CAN SINGLE EMPIRICAL ALGORITHMS ACCURATELY PREDICT INLAND SHALLOW WATER QUALITY STATUS FROM HIGH RESOLUTION, MULTI-SENSOR, MULTI-TEMPORAL SATELLITE DATA?

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ABSTRACT:

Assessing and monitoring water quality status through timely, cost effective and accurate manner is of fundamental importance for numerous environmental management and policy making purposes. Therefore, there is a current need for validated methodologies which can effectively exploit, in an unsupervised way, the enormous amount of earth observation imaging datasets from various high-resolution satellite multispectral sensors. To this end, many research efforts are based on building concrete relationships and empirical algorithms from concurrent satellite and in-situ data collection campaigns. We have experimented with Landsat 7 and Landsat 8 multi-temporal satellite data, coupled with hyperspectral data from a field spectroradiometer and in-situ ground truth data with several physico-chemical and other key monitoring indicators. All available datasets, covering a 4 years period, in our case study Lake Karla in Greece, were processed and fused under a quantitative evaluation framework. The performed comprehensive analysis posed certain questions regarding the applicability of single empirical models across multi-temporal, multi-sensor datasets towards the accurate prediction of key water quality indicators for shallow inland systems. Single linear regression models didn't establish concrete relations across multi-temporal, multi-sensor observations. Moreover, the shallower parts of the inland system followed, in accordance with the literature, different regression patterns. Landsat 7 and 8 resulted in guite promising results indicating that from the recreation of the lake and onward consistent per-sensor, per-depth prediction models can be successfully established. The highest rates were for chl-a ($r^2=89.80\%$), dissolved oxygen ($r^2=88.53\%$), conductivity ($r^2=88.18\%$), ammonium $(r^2=87.2\%)$ and pH $(r^2=86.35\%)$, while the total phosphorus $(r^2=70.55\%)$ and nitrates $(r^2=55.50\%)$ resulted in lower correlation rates.

1. INTRODUCTION

Water quality is a fundamental aspect of global freshwater resources. Information about water quality is needed to assess baseline conditions and to understand trend for water resource management. Therefore, the importance of evaluating and monitoring water quality in terrestrial reservoirs is clear and self-evident. The most commonly used methodology to examine the quality of water is through in-situ sampling and chemical analysis. In-situ sampling lead to accurate estimations but lacks in several other areas. More specifically:

- In-situ measurements fail to provide the spatial distribution of a phenomenon throughout the water body, since the results correspond to the exact location/region from which the sample was taken.

- Water bodies are usually inaccessible on a regular basis.

- In many cases, monitoring one, let alone tens or hundreds of lakes in a region, is a prohibitive process, both financially and logistically.

- The location of the sampling regions usually is not correlated with any phenomena, sensitive regions or management practices.

- Comprehensive monitoring of any crucial phenomena requires a frequent sampling.

To this end, the main advantage of remote sensing technology provides the capability and the required information on a regular basis. Moreover, it provides the means for exploiting information from dates that in-situ sampling was not conducted (*Dekker, Vos, & Peters, 2002, Zheng, Z., Yuanling, 2011*). In particular, monitoring the good environmental status through earth observation data is not new but among the first objectives of remote sensing data exploitation (*Wrigley and Horne, 1974*).

Natural inland waters are optically complex due to the interaction of three main parameters, namely chlorophyll, inorganic suspended solids and dissolved organic matter. The estimation of water concentrations in sensitive shallow systems through the use of multispectral remote sensing imagery can be hindered due to possible errors in consistent correlation. The optical complexity poses many challenges to the accurate retrieval of biogeochemical parameters. The depth of the lake and the aquatic vegetation levels is of significant importance. Many standard chlorophyll-a retrieval algorithms, which are optically dominated by phytoplankton and their breakdown products, tend to fail when applied to more turbid inland and coastal waters whose optically properties are strongly influenced by non-covarying concentrations of non-algal particles and coloured dissolved organic matter (Huang et al., 2015; Palmer et al., 2015; Sass, et al., 2007).

The advent of new generation satellite optical sensors like US Landsat-8 and the upcoming EU Sentinel-2 provides opportunities for developing satellite-based operational monitoring geospatial services globally. However, there are certain challenges regarding the limitations, operational feasibility, inter-calibration between the different sensors and the standardization of procedures for delivering accurate

geospatial value-add maps regarding the good environmental statuts of inland systems.

The establishment of relations between in-situ ground truth and earth observation data is usually based on three approaches (*Duan and Bastiaanssen, 2015; Giardino et al. 2007, Chen et al. 2008, Alparslan et al., 2007, Hellweger et al, 2007, Tyler et al., 2006, Han et al., 2005, Vincent et al, 2004; Young et al., 2011):*

- empirical algorithms, which is based on the creation of a regression models using satellite imagery and water quality parameters,

- semi-empirical approach, which embodies the use of spectral water quality characteristics in the statistical analysis,

- analytical approach, in which key water quality parameters are related to inherent optical properties and therefore to apparent optical properties and top-of-atmosphere radiance.

In this study, we have experimented with multi-temporal Landsat 7 and Landsat 8 high resolution satellite data, coupled with the corresponding hyperspectral data from a field spectroradiometer and in-situ ground truth data with several physico-chemical and key monitoring indicators. All available datasets, covering a 4 years period were processed and fused under a quantitative evaluation framework. The performed comprehensive analysis posed certain questions regarding the applicability of single empirical models across multi-temporal, multi-sensor datasets towards the accurate prediction of key water quality indicators for shallow inland systems. Landsat 7 and 8 resulted in quite promising results indicating that from the recreation of the lake and onward concreate per-sensor, per-depth prediction models can be successfully established.

2. MATERIALS AND METHODS

2.1. Study Area

The study area is located in Greece, on the southeast of Larissa, near the northern slopes of Pelion (Figure 1). It was completely desiccated in 1962 as part of a plan to address the flooding of the surrounding areas and to create new agricultural land. In 2010 it was recreated in order to compensate the profound consequences on the local ecosystem and it now occupies an area of 42.000 acres. It is characterized as shallow and eutrophic while it is constantly pressured by land use changes, hydrological flow modifications and excessive chemical enrichment (*Chamoglou et al. 2014*).

The protection, conservation and management of the site was undertaken by the Management Body of Ecodevelopment Area of Karla – Mavrovouni – Kefalovriso – Velestino (E.A.Ka.Ma.Ke.Ve.) which was established in 2003 and conducted frequent water quality sampling until 2013.

2.2. Multi-temporal Remote Sensing Data and Field Campaigns

Multitemporal high resolution satellite data were collected from the recreation of the Lake and onward. In particular, Landsat 7 (L7) and Landsat 8 (L8) data were acquired. Landsat 7 consists of seven spectral bands, from 0.45 to 2.35 micrometers, with spectral resolutions of 0.06-0.20 micrometers and spatial resolution of 30 meters for Bands 1 to 5 and 7. The thermal infrared band has a 60 meter pixel and wavelengths of 10.40-12.50 μ m. However, the Lake Karla region is heavily affected by the presence of gaps (approximately 20% of image pixels) in all the corresponding L7 paths and rows (Figure 1). The problem is caused by the early failure of the Scan Line Corrector which compensates for the forward motion of the satellite. In addition, Landsat 8 OLI consists of seven spectral bands with wavelengths from $0.43-2.29\mu m$, spectral resolution from 0.02- $0.18\mu m$ and spatial resolution of 30m.

In-situ ground-truth sampling data were systematically collected from 2011 an onward from the lake's Management Body. Among the various field and lab sensors and instruments, the Hach's HQ40d Portable Multi-Parameter Meter carried out the measurements of the physicochemical parameters, while the quantitative determination of water's inorganic nutrient compounds and chlorophyll-a's concentration was performed by applying different determination protocol for each compound, based on standard methods (APHA, 1998) and using the spectrophotometer HACH DR / 3900 (Chamoglou et al. 2014). In-situ hyperspectral reflectance observations were, also, acquired using the GER 1500 (Spectra Vista Corporation, US) portable spectroradiometer which provides spectra with 512 spectral bands distributed in the spectral region from 350nm to 1050nm with 3.2 nm FWHM. The location of every measurement, which was the same with the sampling positions, was recorded using a portable GPS.

This study is focused mainly on the long term monitoring of the following parameters: chlorophyll-a (mg/lt), NO₃ (mg/lt), NH₄ (mg/lt), Total Phosphorus (mg/lt), pH, conductivity (mS/cm), Dissolved Oxygen and temperature (C°). Chlorophyll-a (Chla) is a biological parameter and the necessary pigments used by most photosynthetic organisms for the release of chemical energy. When in vivo form, it exhibits two main absorption maxima positioned at 433nm (blue) and 686 nm (red) of the spectrum (*Hunter et al. 2008*). The concentration of chl-a is used as an indicator for the description of bioproduction and is linearly related to the biomass, the age of algae communities etc. (*Thiemann, et al., 2000*).

Dissolved Oxygen (D.O.) is an important physical and chemical parameter which is used by most organisms for respiration and oxidation of organic substances. It primarily originates in the water from the atmosphere, through the phenomenon of diffusion, and secondarily due to the photosynthesis of aquatic flora. It has a seasonal and daily circle. PH is a physico-chemical parameter expressing the negative decimal logarithm of the hydrogen ion, in particular of hydronium (H_3O^+) in a solution. As most aquatic organisms survive in a relatively small pH range, the parameter is an indicator of the existence of life.

Conductivity is physico-chemical parameter that expresses the ability of the water body to allow the passage of electric current, and gives the total content of water in minerals. Conductivity values are influenced by ion concentration, mobility and electric charge, as well as water temperature. Total Phosphorus (TP) is the sum of the organic and inorganic phosphorus, dissolved or in the form of particles. It is affected by temperature, pH, nitrate and ammonium ions etc. and is usually the limiting factor of primary production, thus of utmost importance for the restoration of the ecological balance of a lake. Finally, nitrates (NO₃) and ammonium (NH₄) are an inorganic chemical parameter and one of nitrogen's forms in the aquatic environment. Their concentration plays a decisive role in the trophic state of the lake.



Figure 1: Lake Karla in central Greece was the study area. Several permanent (with yellow color) and non-permanent (with red color) sampling locations have been employed (top, second from left). Landsat 8 colour composites (RGB 432) before and after the radiometric and atmospheric corrections are, also, shown (top). An example of the processing procedure for the Landsat 7 datasets are presented (bottom). Landsat 7 images before and after the developed gap-filling algorithm are shown. The detected inland water in a binary format and the estimated map with dissolved oxygen concentrations are also demonstrated. Note that all the processing procedure is automated.

2.3. Pre-processing Procedures and Multitemporal Reflectance

Radiometric and atmospheric corrections were performed on the satellite imagery towards the elimination of solar illumination, atmospheric and terrain effects. Digital numbers were converted to top-of-atmosphere reflectance using the absolute radiometric calibration factors and effective bandwidths for each band. Atmospheric correction was then conducted through ATCOR2 and MODTRAN4 for calculating a radiative transfer model for atmospheric transmittance, direct and diffuse solar flux, and path radiance. Several parameters were employed like the aerosol model, as well as satellite and sun geometry information including the satellite inclination, sun azimuth and zenith.

2.4. Relationships between Reflectance and Concentrations

Several empirical regression models were evaluated in order to study and establish consistent relationships between the concentrations of the water quality parameters and the satellite reflectance values.

Several experiments were performed in order to evaluate the potential of establishing relationships between multi-temporal and multi-sensor data. The time difference between the sampling date and the acquisition of the satellite image was up to three days maximum. Three models were developed and evaluated. One containing in-situ sampling locations from the relatively deep parts of the lake, the second containing sampling data from the very shallow parts of the lake and the third including all in-situ sampling data from all lake depths. From every model, linear regression equations were computed for about 140 combinations of Landsat 8 spectral bands and for about 120 combinations of Landsat 7 spectral.

Moreover, concurrent reflectance hyperspectral data from a field spectroradiometer were calculated. These observations were, also, correlated with both the in-situ ground truth and the satellite images. About 120 band ratios and indices were computed and tested.

The overall analysis and comprehensive evaluation posed certain questions regarding the applicability of single empirical models across multi-temporal, multi-sensor datasets. In accordance with the literature, in all cases there wasn't a single linear regression model which could establish concrete relations across multi-temporal, multi-sensor datasets. In particular, only the first model managed to provide high correlations for several water quality indicators for such a shallow and sensitive inland system. The shallower parts of the inland system followed different regression patterns, however a consistent empirical model couldn't be established.

On the contrary, the first model provided quite promising results for most of the examined water quality indicators. The highest correlation rates regarding the hyperspectral reflectance from the field spectroradiometer were for chl-a ($r^{2}=97.6\%$), ammonium ($r^{2}=88.5\%$), nitrates ($r^{2}=85.7\%$), conductivity ($r^{2}=81.7\%$) and dissolved oxygen ($r^{2}=81.9\%$).

Regarding the satellite datasets a number of band ratios, indices and equations established relationships with correlation rates. In Table 1, the highest correlation rates (r^2) that were calculated per satellite sensor (i.e, Landsat 7 or Landsat 8), per water quality indicator (i.e, pH, Chla, etc) and per spectral band combination (e.g., ratio) are shown. Regarding chlorophyll-a the highest rates were calculated for the EXP(R835/R2220), EXP(R835/R660), EXP(R835/R1650), R835/R660. (R835/R660)+R1650, R835/R2220, R835/(R485+R560+R660), EXP(R835/R560), LnR660-LnR835 formulas and for Landsat 7. However, the R835/R660 was selected as was most simple and included bands that seemed to correlated more with chla. For Landsat 8, the higher rates were for the (R480-R655)/R560, R560-R865, EXP(R865/R1610), R480-R560, R560-R480, R440-R560, R560-R440, R560-R655 formulas and the selected of the same reasons was the R480-R560. For both sensors the R835, R660 and R560 spectral bands (and their neighbours) were involved in most high correlated models.

Regarding NH₄ concentrations, the high rates for Landsat 7 were the EXP(R600/R835), R600/R835, EXP(R660/R835), EXP(R600/R1650), EXP(R660/R1650), (R600-R835)/R660, EXP(R600/R2220), R660/R835 and R600-R835 formulas, while the one employed was the R600/R835. Regarding Landsat 8, the highest rates were for the (R480-R655)/R560, R480-R560, R560-R480, EXP(R865/R1690), R560-R865, R440-R560, R560-R440, R560-R655, R480/R2200 formulas. The first one was employed for calculating the corresponding maps. For both sensors the R560, R835 and R660 spectral bands (and their neighbours) were involved in most high correlated models.

Regarding the pH parameter, for Landsat 7 the highest rates were for the LnR485-LnR2220, R485-R2220, R485/R2220, R485-R1650, EXP(R2220), R2220, LnR2220 and EXP(R485/R2220) formulas, while for Landsat 8 the highest correlations were for the LnR865-LnB6, R865/R1690, R440-R560, R560-R440, R865/R2200, R480-R560, R560-R480, R655/R2200, R480/R2200 and LnR440-LnR2200. For both sensors the R485 and R2200 spectral bands (and their neighbours) were involved in most high correlated models.

3. EXPERIMENTAL RESULTS AND VALIDATION

Regarding the evaluation of the employed empirical algorithms the overall validation indicated that several water quality indicators could quite accurately estimated through high resolution multispectral data. In particular, the highest rates were for chl-a (r^2 =89.80%), dissolved oxygen (r^2 =88.53%), conductivity (r^2 =88.18%), ammonium (r^2 =87.2%) and pH (r^2 =86.35%), while the total phosphorus (r^2 =70.55%) and nitrates (r^2 =55.50%) resulted in lower correlation rates.

Note that algorithms which included the EXP form, while in many cases provided high correlations, proved to be sensitive and unable to estimate correctly the corresponding parameters especially in images with a certain cloud cover. In particular, images with important cloud cover had to be excluded due to certain inaccurate reflectance calculations and relative radiometric calibration.

Experimental results regarding chla concentrations demonstrated quite promising correlations i.e, for L7 [r^2 =89.80%, (R835/R660)] and L8 [r^2 =76.65%, (R480-R565)]. These quantitative results were also verified from the performed

comparison between the delivered maps from L7 and L8 for close dates. In particular, the two sensors and the employed persensor model estimated the same concentration levels when only one day temporal difference. Few higher differences were calculated in the quite shallow parts of the lake. In general, when comparing with the in-situ ground truth data the calculated chla levels were slightly overestimated with L7 data and slightly underestimated with L8 data.







Figure 2: Multi-temporal geospatial maps with the estimated concentrations for certain key water quality indicators. It can be observed that chlorophyll-*a* presented slight variations throughout the year. TP reached certain peaks in March and then dropped to lower rates. Conductivity resulted in high rates throughout the year although from June and afterwards there was a minor decrease. Dissolved oxygen reached a maximum in March (as TP) and then decreased stably.

Regarding the DO estimation the experimental results indicated high correlation rates i.e, $[r^{2}= 88.53\%, (R560+660)/2$ for L7 and $r^{2}=80.49\%, (R480/R655)$ for L8]. This was also confirmed by the comparative analysis between the two sensors for maps of closing dates. The conductivity was estimated, also, for both sensors with high rates $[r^{2}=66.02\%, (R485-R835)/(R660-R835)$ for L7 and $r^{2}=88.18\%, (R480-R655)/R560$ for L8].

Moreover, regarding the estimation of NH₄ concentrations high correlations were established [$r^2=94.32\%$, (R560/R835) for L7 and $r^2=80.64\%$, (R480-R655)/R560 for L8] by the regression models. However, when all the multi-temporal maps were computed for all the acquired data for the 4 years period, some negative values where calculated indicating that the established relation was sensitive to certain optical variations.

The pH parameter was estimated, also, with high correlation rates $[r^{2}=82.46\%, (R485/R2220]$ for L7 and $r^{2}=86.35\%$,

(R865/R1610)] and delivered consistent and stable maps across the multi-temporal dataset.

The TP and NO₃ parameters were calculated with lower rates than the aforementioned ones. In particular, the TP was estimated with a higher rate r^2 =70.55% (R660/R835) for the L7 datastes and with a lower one r^2 =50.82% (R560-R1610) for L8. For the estimation of NO₃ concentrations the calculated correlation was at r^2 =55.50% (R835/R2220) for L7 and r^2 =55.50% (LnR1610-Ln2200) for L8.

Generally speaking, chla resulted to high correlations and included the RED and NIR bands. NO_3 mainly the SWIR2, NH_4 the GREEN and BLUE, the TP for GREEN and the pH for SWIR2, BLUE, GREEN and RED. These observations are, generally, in accordance with the literature. In particular, there is a number of studies that established correlations for e.g., chla between the Landsat ETM1, ETM2, ETM3 and ETM4 bands,

while the models were constructed using genetic algorithms, multilinear regression with correlations ranged from $r^2 = 0.58$ to 0.95 (*Chen et al. 2008, Alparslan et al., 2007, Hellweger et al, 2007, Tyler et al., 2006, Han et al., 2005, Vincent et al, 2004*).

4. CONCLUSIONS

We have experimented with Landsat 7 and Landsat 8 multitemporal satellite data, coupled with hyperspectral data from a field spectroradiometer and in-situ ground truth data with several physico-chemical and other key monitoring indicators. All available datasets, covering a 4 years period, in our case study Lake Karla in Greece, were processed and fused under a quantitative evaluation framework. The performed comprehendsive analysis posed certain questions regarding the applicability of single empirical models across multi-temporal, multi-sensor datasets towards the accurate prediction of key water quality indicators for shallow inland systems. Landsat 7 and 8 resulted in quite promising results indicating that from the recreation of the lake and onward concrete per-sensor, per-depth prediction models can be successfully established. The highest rates were for chl-a (r²=89.80%), dissolved oxygen (r²=88.53%), conductivity ($r^2=88.18\%$), ammonium ($r^2=87.2\%$) and pH $(r^2=86.35\%)$, while the total phosphorus $(r^2=70.55\%)$ and nitrates ($r^2=55.50\%$) resulted in lower correlation rates.

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