How can we achieve a better world by incorporating the modern techniques of continuous optimization within spatial analysis?

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Abstract

Global challenges have strong impact on world development. They are often related with our nature and environment, and have spatial characteristics. Spatial technologies provide us powerful tools to deal with these problems. They offer enough flexibility to handle substantial amount of spatial data and wide range of modeling capabilities. Remotely sensed data is the most significant data source used in spatial technologies. However, it is often associated with uncertainties due to atmospheric effects (i.e., absorption and scattering by atmospheric gases and aerosols). Methods based on rigorous treatment of radiative transfer models still have some drawbacks in removing the effects of atmosphere on large numbers of satellite images. In our paper, a different approach is represented for the regional atmospheric correction by employing nonparametric regression splines within the frame of modern techniques of continuous optimization and conic quadratic programming. Atmospheric correction models obtained through conic multivariate adaptive regression splines are applied on a set of satellite images. The results are compared with the ones obtained by both multivariate adaptive regression splines and a radiative transfer-based method.

Keywords: *MARS, CMARS, Conic quadratic programming, Remote sensing, Atmospheric correction, Radiative transfer*

Introduction

World development and spatial technologies

Whole series of problems, like *global warming*, drastic changes in *weather* and *climate*, devastating impacts of *natural disasters* (i.e., *typhoon attacks*, *floods*, or *tsunamis*), downsizing in *agricultural* areas, expanding *urbanization*, *pollution* of world's *natural resources* etc., are at alarming levels. These *global challenges* often exhibit spatial characteristics, and closely related to our nature and environment.

It is inevitable for us to consider these problems within the *world development* perspective, and in order to tackle them, we need more information about the interaction between human and environment. Hence, we require effective spatial tools to deepen our understanding in such natural and environmental phenomena, where we have to "mine" for the inherent structure of the data in both time and spatial domains.

Since the day it emerged (i.e., 1960s), *geographical information systems* (*GIS*), together with the parallel developments in *remote sensing* (*RS*) technologies, have been offering unique capabilities for editing, managing, analyzing and automating different kinds of spatial data that provides valuable information required for decision making in diverse areas [1].

These technologies have been intensively employed in studies related to *global warming* [2], sustainable management of *natural* and *water resources*, [3-7], *emergency response systems* for natural events [8-9], and *weather* and *climate* modelling [10-12].

GIS and *RS* have also an increasing importance in *economic development*, where they help route *financial* markets and the behavior of firms in today's global economy, like *financial* and *environmental* analysis of investments in *energy* markets [13-14], *real estate* business [15-16], *urban development* planning [17-18], *agriculture* [19-20], *farmin*g industry and *rural area management* [21-23], and in *oil* and *mining* industry as well [24-25].

Remotely-sensed image data have been used as a primary information source in spatial technologies. However, a fundamental problem in *RS* is the perturbations on surface reflectance data due to *absorption* and *scattering* by atmospheric gases and molecules [4, 26-27]. So, in order to make correct analysis and interpretation of remotely sensed images, the reflectance values of the image pixels must accurately represent the ground surface reflectance values. Failure to correct for the atmospheric effects can inevitably lead to different surface reflectance values, and will definitely have a significant effect on any conclusions drawn from such data. This issue is particularly important in the evaluation of long time series, over which the atmospheric parameters do not remain constant [28-29].

A brief remark on radiative transfer models

Numerous methods and algorithms based on *radiative transfer* (*RT*) models have been proposed by various authors in order to remove atmospheric effects from images taken by sensors with different technical specs and operational objectives [30-34].

Generally speaking, the goal of *RT*-based correction schemes is to remove the influence of the atmosphere by modifying *top of atmospheric* (*TOA*) radiance measurement recorded by a sensor. Aerosol and water vapor content of the atmosphere have a substantial effect on atmospheric *absorption* and *scattering*. Besides, the *view zenith angle* (*VZA*) and *solar zenith angle* (*SZA*) also play a crucial role in determining the effects of the atmosphere (Figure 1). When the zenith angle is far from nadir, then the ray path travelled by the photon through the atmosphere gets larger, which increases the probability of an *absorption* or *scattering* event in turn [28, 35-36].

-Figure 1 inserted here-

Fig. 1 Geometry of the problem

Even though no atmospheric correction scheme can completely nullify the effects of the atmosphere, the radiative transfer in clear atmosphere is now well understood and a significant amount of work has been done in improving the accuracy and quality of correction algorithms [28, 37].

However, we should emphasize that the high accuracy available with detailed *RT* models may not actually be reached when working over large areas, due to unknown atmospheric parameters. For large areas and long time periods, these models still need faster methods in order to derive surface reflectances and to retrieve atmospheric parameters.

Additionally, in images, acquired by instruments with high temporal resolution and large field of view, each pixel has a different observational geometry and each atmospheric parameter has to be calculated for each pixel [29, 37-38]. Hence, it is highly costly and time consuming to employ models based on a rigorous treatment of the *RT* problem, like *Second Simulation of a Satellite Signal in the Solar Spectrum* (*6S*) [39], for the atmospheric correction of bulk numbers of such satellite images in real-time.

The *Simplified Model for Atmospheric Correction* (*SMAC*) was first introduced nearly two decades ago as an alternative approach to tackle these problems. It is based on the parametrization of detailed *RT* models [38]. Despite its age and lower level of accuracy as compared to *6S*, it is still a preferred atmospheric correction tool for many research groups due to its high speed [28-29].

Nonparametric regression splines with continuous optimization and conic quadratic programming

In our paper, we, for the first time ever, adjust, refine and employ the new regression and classification tool of data mining, *conic multivariate adaptive regression splines* (*CMARS*) [40], on a subject of *RS*. Developed as an alternative approach to *multivariate adaptive regression splines* (*MARS*) [41], *CMARS* converts the second stage of the *MARS* algorithm (i.e., backward step) into a *Tikhonov regularization* (*TR*) problem based on *penalized residual sum of squares* (*PRSS*) approach and solves the problem through *conic quadratic programming* (*CQP*). Herewith, the number of data and the amount of conditions grows, compared with earlier applications of *CMARS*.

In our research, we try to benefit from the dataset topologically and geometrically, intelligently, to “get into” it smartly, taking benefit from any structural features of this set. In this regard, the *CMARS* algorithm seems to be a very good choice as, i.e., in each dimension of the input variables, we build up a piecewise linear “zigzag” function, where the linear parts represent and approximate the data over whole intervals. This basic strategy is followed adaptively and multivariately [42]. As we are regularizing the *CMARS* approach, addressing first- and second-order derivatives, we go for “easy” models, by penalization; we turn this regularization into the language of a *CQP* model. As an expression of that easiness, there is the (to some sense enforced, by the entire complexity bounded) “flatness” of our model. We may say: we force the components of the unknown parameters’ vector to be 0 or, as much as possible, be nearby to vanish. This also implies that we try to have the smallest possible number of “significant” coefficients in our model. *MAR*S follows this goal through an “index” called *generalized cross-validation*; with *CMARS*, we follow this aim by an integrated framework of *conic* and *global optimization* [42].

A second class of parameters is the *penalty parameters* or, equivalently, upper bounds of the complexity. We already reduced these parameters by just single values, per class of variables, and no longer individually per basis functions, which means a strong reduction of the entire numbers of parameters, too. But we still do have the opportunity of activating these different parameters in a more individual manner, in the frame of the whole model and its complexity. With all of this, we may “tune”. Actually, our work on the number of parameters can also be considered as a *model selection*, the determination of dimensions included [42]. In view of the choice of those upper bound parameters, we gain from our experiences with statistical “performance” or “comparison” measures in earlier research works on *CMARS* and its robust counterpart *RCMARS* [43].

Advantage of using splines

The use of *spline functions* offer great advantages, in general, and in the context of our modelling in *RS*, as will be explained now compactly [42]: *(I)* Splines, from the perspective of just one dimension (input variable), are “piecewise polynomials”. If we merely used polynomials, then they would usually converge to plus or minus infinity when the absolute values of the (input) variables grow large. Since real-life processes stay in bounded margins (even if these bounds may be very large) generally, polynomials would need to have a high degree to oscillate sufficiently in order to remain within some reasonable margin. However, with high-degree polynomials it is hard and costly to work, in particular, as the real-life challenges are multivariate, which may need multiplications and, hence, a rapid increase in degree of the occurring multivariate splines. Using splines however permits us, in every dimension, to keep the degree of the polynomial “pieces” very low. Splines are indeed quite “flexible” and sufficiently “elastic” in order to approximate complex and high-dimensional data structures. We often even call them “smoothing splines”, since they “smoothly” approximate discrete data. *(II)* The splines of our *CMARS* are more “smooth” even in the sense that their oscillation is kept under control via a penalization of their integrals of squared first- and, especially, second-order derivatives, i.e., their complexity; then we discretize the integrals, obtain a program of *TR* which we eventually represent as a program of *CQP*. *(III)* The multivariate splines of our *CMARS* are multiplication products of “zig-zagging”, piecewise linear functions, which are of degree 1 (or 0) piecewise, and we can carefully determine how many dimensions we include into the process of multiplications of those 1-dimensional splines. Indeed, both these very low dimensional degrees and the controlled multiplication amount to a special care in order to prevent the complexity of our model from becoming too high. Let us recall that reducing the complexity can also be expressed as an increase in stability. *(IV)* Those multiplications are an expression of the fact that there are input variables, which are dependent and together in groups, contributing to an explanation of response variable by those explanatory input variables. *(V)* Eventually, in contrast to the use of a “stiff” model formulas (motivated in the tradition of physics and other basic sciences) and in our paper recalled by the formulas (1)-(4), our *CMARS* approach is very *adaptive* and “getting into” the complex dataset with its basic topological subsets and characteristics of shape.

Our motive

With this paper we recommend our adaptive tool for regression and classification, *CMARS*, especially, as a strong alternative to *traditional formula-based approaches* who have their scientific origins in the *natural sciences*, especially, in *physics*. However, we very much respect and appreciate those formulas as they represent important relations between essential, "natural" dimensions, though on a certain level of abstraction and, sometimes, simplification. Our *CMARS* approach of learning and modeling is based on both the empirical data and the mathematics

of *applied probability* and, especially, *optimization theory*, whereby *accuracy* becomes compromised with *stability*. But we herewith do also deliver formulas again, as in the *traditional approaches*; the formulas now are our *CMARS* models.
In order to accomplish our goals in this study, *CMARS* is applied to build a model for the atmospheric correction of a *Moderate-resolution Imaging Spectroradiometer* (*MODIS*) image data set. We also employ *MARS* for the same purpose, since it has many successful applications in economy, technology, and many other branches of science where complex relationships among variables are modeled [44-50]. The atmospheric correction models obtained through *CMARS* and *MARS* algorithms are applied on predefined areas of 12 *MODIS* images taken over the Alps. *SMAC* algorithm is also used in order to obtain the atmospherically corrected surface reflectance values for the same areas. Then, the results are compared against the surface reflectance values of *MODIS Level 2G* products [51], which are already corrected for the atmospheric effects via *6S*, and the results are given in terms of *root-mean-square error* (*RMSE*) values.
The remainder of this paper is organized as follows. *6S* and *SMAC* algorithms are briefly introduced in Section 2. Section 3 gives basic overview of *MARS* and *CMARS*. Then, in Section 4, the methodology and the results are represented. Finally, Section 5 concludes this paper, and gives an outlook to future studies.

6S and SMAC Methods

Atmospheric correction algorithms have evolved a lot during the last three decades, starting from the empirical line method to the recent *RT*-based algorithms; however, we do not intend to cover all these methods in a comprehensive manner. Instead, *6S* and *SMAC* methods are briefly introduced based on [28-29, 38-39, 52-54].

6S

Solar radiance reflected by a target is seriously modified by gaseous absorption, molecular scattering and aerosols in the atmosphere. In addition, *VZA* and *SZA* also play a major role in determining the effects of the atmosphere.
As an *RT*-based correction algorithm, the latest vector version of *6S* code (its current vector version is *6SV*) is widely used and has been extensively tested. *6SV*

is the basic code employed for the correction of *MODIS Level 1B* land surface reflectance products [55].

TOA reflectance, *SZA*, *VZA* and relative azimuth between the sun and the satellite direction, 3 variables defining the atmospheric condition: *atmospheric optical depth* (AOD), *water vapor* (*uWV*) and *ozone* (uO_3) content are required as input for *6SV*. The atmospherically corrected surface reflectance value of a target pixel is given by

$$\rho_s\left(\theta_s,\theta_v,\Delta\varphi\right) := \frac{\rho_s'}{1+S\rho_s'}, \qquad (1)$$

with

$$\rho_s' := \frac{\dfrac{\rho_{TOA}\left(\theta_s,\theta_v,\Delta\varphi\right)}{T_G} - \rho_a\left(\theta_s,\theta_v,\Delta\varphi\right)}{T_{\theta_s}T_{\theta_v}}. \qquad (2)$$

Here, ρ_s is the atmospherically corrected surface reflectance, S is the *spherical albedo* of the atmosphere. T_G denotes the *gaseous transmission*, $T\left(\theta_s\right)$ and $T\left(\theta_v\right)$ are the *total downward* and *upward atmospheric transmittances* respectively. ρ_a is the *atmospheric reflectance*.

SMAC Algorithm

Real-time atmospheric correction of large datasets, collected by sensors with high-temporal resolution, via detailed *RT* codes, like *6SV,* is operationally impractical. So, *SMAC* was proposed as an alternative method nearly two decades ago. Even though *6SV* and *SMAC* operate in a similar manner, the former is based on the rigorous treatment of the *RT* problem. *SMAC* employs the simplified forms of the formulas used in *6SV* to calculate the process variables. This leads to reduced complexity and quick atmospheric correction on a large data set. However, since *SMAC* does not include many components that are modeled within *6SV* in a more complex manner, the accuracy of the atmospheric correction is degraded, as compared to *6SV*.

Apart from a series of predefined coefficients, dependent upon the *RS* instrument, *SMAC* requires 7 input variables: *TOA* reflectance (ρ_{TOA}), *SZA* (θ_s), *VZA* (θ_v), *relative azimuth* between the sun and the satellite ($\Delta\varphi$), *AOD* (τ_{550}), *uWV* and *uO₃*. Then, the corrected surface reflectance is expressed as

$$\rho_s(\theta_s,\theta_v,\Delta\varphi) := \frac{\rho_s'}{T_G T(\theta_s) T(\theta_v) + S\rho'}, \qquad (3)$$

with

$$\rho_s' := \rho_{TOA}(\theta_s,\theta_v,\Delta\varphi) - T_G \rho_a(\theta_s,\theta_v,\Delta\varphi). \qquad (4)$$

Despite its age and lower level of accuracy, *SMAC* approach is still used by many research groups and projects, since it can perform an atmospheric correction in a short time. To give a specific example, *SMAC* can process a single *Meteosat Second Generation* subset 3000 times faster than *6SV*.

There are other correction techniques [56-58] that provide accurate results and are still significantly faster than *6SV*. However, these techniques are often commercial and provide little access to the inner structure of the algorithm. On the other hand, *SMAC* is available as a free and open-source code. This means that it can easily be implemented in an operational data preprocessing computer and can be modified according to user requirements.

In addition, when new sensors are introduced, only the band-specific coefficients need to be updated while the routines remain the same; this is another attractive feature of *SMAC* algorithm that makes it still popular.

Basic Overview on MARS and CMARS

We are interested in the multi-criteria antagonism (tradeoff) between *accuracy* and *stability*. Stability may be called: a *small complexity*. This tradeoff is keeping the complexity under "control", realized by us through *CMARS* in different ways: by *(i)* restraining the discretized integral of first- and second-order derivatives of the basis functions within some margin or "tolerance" (under a chosen and prescribed upper bound), but also *(ii)* using modern optimization theory (*model-based* approach) for a more integrated approach of both the forward and the backward step which we have in *MARS*. By this, we are closer also to exploiting the "power" of differential and integral *calculi* and to future developments in those calculi and in optimization theory. In future, we can also do modifications and elaborations by new and forthcoming principles and techniques of *discretization* [42].

So, in this section, within the aforementioned context, the reader can find the fundamentals of *MARS* and *CMARS* algorithms based on [40-43, 59-62].

MARS

Nonparametric regression and classification techniques are mostly the key data mining tools in explaining real-life problems and natural phenomena where many effects often exhibit a nonlinear behavior. As a form of regression analysis, *MARS* is a nonparametric regression technique widely used in data mining and estimation theory in order to built flexible regression models for high-dimensional nonlinear data. In *MARS* model building, piecewise *linear basis functions* (*BFs*) are fitted in such a way that additive and interactive effects of the predictors are taken into account to determine the response variable.

MARS uses two stages when building up regression model, namely, the *forward* and the *backward step* algorithms. In *forward step*, *BFs* are added up until the highest level of complexity is reached. Since the first step creates an over-fit model, preferred and eventual model is obtained by the elimination of *BFs* in *backward step*. Selection of *BFs* is data-based and specific to the problem in *MARS*, which makes it an adaptive regression procedure suitable for solving high-dimensional problems.

MARS uses expansions of the truncated piecewise linear basis functions of the form $\left(\pm\left(x_j-\tau\right)\right)_+$, where x_j is the *j*th component of *p*-dimensional variable $\boldsymbol{x}$, τ is the associated knot location of x_j. The '±' symbol indicates that only the positive or the negative parts are used, respectively, and x, $\tau \in \mathbf{R}$.

The relation between input and response in general model is expressed as

$$Y = f(\boldsymbol{x}) + \varepsilon, \quad (5)$$

where *Y* is a response variable, $\boldsymbol{x} = \left(x_1, x_2 \ldots, x_p\right)^T$ is a vector of predictors and ε is the error term in the observation with zero mean. *MARS* builds reflected pairs for each input $x_j \left(j = 1, 2, \ldots, p\right)$ with *p*-dimensional knots $\boldsymbol{\tau}_i = \left(\tau_{i,1}, \tau_{i,2}, \ldots, \tau_{i,p}\right)^T$ at each input data vectors $\bar{\boldsymbol{x}}_i = \left(\bar{x}_{i,1}, \bar{x}_{i,2}, \ldots, \bar{x}_{i,p}\right)^T$ of that input $i = 1, 2, \ldots, N$. Then, the collection of *BFs* is:

$$C := \left\{ \left(x_j - \tau\right)_+ ,\ \left(\tau - x_j\right)_+ ,\ \tau \in \left\{ x_{1,j}, x_{2,j}, \ldots, x_{N,j} \right\}\ \left(j \in \{1, 2, \ldots, p\}\right) \right\}, \tag{6}$$

where *N* is the total number of observations, *p* is the dimension of the input space. In order to reach spline fitting in higher dimensions, the tensor products of univariate spline functions are employed, leading to multivariate spline *BFs* in the following form:

$$B_m\left(\boldsymbol{x}^m\right) := \prod_{j=1}^{K_m} \left[s_{\kappa_j^m} \cdot \left(x_{\kappa_j^m} - \tau_{\kappa_j^m} \right) \right]_+ , \tag{7}$$

where K_m is the interaction degree of the *m*th *BF* and $\boldsymbol{x}^m$ denotes the vector of independent variables contributing to the *m*th *BF*. $x_{\kappa_j^m}$ is the corresponding input variable of the *k*th truncated linear function in the *m*th *BF*, the corresponding knot value for the variable $x_{\kappa_j^m}$ is given by $\tau_{\kappa_j^m}$, and finally $s_{\kappa_j^m} \in \{\pm 1\}$.

The *forward* and the *backward step* algorithms of *MARS* are used for the estimation of model function $f\left(\boldsymbol{x}\right)$. In the *forward step*, the use of functions from the set *C* and their products are allowed to represent *interaction*, which generates a maximal model that overfits the data. The initial model is in the following form:

$$f\left(\boldsymbol{x}\right) = \beta_0 + \sum_{m=1}^{M} \beta_m B_m\left(\boldsymbol{x}^m\right), \tag{8}$$

where B_m is either a function or product of two or more functions from the set *C*. The number of *BFs* in the current model is indicated by *M*, and β_0 is the intercept.

In order to compare the possible *BFs*, a *lack-of-fit* (*LOF*) criterion is used. For generating an estimated best model $\hat{f}_\alpha$ with the optimal value α, where α represents some complexity of the estimation, *MARS* algorithm first adds basis functions and products of the basis functions in the *forward step*. Then, the least significant ones are deleted in the *backward step*. To find the value for α, *MARS* uses *generalized cross-validation* (*GCV*) indicating the *LOF* and it is given as $GCV(\alpha) := \sum_{i=1}^{N}\left(y_i - \hat{f}_\alpha(\boldsymbol{x}_i)\right)^2 \Big/ \left(1 - Q(\alpha)/N\right)^2$. Here, N is the number of sample observations, $Q(\alpha) = u + dK$ with K representing the number of knots which are selected in *forward step*. The number of linearly independent functions in the model is given by u, and d denotes a cost for each *BF* optimization. While a larger $Q(\alpha)$ value creates a smaller model with less number of *BFs*, a smaller $Q(\alpha)$ value generates a larger model with more *BFs*. Using the *LOF* criterion, the best model is chosen according to backward step that minimizes *GCV*.

CMARS

CMARS has been developed as an alternative method to *MARS* by utilizing statistical learning, inverse problems and multiobjective optimization theories. Instead of applying backward step of *MARS*, *PRSS* with the *BFs* is built up during forward step. Then, penalty terms are added to the least squares estimation to control the *LOF*. This introduces an alternative approach to the complexity and the stability of the problem.

PRSS summed up during the forward pass stage of *MARS* has the following form:

$$PRSS := \sum_{i=1}^{N}\left(y_i - f(\overline{\boldsymbol{x}}_i)\right)^2 + \sum_{m=1}^{M_{\max}} \varphi_m \sum_{\substack{|\delta|=1 \\ \delta=(\delta_1,\delta_2)^T}}^{2} \sum_{\substack{r<s \\ r,s\in V_m}} \int_{Q_m} \lambda_m^2 \left[G_{r,s}^{\delta} B_m\left(\boldsymbol{h}^m\right)\right]^2 d\boldsymbol{h}^m.$$

(9)

Here, $V_m := \left\{\kappa_j^m \,|\, j = 1,2,\ldots,K_m\right\}$ denotes the variable set related with the mth *BF*, $\boldsymbol{h}_m = \left(h_{m_1}, h_{m_2}, \ldots, h_{m_{K_m}}\right)^T$ is the vector of variables contributing to the mth *BF*. Furthermore, $\varphi_m \geq 0$ are penalty parameters, and Q_m are suitable integration domains $(m = 1,2,\ldots,M_{\max})$. Finally, $G_{r,s}^{\delta} B_m\left(\boldsymbol{h}^m\right) := \left(\partial^{\delta} B_m / \partial^{\delta_1} h_r^m \partial^{\delta_2} h_s^m\right)\left(\boldsymbol{h}^m\right)$ for $\delta = (\delta_1,\delta_2)^T$, $|\delta| := \delta_1 + \delta_2$, where $\delta_1, \delta_2 \in \{0,1\}$. The trade-off between accuracy and complexity in this optimization problem is established through the penalties φ_m, and *PRSS* can be approximated as

$$PRSS \approx \left\|\boldsymbol{y} - \boldsymbol{B}(\tilde{\boldsymbol{g}})\lambda\right\|_2^2 + \sum_{m=1}^{M_{\max}} \varphi_m \sum_{i=1}^{(N+1)^{K_m}} L_{im}^2 \lambda_m^2. \quad (10)$$

Here, $\boldsymbol{y} := (y_1, y_2, \ldots, y_n)^T$ is the vector of responses, $\boldsymbol{B}(\tilde{\boldsymbol{g}}) = (\boldsymbol{B}(\tilde{\boldsymbol{g}}_1), \boldsymbol{B}(\tilde{\boldsymbol{g}}_2), \ldots, \boldsymbol{B}(\tilde{\boldsymbol{g}}_N))^T$ is an $(N \times (M_{\max} + 1))$-matrix, and $\|\bullet\|_2$ is the Euclidian norm. Rather than using distinct penalty parameters for each derivative in (10), only one penalty parameter $(\varphi = \varphi_m := \phi^2)$ can be employed, and then the new form of *PRSS* is expressed as

$$PRSS \approx \left\| \boldsymbol{y} - \boldsymbol{B}(\tilde{\boldsymbol{g}})\lambda \right\|_2^2 + \varphi \left\| \boldsymbol{L}\lambda \right\|_2^2, \qquad (11)$$

where $\boldsymbol{L}$ is a diagonal $((M_{\max} + 1) \times (M_{\max} + 1))$-matrix and λ denotes an $((M_{\max} + 1) \times 1)$-parameter vector estimated through the data points. The *PRSS* problem turns into a classical *TR* problem with $\varphi > 0,\ \varphi = \phi^2$ for some $\phi \in \mathbf{R}$.

The *TR* problem in (11) can be treated by *CQP* with a convenient choice of bound $\tilde{Z} \in \mathbf{R}$:

$$\begin{aligned} &\underset{h,\lambda}{\text{minimize to}} \quad h, \\ &\text{subject to } \left\| \boldsymbol{y} - \boldsymbol{B}(\tilde{\boldsymbol{g}})\lambda \right\|_2 \le h, \ \left\| \boldsymbol{L}\lambda \right\|_2 \le \sqrt{\tilde{Z}}. \end{aligned} \qquad (12)$$

At this point, one has to note that a careful learning process must be followed in order to obtain the values of bound $\tilde{Z}$. By applying the modern methods of continuous optimization, the *CQP* can be written in this basic notation:

$$\begin{aligned} &\underset{\boldsymbol{x}}{\text{minimize}} \quad \boldsymbol{c}^T \boldsymbol{x}, \\ &\text{subject to } \left\| \boldsymbol{G}_i \boldsymbol{x} - \boldsymbol{g}_i \right\|_2 \le \boldsymbol{p}_i^T \boldsymbol{x} - q_i \ \ (1, 2, \ldots, k) \end{aligned} \qquad (13)$$

The parametrical upper bound $\tilde{Z}$ in the second constraint of the *CQP* and the penalty parameter φ in the *PRSS* are linked, and the value for φ can be obtained via *TR*. The authors emphasize the high importance of the goal of numerical precision (accuracy) as a core target inside of the tradeoff stated above. In *CMARS*, via the "control parameter" given by some upper bound of the complexity term in our *CQP* optimization program, we may tune and regulate the importance that we grant and demand for the stability (lower complexity) goal and, by this, for the antagonistic accuracy goal [42].

Methodology and Results

Data Set and Retrieval of Necessary Parameters

The *MODIS* instrument capture daily data in 36 spectral bands ranging in wavelength from 0.4 μm to 14.4 μm at varying spatial resolutions (bands 1 and 2: 250 m, bands 3-7: 500 m, bands 8-36: 1000m) in order to investigate earth's global dynamics such as radiation budget, cloud cover and atmosphere. *MODIS* surface reflectance product (*MOD09/MYD09*) [51] comprises the atmospherically corrected surface reflectance values for the first seven bands, and the vector version of *6S* (*6SV*) is the basic correction algorithm behind this product [52]. The algorithm takes the *TOA* reflectance values from *MODIS Level 1B* product [55], and makes a series of corrections for the absorption and scattering by atmospheric gases and molecules. It also takes into account the coupling between atmospheric and surface bi-directional reflectance function and adjacency effect [39].

Another product family of *MODIS* is the *Level-3 daily atmospheric products*, from which *AOD*, *uWV* and uO_3 can be retrieved in order to be employed as input in *SMAC*. All these features make *MODIS* an attractive and convenient platform for this study.

12 *MODIS* images taken by *Terra* satellite between 2001 and 2008 are selected as data set. However, instead of using the full *MODIS* scene covering the south central part of Europe, it is preferred to work on a smaller subset that focuses on the Alps and their close neighborhood (Figure 2). Detailed information about the data set can be found in Table 1. At this point, we emphasize that all the calculations and operations are performed on the 4th reflective solar band (0.545 – 0.565 μm).

-Figure 2 is inserted here-

Fig. 2 Study area (S11: 06.11.2002)

-Table 1 is inserted here-

TOA reflectance values are retrieved from *Terra Level 1B* product *MOD02HKM* [55], which comprises the 3rd, 4th, 5th, 6th and 7th reflective solar bands at 500 m spatial resolution. Atmospheric parameters required to perform atmospheric correction through *SMAC* algorithm (i.e., *AOD*, *uWV* and *uO3*) are obtained from *Terra Level 3 daily atmospheric products* [63].

The results obtained by *MARS*, *CMARS* and *SMAC* methods are tested against *Terra Level 2G* surface reflectance products (*MOD09GA*) [51]. The atmospheric correction algorithm used in *MOD09GA* is based on *6SV* method. *6SV* has been seriously cross-checked with other complex correction algorithms and has given highly accurate results under various conditions. So, *MOD09GA* is preferred as a reference in the comparison of the results.

MARS and CMARS Model Training

In the model training phase, on each image in the training set, a training polygon with fixed dimension (i.e., rectangular in shape with an area of 483000 km^2), which includes all basic land-cover types, are drawn. In each training polygon, 5000 points are randomly generated, and for each point, *TOA* reflectance value and atmospherically corrected surface reflectance value are extracted from *MOD02HKM* and *MOD09GA* products, respectively, together with the corresponding geographic longitude and latitude. As seen in Table 1, each month appears once in the dataset. So, month value of the image, from which the corresponding model training parameters are retrieved, is also written in that point data file. In the next step, the training data from each of the training polygons are combined in a single text file, which results in 60000 data points on aggregate.

In *MARS* model building, $\boldsymbol{x} = (\lambda, \phi, \kappa, \zeta)^T$ is the vector of predictor variables, where λ and ϕ represents the geographic latitude and longitude, respectively, κ is the *TOA* reflectance value, and ζ is the month indicator ($\zeta = 1, 2, \ldots, 12$). The observation equation for *MARS* is given by $y_i = \mathrm{SRef}(\boldsymbol{x}_i) + \varepsilon_i$ $(i = 1, 2, \ldots, N)$, where y_i is the atmospherically corrected surface reflectance obtained from *MOD09GA* at $\boldsymbol{x}_i = (\lambda_i, \phi_i, \kappa_i, \zeta_i)^T$ with a measurement error ε_i. SRef is the function that gives the surface reflectance predicted by *MARS,* and N is the total number of observations.

Since *MARS* algorithm allows users to define model-building dimensions such as maximal number of terms, the degree of interaction among predictor variables, different settings are applied, and the model that gives the minimum *GCV* value and the maximum *adjusted R^2* [64] value are chosen. All settings employed in the model training are given in Table 2. Salford Systems MARS® Ver. 3 [65] is used for *MARS* model building.

-Table 2 is inserted here-

In *CMARS*, all of the *BFs* obtained in the forward pass of *MARS* are considered for the formulation of *PRSS* in the form of a *CQP* problem, and then it is solved by using MOSEK™ software [66].

Model Testing and Comparison of the Results

After constructing *MARS* and *CMARS* models through the training phase, the obtained models are tested on each image in the data set. For testing, both models are applied on a predefined area with a size of 53700 km^2 on each image. In addition to *MARS* and *CMARS* models, *SMAC* algorithm is also employed for each test area (Figure 3). Then, the surface reflectance values produced by *MARS*, *CMARS* and *SMAC* algorithms for each test area are compared with the ones given by *MOD09GA* product in terms of *RMSE*. The results can be found in Table 3.

-Figure 3 is inserted here-

Fig. 3 Test area images for S11(06.11.2002): a) CMARS, b) MARS, c) SMAC, d) MOD09GA

-Table 3 is inserted here-

It is evident that *CMARS* (and *MARS*) outperforms the "traditional" approach *SMAC*.

Even though *CMARS* seems to give similar performance as *MARS*, as it may be inferred from the results at first sight; one must not miss the fact that *MARS* has already been in the statistical learning and data mining community for nearly two decades and it is "well-prepared" and "very well-elaborated" for dealing with huge data sets.

However, as being obvious from the results, we have solidified the competitiveness of *CMARS*, even on very huge and complex real-life data. By *CMARS*, we know that our models are more accurate, robust and stable than *MARS*, since it is more model-based and employs the modern techniques of continuous optimization.

Moreover, via the tradeoff between precision and stability, *CMARS* lets us open our investigations to real-world challenges which include noise in the response (*output*) variable, namely, to the Theory of Inverse Problems, to Data Mining and to Statistical Learning.

Conclusions and Outlook

In this paper, we try to shed light onto the areas of data-mining and optimization within a real-life perspective by taking the unique advantages of spline functions. Natural phenomena and real-life problems often exhibit a nonparametric and multivariate behavior, in which the curse of dimensionality may easily prevail. This means, controlled successive multiplications may sometimes be inevitable and useful to represent the multi-dimensional interaction of the model.

High dimensional and complex data sets can be wisely handled with the inherent smoothing characteristic of splines. As illustrated in our case, splines applied in *CMARS* are even made smoother through *TR* and *CQP*, and enable us to adaptively penetrate into our complex and large data set.

In the works [40, 59, 62] on *CMARS*, the authors firstly demonstrated the remarkable competitiveness of *CMARS*, when compared with *MARS*, with respect to various "comparison measures" of performance, in particular, statistical performance measures. Those measures not only covered *accuracy*, but also *stability* [42].

The accuracy goal is fostered in another special and powerful way in this paper: by the use of the very elaborated and strong (in theory and in real-life performance) *Interior Point Methods*, which benefit from the well-structuredness of our convex problem, given here by the class *CQP* [42].

On the other hand, it is a clear fact that MARS still performs well and gives satisfactory results as our CMARS on the data set. This has already been expected because that is what MARS was designed for: to overcome large and complex data.

However, within the light of our obtained results, we have a growing confidence in CMARS, since it enables us to accomplish two crucial tasks simultaneously; (*i*) to process large and complex real-life data, (*ii*) and to obtain more robust and stable models.

Moreover, with *CMARS* we are now "hosted" in optimization theory and its scientific community; furthermore, we even have a promise of future benefitting from *Robust Optimization*, which we can apply through the *robust* counterpart of *CMARS*, our *RCMARS* [43]. *RCMARS* will additionally permit to imply into our modelling the uncertainty in the *input* variables, which typical for real-life problems also [41].

As a future work, we would definitely, and intensively like to concentrate on the application of *CMARS* on even larger datasets with different wavelength bands. Moreover, *RCMARS* will be considered as another new and powerful data mining tool in order to cope with the uncertainties in our huge dataset by applying the principles of robust optimization.

Spatial technologies (i.e., *GIS* and *RS*) are powerful tools with data management, geo-processing, modeling and visualization capabilities. Furthermore, the rapid advances in these technologies give us the opportunity of more effective planning and decision making.

As our study showed us, once we manage to integrate the dynamical progress of scientific advances in modern continuous optimization with the spatial technologies, we can improve our ability to deal with *global challenges* hindering *development*. So, there is still room for us to enhance our understanding of the value of spatial data and to find better methods for incorporating the modern techniques of continuous optimization with *GIS* and *RS*, in order to increase our *quality of life* and provide a *better future* for the next generations.

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