i,2}, \ldots, \nabla_{i,p})^T$ $(i = 1, 2, \ldots, N)$. Herewith, the new values of piecewise linear BFs with uncertainty are shown in the following:

$$\breve{x}_{ij} \to \breve{\breve{x}}_{ij}; \qquad \breve{\breve{x}}_{ij} = \bar{x}_j + \nabla_{ij}, \ \ |\nabla_{ij}| \leq \delta_{ij} \ \ (j = 1, 2, \ldots, p; \ i = 1, 2, \ldots, N),$$

where $\bar{x}_j$ is the arithmetic mean of the components of the vector $\breve{\boldsymbol{x}}_{\boldsymbol{j}}$ $(j = 1, 2, \ldots, p)$. Here, the amount of perturbational term in each dimension is limited by δ_{ij} which is the semilength of CI for input data. In a similar way, the output data vector $\breve{\boldsymbol{y}} = (\breve{y}_1, \breve{y}_2, \ldots, \breve{y}_N)^T$ is defined as $\breve{\breve{\boldsymbol{y}}} = (\breve{\breve{y}}_1, \breve{\breve{y}}_2, \ldots, \breve{\breve{y}}_N)^T$, including the perturbational increment $\hbar = (\hbar_1, \hbar_2, \ldots, \hbar_N)^T$ $(i = 1, 2, \ldots, N)$. Now, our new output values can be described by:

$$\breve{y}_i \to \breve{\breve{y}}_i; \qquad \breve{y}_i = \bar{y} + \hbar_i, \ \ |\hbar_i| \leq \wp_i \ \ (i = 1, 2, \ldots, N),$$

where $\wp_i$ is the semilength of the CI for the output data and the amount of perturbational increment is restricted by $\wp_i$. Here $\bar{y}$ is the mean over the vector $\breve{\boldsymbol{y}}$, again with respect to its coordinates (for details, cf. [9] as a related study).

When we imply the uncertainty sets $U_1 \subseteq \mathbb{R}^{N \times M}$ and $U_2 \subseteq \mathbb{R}^N$, determined in Subsection 3.2, into the data $(\breve{\breve{\boldsymbol{x}}}_i, \breve{\breve{y}}_i)$, the piecewise linear BFs in Eqn. (1) are constructed based on the new data that incorporate uncertainties, and the multiplicative form of the mth BF can be stated in the following way:

$$T_m(\breve{\breve{\boldsymbol{x}}}_{\boldsymbol{i}}^{\boldsymbol{m}}) := \prod_{k=1}^{K_m} [\breve{\breve{x}}_{iv(k,m)} - \varphi_{km})]_{\pm} \ \ (i = 1, 2, \ldots, N). \tag{7}$$

If we estimate the BFs $[\breve{\breve{x}}_{iv(k,m)} - \varphi_{km}]_{\pm}$ in (7), we can evaluate them by the following special terms of estimation:

$$[\breve{\breve{x}}_{iv(k,m)} - \varphi_{km}]_{\pm} \leq [\breve{x}_{iv(k,m)} - \varphi_{km}]_{\pm} + [\nabla_{iv(k,m)} + (\pm\Phi_{iv(k,m)})]_{\pm}, \tag{8}$$

where $\Phi_{iv(k,m)}$ is interpreted and applied as *control parameters*. Here, the amount of the value of $\Phi_{iv(k,m)}$ is limited by a value $\eta_{iv(k,m)}$ because the value of is directly affect the size of uncertainty set U_1, and our uncertainty sets are unknown but bounded. When we take into account the *risk friendly* case, we can choose the value of $\Phi_{iv(k,m)}$ between 0 and the absolute value of $\Phi_{iv(k,m)}$. Otherwise, considering the risk averse case, " worst case", for the value of $\Phi_{iv(k,m)}$, it is equal

to $\eta_{iv(k,m)}$. To predict the values $T_m(\breve{\boldsymbol{x}}_{\boldsymbol{i}}^{\boldsymbol{m}})$ and $T_m(\breve{\breve{\boldsymbol{x}}}_{\boldsymbol{i}}^{\boldsymbol{m}})$, we may use (8) in the subsequent form, where all the "+" and "-" signs belong to each other, respectively:

$$\begin{aligned}\underbrace{\prod_{k=1}^{K_m}[\breve{\breve{x}}_{iv(k,m)}-\varphi_{km}]_{\pm}}_{=:T_m(\breve{\breve{\boldsymbol{x}}}_i^m)} \leq \underbrace{\prod_{k=1}^{K_m}[\breve{x}_{iv(k,m)}-\varphi_{km}]_{\pm}}_{=:T_m(\breve{x}_i^m)} + \\ \sum_{B\subsetneqq\{1,\ldots,K_m\}}\prod_{b\in B}[\breve{x}_{ib}-\varphi_b]_{\pm}\prod_{a\in\{1,\ldots,K_m\}/B}[(\pm\Phi_{ia})+\nabla_{ia})]_{\pm}.\end{aligned} \tag{9}$$

Afterward, we can construct the bounding form with symmetry given below:

$$\left.\begin{aligned}T_m(\breve{\breve{\boldsymbol{x}}}_{\boldsymbol{i}}^{\boldsymbol{m}})-T_m(\breve{\boldsymbol{x}}_{\boldsymbol{i}}^{\boldsymbol{m}})\leq\hat{u}_{im}\\ T_m(\breve{\boldsymbol{x}}_{\boldsymbol{i}}^{\boldsymbol{m}})-T_m(\breve{\breve{\boldsymbol{x}}}_{\boldsymbol{i}}^{\boldsymbol{m}})\leq\hat{\hat{u}}_{im}\end{aligned}\right\}\Rightarrow\left|T_m(\breve{\breve{\boldsymbol{x}}}_{\boldsymbol{i}}^{\boldsymbol{m}})-T_m(\breve{\boldsymbol{x}}_{\boldsymbol{i}}^{\boldsymbol{m}})\right|\leq\max\{\hat{u}_{im},\hat{\hat{u}}_{im}\}. \tag{10}$$

So, for each BF, the uncertainty value $|u_{im}|$ may be evaluated in the subsequent way:

$$\begin{aligned}|u_{im}| &\leq \sum_{B\subsetneqq\{1,\ldots,K_m\}}\prod_{b\in B}\underbrace{|\breve{x}_{ib}-\varphi_b|}_{\leq \mathrm{H}_{ib}\delta_{ib}}\prod_{a\in\{1,\ldots,K_m\}/B}\underbrace{(|\pm\Phi_{ia}+\nabla_{ia}|)}_{\leq\eta_{ia}+\delta_{ia}}\\ &\leq \sum_{B\subsetneqq\{1,\ldots,K_m\}}\prod_{b\in B}\mathrm{H}_{ib}\delta_{ib}\prod_{a\in\{1,\ldots,K_m\}/B}(\eta_{ia}+\delta_{ia})\\ &\leq \sum_{B\subsetneqq\{1,\ldots,K_m\}}\prod_{a\in B}\underbrace{\mathrm{H}_{ib}}_{\leq\mathrm{H}_i}\prod_{b\in B}\delta_{ib}\prod_{a\in\{1,\ldots,K_m\}/B}(\eta_{ia}+\delta_{ia})\\ &\leq \sum_{B\subsetneqq\{1,\ldots,K_m\}}\mathrm{H}_i^{|B|-1}\prod_{b\in B}\delta_{ib}\prod_{a\in\{1,\ldots,K_m\}/B}(\eta_{ia}+\delta_{ia}).\end{aligned} \tag{11}$$

Here the cardinality of the set B is denoted through $|B|$ and H_i is also considered to be employed as *control parameters*. The value of H_i will be 2 in cases without outliers, but for outliers, it will be greater than 2. For such a case, we must choose a different value for H_i. This robustification concept can be visualized in Figure 1(for more details we refer to cf. [9] as related subject).

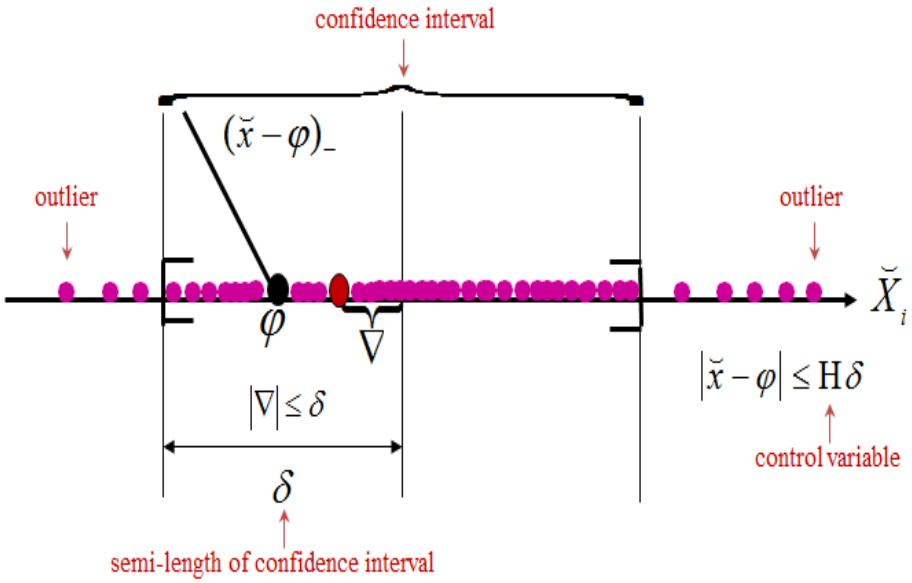


Figure 1: The CIs for BF and perturbational term for input data.

3.2 Polyhedral Uncertainty and Robust Counterpart for MARS

In order to work on the robustness problem, our multiplicative form of BF and output vector that include uncertainty are represented as a family of matrices $\boldsymbol{T}(\breve{\breve{\boldsymbol{x}}}) = \boldsymbol{T}(\breve{\boldsymbol{x}}) + \boldsymbol{U}$ and vectors $\breve{\breve{\boldsymbol{y}}} = \breve{\boldsymbol{y}} + \boldsymbol{v}$. Here, $\boldsymbol{U}$ and $\boldsymbol{v}$ are lying in unknown but bounded sets U_1 and U_2, respectively. Whenever *polyhedral* uncertainty is employed for MARS, addressing uncertainty sets U_1 and U_2, the RC can be represented by

$$\underset{\boldsymbol{\alpha}}{\text{minimize}} \ \max_{\substack{\boldsymbol{A}\in U_1 \\ \boldsymbol{b}\in U_2}} \ \left\|\boldsymbol{b}-\boldsymbol{A}\boldsymbol{\beta}\right\|_2^2, \tag{12}$$

where U_1 is a polytope with $2^{N\cdot M}$ vertices $\boldsymbol{A}^1, \boldsymbol{A}^2, \ldots, \boldsymbol{A}^{2^{N\cdot M}}$. In fact, it is not known as a singleton, but establishes a convex bounded uncertain domain defined as

$$U_1 = \left\{ \sum_{j=1}^{2^{N\cdot M}} \lambda_j \boldsymbol{A}^j \mid \lambda_j \ge 0 \ (j \in \left\{1,2,\ldots,2^{N\cdot M}\right\}), \ \sum_{j=1}^{2^{N\cdot m}} \lambda_j = 1 \right\}, \tag{13}$$

i.e., $U_1 = \text{conv}\left\{\boldsymbol{A}^1, \boldsymbol{A}^2, \ldots, \boldsymbol{A}^{2^{N\cdot M}}\right\}$ being the convex hull. Furthermore, U_2 is a polytope with 2^N vertices $\boldsymbol{b}^1, \boldsymbol{b}^2, \ldots, \boldsymbol{b}^{2^N}$ and it is given by

$$U_2 = \left\{ \sum_{i=1}^{2^N} \ell_i \boldsymbol{b}^i \mid \ell_i \ge 0 \ (i \in \left\{1,2,\ldots,2^N\right\}), \ \sum_{i=1}^{2^N} \ell_i = 1 \right\}, \tag{14}$$

where $U_2 = \text{conv}\left\{\boldsymbol{b}^1, \boldsymbol{b}^2, \ldots, \boldsymbol{A}^{2^N}\right\}$ is the convex hull (for closer details cf. [9, 12] as related subject). Therefore, equivalently to our robustified problem, the robust CQP problem is stated as:

$$\begin{aligned} &\underset{t,\boldsymbol{\beta}}{\text{minimize}} \;\; t \\ &\text{subject to} \quad \left\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{\beta}\right\|_2 \leq t \quad \forall \underbrace{\boldsymbol{A}}_{=\sum_{j=1}^{2^{N\cdot M}} \lambda_j \boldsymbol{A}^j} \in U_1, \; \underbrace{\boldsymbol{b}}_{=\sum_{i=1}^{2^N} \ell_i \boldsymbol{b}^i} \in U_2. \end{aligned}$$

If U_1 and U_2 are polytopes, defined by their vertices through $\boldsymbol{A}^1, \boldsymbol{A}^2, \ldots, \boldsymbol{A}^{2^{N\cdot M}}$ and $\boldsymbol{b}^1, \boldsymbol{b}^2, \ldots, \boldsymbol{b}^{2^N}$, respectively, our robust CQP for RMARS model can equivalently be presented by a standard CQP problem [26] as follows:

$$\begin{aligned} &\underset{t,\boldsymbol{\beta}}{\text{minimize}} \;\; t \\ &\text{subject to} \quad \left\|\boldsymbol{b}^i - \boldsymbol{A}^j\boldsymbol{\beta}\right\|_2 \leq t \;\; (i = 1, 2, \ldots, 2^N; j = 1, 2, \ldots, 2^{N\cdot M}), \end{aligned} \tag{15}$$

To not increase the complexity of optimization problems involved, in this study, we select the uncertainty set U_1 and U_2 as *polyhedral* for the input and the output data to study our robustified problem in the following sections.

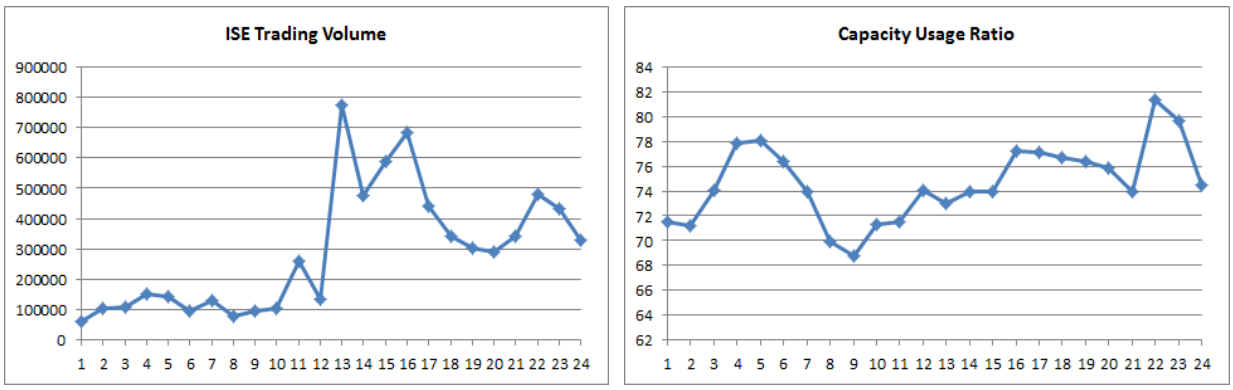
4 Numerical Experience with RMARS in Finance

As a numerical experiment that may serve to illustrate the implementation of RMARS algorithm developed, we use a small dataset as a sample from the real-world financial market data. It is chosen for our empirical part as time-series data from the website of Central Bank of the Republic of Turkey [27]. The data contain four economic indicators (independent variables) which are the most commonly used ones for the interpretation of an economic situation. These are:

x_1 : ISE Trading Volume, x_2 : Capacity Usage Ratio,
x_3 : Credit Volum, x_4 : Federal Funds Interest Rate.

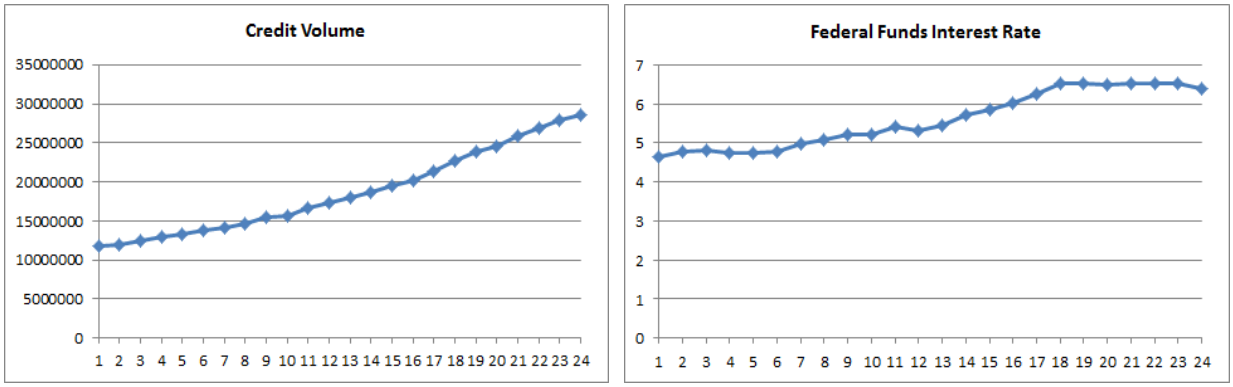
Here, ISE Trading Volume stands for the number of shares or contracts of a security traded within of a predefined time-window for a month; Capacity Usage Ratio means the ratio of the production capacity of the regarded economy to the maximum capacity of that economy. ISE 100 stock index is the dependent (output or response) variable Y that we try to assess based on our dataset. It consists of 100 stocks that have been chosen among the stocks of companies which are listed on the National Market, and the stocks of real estate investment trusts and venture capital investment trusts, which are listed on the Corporate Products Market. It covers ISE 30 and ISE 50 stocks. As it is a statistical measure of change in an economy or a securities market, we will use that index. For financial markets, an *index* is an imaginary portfolio of securities, representing some market or a portion of it. It possesses its own traditional methods of calculation and, in general, it is represented by a deviation from a base value. Thus, the relative change (in percentage terms) is more important than the absolute value (in actual numerical terms). This

dataset includes 24 observations and the characteristics of our independent variables in time can be seen in Figures 2-3 for a visualization of the dataset.



(a) (b)

Figure 2: Graph for the characteristic of variables (a) x_1 and (b) x_2.



(a) (b)

Figure 3: Graph for the characteristic of variables (a) x_3 and (b) x_4.

With this data the largest model is constructed by the forward stepwise stage of Salford MARS Version 3 [25]. After backward stepwise elimination of MARS, the final model is represented as follows:

$$\hat{y} = \beta_0 + \sum_{m=1}^{M} \beta_m T_m(\boldsymbol{x}^m) = \beta_0 + \beta_1 \max\{0,\ x_3 - 0.1672\} + \beta_2 \max\{0,\ 0.1672 - x_3\}$$
$$+\beta_3 \max\{0,\ x_4 + 0.4200\} + \beta_4 \max\{0,\ x_1 + 0.6803\}.$$

To apply the RO technique on MARS model, firstly uncertainties are evaluated for all input values using Eqn. (11) and all output values. Here these input and output values presented by

CIs. Next, we include perturbations (uncertainties) into the real input data $\breve{\boldsymbol{x}}_i$ in each dimension and into the output data $\breve{y}_i$ $(i = 1, 2, \ldots, 24)$. For this aim, using Eqns. (13)-(14), the uncertainty matrices and vectors based on *polyhedral uncertainty sets* are built. Consequently, we construct different uncertainty matrices, $\boldsymbol{U}$ and $\boldsymbol{A}$, for the input data and different uncertainty vectors, $\boldsymbol{v}$ and $\boldsymbol{b}$, for the output data by using six different uncertainty scenarios which are given by the CIs ± 3, $\pm 3/2$, $\pm 3/4$, $\pm 3/6$, $\pm 3/8$ and as a special case, mid-point (zero) value of our interval. For instance, according to CI ± 3, the matrices of input data, $\boldsymbol{U}$, $\boldsymbol{A}_{upper}$, $\boldsymbol{A}_{lower}$, addressed in Section 3.2 are of the following forms:

$$\boldsymbol{U} = \begin{bmatrix} u_{11} & \ldots & u_{14} \\ u_{21} & \ldots & u_{24} \\ \vdots & \vdots & \vdots \\ u_{231} & \ldots & u_{232} \\ u_{241} & \ldots & u_{242} \end{bmatrix} \in \begin{bmatrix} 0 & [-2.46, 2.46] & 0 & 0 \\ 0 & [-2.48, 2.48] & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ [-2.30, 2.30] & 0 & [-2.45, 2.45] & [-3.05, 3.05] \\ [-2.17, 2.17] & 0 & [-2.60, 2.60] & [-2.55, 2.55] \end{bmatrix},$$

$$\boldsymbol{A}_{upper} = \boldsymbol{T}(\breve{\boldsymbol{x}}) + \boldsymbol{U}_{upper} = \begin{bmatrix} 1 & 0 & 3.89 & 0 & 0 \\ 1 & 0 & 3.89 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 3.85 & 0 & 4.12 & 4.42 \\ 1 & 3.85 & 0 & 4.12 & 4.42 \end{bmatrix},$$

$$\boldsymbol{A}_{lower} = \boldsymbol{T}(\breve{\boldsymbol{x}}) + \boldsymbol{U}_{lower} = \begin{bmatrix} 1 & 0 & -1.03 & 0 & 0 \\ 1 & 0 & -1.07 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & -0.75 & 0 & -0.77 & -1.68 \\ 1 & -0.50 & 0 & -1.07 & -2.68 \end{bmatrix}.$$

Likewise, based on CI ± 3, the uncertainty vectors of output data, $\boldsymbol{v}$, $\boldsymbol{b}_{upper}$, $\boldsymbol{b}_{lower}$, are represented as follows:

$$\boldsymbol{v} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_{23} \\ v_{24} \end{bmatrix} \in \begin{bmatrix} [-3, 3] \\ [-3, 3] \\ \vdots \\ [-3, 3] \\ [-3, 3] \end{bmatrix}, \boldsymbol{b}_{upper} = \breve{\boldsymbol{y}} + \boldsymbol{v}_{upper} = \begin{bmatrix} 1.61 \\ 1.76 \\ \vdots \\ 3.52 \\ 2.88 \end{bmatrix}, \boldsymbol{b}_{lower} = \breve{\boldsymbol{y}} + \boldsymbol{v}_{lower} = \begin{bmatrix} -4.39 \\ -4.27 \\ \vdots \\ -2.49 \\ -3.12 \end{bmatrix}.$$

Since the uncertainty matrix for input data has a very big size; and our computer capacity is not enough to solve our problem for this uncertainty matrix, we formulate RMARS for each observation using a certain *combinatorial approach* which is called as *weak robustification*. This approach was introduced in [9]. Therefore, we obtain different *weak RMARS* (*WRMARS*) models to handle that difficulty of complexity. Actually, we have a *tradeoff* between tractability

and robustification. As a result, we obtain 24 different WRMARS models and solve them with MOSEK program [28].Then, we estimate the parameters values $\beta_0, \beta_1, \beta_2, \beta_3$ and β_4 using a selected WRMARS model which has the *highest* t value in Eqn. (15) by applying the *worst-case* approach. Finally, we evaluate the regression coefficients and estimation errors based on *Average Absolute Error* (*AAE*) and *Root Mean Squared Error* (*RMSE*) for different uncertainty scenarios. All of the parameter values and estimation errors for MARS and RMARS are represented in Table 1.

Table 1: Parameter values and estimation errors of MARS and RMARS.

$\boldsymbol{U}, \boldsymbol{v}$	± 3	$\pm 3/2$	$\pm 3/4$	$\pm 3/6$	$\pm 3/8$	zero	MARS
$\boldsymbol{\beta}_0$	-0.6197	-0.7644	-0.6660	-0.5111	-0.4418	-0.3470	-0.3470
$\boldsymbol{\beta}_1$	0.3348	0.2501	-0.3292	-0.5921	-0.7074	-0.8843	-0.8843
$\boldsymbol{\beta}_2$	0.0000	0.0000	-0.1852	-0.3686	-0.4494	-0.5722	-0.5722
$\boldsymbol{\beta}_3$	0.0000	0.0000	0.4600	0.6262	0.6986	0.8120	0.8120
$\boldsymbol{\beta}_4$	0.6529	0.8691	0.7403	0.6508	0.6121	0.5498	0.5498
AAE	0.4048	0.3215	0.1937	0.1385	0.1254	0.1123	0.1123
RMSE	0.4880	0.4204	0.2496	0.1781	0.1559	0.1414	0.1414

As we can see in Table 1, RMARS produces less accurate results than MARS in terms of AAE and RMSE when the CIs on the variable are very wide. However, as the CIs are narrower, the performance results approach to that of MARS.

According to our *main purpose*, we also calculate ***estimation variances*** (***EVs***) for different uncertainty scenarios. EV is the variance of the estimated response values and smaller value of EV provide us the better result. It is evaluated using the following formula:

$$EV := \frac{\sum_{i=1}^{N}(\hat{y}_i - \bar{\hat{y}})}{N-1},$$

where N is number of observations; $\hat{y}_i$: the ith estimated response value; $\bar{\hat{y}}$: the mean of the estimated response values. Based on six different uncertainty scenarios, the values of EV evaluated for our numerical experiment are presented in Table 2.

Table 2: Estimation variance of MARS and RMARS.

$\boldsymbol{U}, \boldsymbol{v}$	± 3	$\pm 3/2$	$\pm 3/4$	$\pm 3/6$	$\pm 3/8$	zero	MARS
EV	**0.4469**	**0.7060**	**0.8111**	**0.8805**	**0.9178**	**0.9791**	**0.9791**

As we may deduce from the results in Table 2, RMARS has a much smaller variance than MARS if the CIs on the variable are very wide. As the CIs are narrower, EV increases but,

RMARS still has a smaller variance than MARS. Therefore, we can say that RMARS has a considerably smaller EV than MARS for different uncertainty scenarios, as we expect.

While developing RMARS models, a sensitivity study is conducted to define the most suitable confidence limits on both input and output data. For this purpose, different uncertainty matrices for the input data, $\breve{\boldsymbol{x}}$, and different uncertainty vectors for the output data, $\breve{\boldsymbol{y}}$, are obtained by using six different intervals. Above results in Tables 1 and 2 indicate that solutions obtained are sensitive to the limits of CIs. When we use the mid-point of our interval values for both input and output data, which is the certain data case (zero interval), we receive the same parameter estimates, and thus, the same model performances and EV as the ones by MARS. This can disclose that MARS is a ***special case*** of RMARS.

We have a smaller EV when the lengths of the CIs are wide whereas we receive better performance results when the lengths of the CIs are narrow. According to these result, we can observe the tradeoff between *accuracy* (expressed by AAE and RMSE) and *robustness* (given by EV). Also, to analyze this tradeoff clearly, we evaluated the values of Residual Sum of Squares (RSS) and EV based on various different uncertainty scenarios and represented the results graphically in Figure 4.

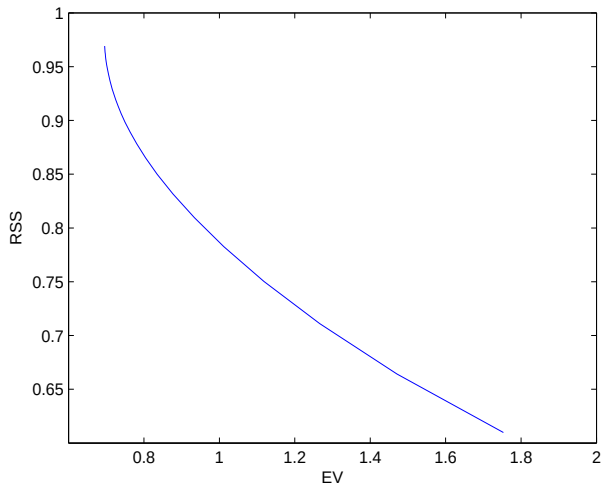


Figure 4: The efficiency frontier between estimation error and estimation variance

This figure demonstrates the tradeoff between accuracy (given as RSS) and robustness (represented by EV). In finance and economics, this is the so-called *efficiency frontier*.

5 Simulation Study

In the previous sections, we represented and investigated scientifically MARS and RMARS in detail and we applied them on a financial dataset. In this section, we compare these methods using different datasets created by Monte-Carlo simulation based on *variation* of the parame-

ter estimates. Furthermore, in order to see the variation of model performance with parameter estimates, the estimation errors of simulation models are evaluated based on AAE and RMSE.

Monte-Carlo simulation permits to model situations which present uncertainty and conduct them many times on a computer. It also includes a risk study through a preparation of models of possible results by substituting a range of values - we may say: a probability distribution - for any factor which implies uncertainty. Monte-Carlo simulation generates distributions of possible outcomes. Through the use of probability distributions, variables may have different probabilities of the outcomes that occur. *Probability distributions* mean a much more realistic kind of representing uncertainty in variables of a risk analysis that belongs to each decision which we are making. Continuously, we are confronted with uncertainty, with ambiguity and ***variability***. It is impossible to precisely estimate the future, even if nowadays we can access an unprecedented amount of information. Monte-Carlo simulation permits us a survey of nearly all the outcomes of our possible decisions and an impact assessment of risk; this allows for a more qualified decision making in the presence of uncertainty [29].

In this study, we select normal distribution as a probability distribution to obtain random input variables. For the simulation study of MARS, firstly, we develop a mathematical model. This model is the *process model* and represented as follows:

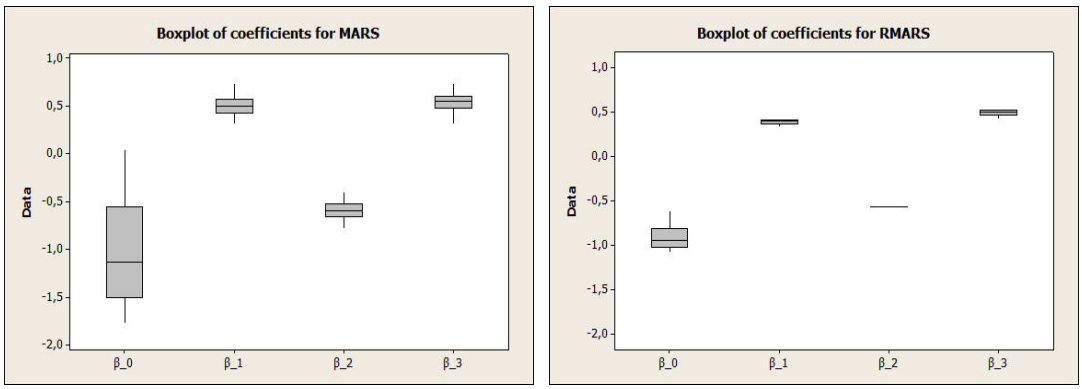
$$Y = -3050 + 0.02x_1 + 50x_2 - 0.0009x_3 + 8400x_4 + 30x_2x_4 + \varepsilon. \tag{16}$$

Afterward, using Minitab package program [30] generated random input variables chosen from suitable distribution function which are expected to determine the variables. Here we simulate values of a *normal random variable*. Then, using Eqn. (16), we monitor preferred output variables which become distributions whose properties are described by the model and the distributions of the random variables. So, we generate thirty different simulated datasets to employ simulation for MARS and thirty different MARS models are constructed using Salford Systems MARS [25]. Finally, parameter values of MARS models are estimated according to these simulated datasets. Some selected MARS models obtained are of the following form:

$$\begin{aligned}
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 2.25\} + \beta_2 \max\{0,\ x_3 + 1.86\} + \beta_3 \max\{0,\ x_4 + 2.18\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 1.47\} + \beta_2 \max\{0,\ x_3 + 2.84\} + \beta_3 \max\{0,\ x_4 + 2.45\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 3.07\} + \beta_2 \max\{0,\ x_3 + 1.78\} + \beta_3 \max\{0,\ x_4 + 2.63\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 2.39\} + \beta_2 \max\{0,\ x_3 + 1.62\} + \beta_3 \max\{0,\ x_4 + 1.51\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 2.21\} + \beta_2 \max\{0,\ x_3 + 1.98\} + \beta_3 \max\{0,\ x_4 + 3.27\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 1.98\} + \beta_2 \max\{0,\ x_3 + 2.07\} + \beta_3 \max\{0,\ x_4 + 1.49\},\\
\hat{y} &= \beta_0 + \beta_1 \max\{0,\ x_1 - 2.74\} + \beta_2 \max\{0,\ x_3 + 2.20\} + \beta_3 \max\{0,\ x_4 + 1.70\}.
\end{aligned}$$

For simulation study of RMARS, firstly, thirty different interval values are determined and, hence, under polyhedral uncertainty sets, thirty different uncertainty scenarios are obtained by using these values. The values of the CIs are $\pm 3/2$, $\pm 3/2.1$, $\pm 3/2.2$,..., $\pm 3/4.6$, $\pm 3/4.8$, $\pm 3/5$. Then RMARS models are constructed by running a MATLAB code written by us and MOSEK software [28] is used to solve the CQP problems for RMARS models. Finally, parameter values of RMARS models are also predicted based on thirty different uncertainty scenarios.

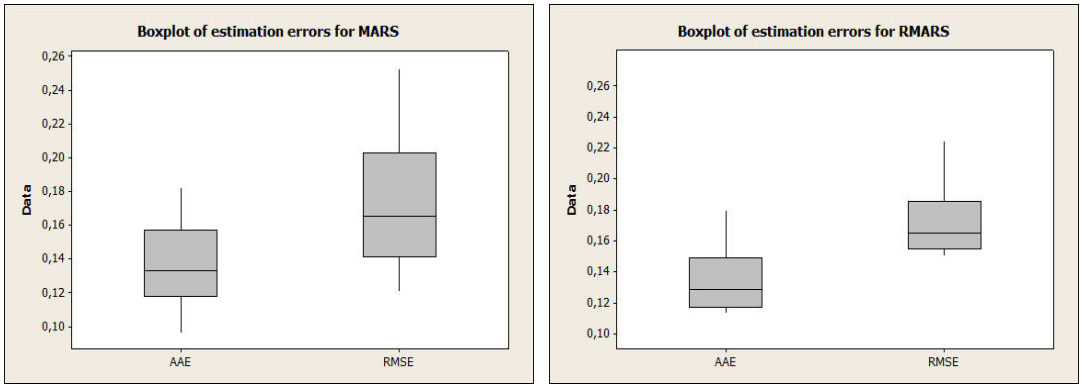
In RMARS, our aim is to decrease the *estimation variance* by implying full robustification in MARS even though the estimation errors of RMARS can be slightly higher than that of MARS when we incorporate perturbation (uncertainty) into the input and output data based on polyhedral uncertainty set. For this simulation study, the results for the variance of parameter estimates can be understood in Figure 5.



(a) (b)

Figure 5: The graphical representation for the variance of parameter estimates of (a) MARS and (b) RMARS.

As we observe in Figure 5, the variability of the model parameter estimates of the RMARS is much less than that of MARS. For this simulation study, the variance of model performance can be learned in Figure 6 for our two methods.



(a) (b)

Figure 6: Based on AAE and RMSE, the graphical representation for the variance of model performance criteria of (a) MARS and (b) RMARS.

As we can deduce from Figure 6, similar to variability of the model parameter estimates, the variability of model performance of the RMARS is less than that of MARS.

6 Conclusion and Future Outlook

In this study, we first study on the theory and methods of RMARS, a newly developed method for modeling uncertain data. We run the code for the data that include uncertainties, and then evaluate the results with respect to accuracy and stability (based on *variance*). Then, we represent the results of the sensitivity analysis on the parameter estimates, and thus, the model performances and estimation variances. We solve our optimal problem and robustify MARS by using our RO approach, but also a combinatorial approach, which is the *weakly robust* case, to handle uncertainties that may exist in data and to make our rich approach feasible. As an innovation of this work, our robustification even enters into the input variables and, herewith, in the model design, we can say: the scenarios. By further "control" parameters, we offer a *tuning* of how much risk averse the modeler wishes us to be.

We apply MARS and RMARS method on a financial dataset taken from *Central Bank of the Republic of Turkey*. RMARS has a considerably smaller variance than MARS for different uncertainty scenarios while MARS produces slightly more accurate results than RMARS. As the CIs on the variables are narrower, the performance results approaches to that of MARS. In this way, we purpose to decrease the ***estimation variance***. In order to demonstrate this based on replicated datasets, we take into account a simulation study. For this aim, we generate thirty different datasets by Monte-Carlo simulation, and present our results graphically. Results indicate that RMARS models have ***much less variability*** in parameter estimates, and thus, in accuracy measures as we expect.

We work on this RMARS in terms of *polyhedral uncertainty*. This provides us back to CQP naturally. Our new RMARS can be regarded as a more "*handy*" alternative to RCMARS. In our future study, we are also going to work on RMARS and RCMARS under ellipsoidal uncertainty. This may cause an increase in our model complexity but will give us a more robust approximation and prediction than polyhedral uncertainty. We will study on real-world applications of this approach to validate and to investigate the performance of our RMARS and RCMARS and to compare these methods with respect to accuracy and variance. For those forthcoming studies, we will consider using parallel computing to handle limitations of the computer capacity. Furthermore, we can use *Robust Generalized Partial Linear Model* (*RGPLM*) like Robust Conic GPLM (RCGPLM) [31, 32] which lead to some decrease of some complexity of the algorithm RCMARS, since we also have to solve an extra problem (by Software MARS [25]), etc.), namely, knot selection (not required for the linear part) in MARS and RMARS.

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