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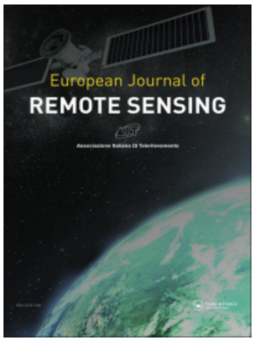

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Evaluation of Landsat-8 OLI and Sentinel-2 MSI images for estimating the ecological quality of port waters

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ABSTRACT
Recent research has demonstrated that the TRophic IndeX (TRIX) is informative on the ecological quality of Mediterranean port waters and can be estimated by the processing of multispectral observations collected in situ. The current study investigates the alternative use of multispectral data acquired by medium-high spatial resolution optical satellite sensors, i.e. the Landsat-8 (L8) Operational Land Imager (OLI) and the Sentinel-2 (S2) MultiSpectral Instrument (MSI). The study analyzes the impact of the main factors influencing TRIX estimation using datasets collected in several Mediterranean ports and particularly in those of Civitavecchia and Viareggio (Central Italy). The experimental results indicate that the spectral configurations of OLI and MSI have a marginal impact on TRIX estimation, while major effects are caused by the different spatial and temporal features of the two sensors. The enhanced spatial properties of MSI are important particularly in the smaller port of Viareggio; the higher acquisition frequency of this sensor brings significant advantages for operational monitoring applications. Overall, the accuracy of TRIX estimation based on in situ spectral measurements is reduced significantly by the use of OLI images and only marginally by that of MSI images. Both image types represent an advancement for the operational monitoring of port waters.

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Introduction

The effects of both global climate change and anthropogenic activities have increased the importance of defining efficient practices to conserve and improve the ecological status of water bodies (IPCC, 2019). Seaports are sheltered areas where man-made infrastructures have modified the natural conditions of the water bodies for commercial, recreational and military navigation purposes. Since most of global trade is carried by sea, ports have always played a key role for world economic and social development. This has promoted appropriate policies to monitor, regulate and address the various environmental impacts associated to the increasing traffic of maritime transportation (see for details: https://www.imo.org).

In the context of quality assessment and protection of inland and marine waters, the European Directives: EC-WFD (2000), EC-MSFD (2008), EC-IMP (2013) and related further implementation developments, established the framework for monitoring water bodies. With the adoption of the Marine Strategy Framework Directive (MSFD) the member states of the European Community are obliged to achieve and maintain a "Good Ecological Status" (GES) of all European seas by 2020 (Vanhellemont & Ruddick, 2015). Port waters are substantially altered by human activities and addressed in the category of Heavily Modified Water Bodies (EC-HMWB, 2003). In this case, an improvement in environmental conditions is achieved only with some mitigation measures allowing to reach the "Good Ecological Potential" (GEP), which represents the best ecology that permits human activities to continue (Ondiviela et al., 2012).

Among the most critical aspects, concerning the ecological quality of port waters there is eutrophication, i.e. the abnormal increase of nutrient concentration due both to waste discharges and to resuspension of sediments, which can induce anomalous phytoplankton blooms and anoxia phenomena (Karydis, 2009). The methods applied to monitor and control trophic condition and eutrophication in transition and coastal waters include a series of physical-chemical and biological investigations, whose final result can be summarized through a bad-good quality scale expressed by specific indices.

Among these, one of the most widely utilized is the TRophic IndeX (TRIX) proposed by Vollenweider et al. (1998). This index integrates numerous water parameters related to the trophic processes occurring in marine ecosystems, such as Chlorophyll *a*, Dissolved Oxygen, Nitrogen and Phosphorus. TRIX therefore provides exhaustive information on biological response (biomass), environmental disturbance (oxygen) and pressure (nutrients) of seawaters covering a wide range of trophic conditions from oligotrophy to hypereutrophy. After being adopted by the

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Italian legislation to classify the coastal waters into four classes, TRIX was used in the context of a common Mediterranean strategy for eutrophication monitoring (UNEP-MAP, 2007).

TRIX was then revised to meet the requirements of the European Water Framework Directive 2000/60 (Pettine et al., 2007) and thereafter discussed and applied for characterizing the ecological status of many other coastal and transitional water bodies (Cabrita et al., 2015; Giovanardi & Vollenweider, 2004; Primpas & Karydis, 2011; Salas et al., 2008).

Due to the need to collect and analyse various water parameters, however, the field-based assessment of TRIX is costly and labour-intensive. This represents a limit at the operational application of the index for the long-term monitoring of port waters, which should be preferably carried out with high spatiotemporal resolution. The relationships between the variables involved in the computation of TRIX, particularly Chlorophyll *a* concentration and water spectral reflectance (Soja-Woźniak et al., 2020), provide the basis for an alternative method to estimate TRIX. The study conducted by Massi et al. (2019) addressed this issue, demonstrating that an efficient characterization of TRIX in Mediterranean ports can be obtained by the analysis of reflectance spectra collected in situ.

A direct extension of such study would concern the application of a similar method to multispectral satellite sensors (IOCCG, 2000), which would obviously imply further advantages in terms of labor and economic costs. Medium spatial resolution optical imagery is historically available from the Landsat satellite series. The last satellite of this series, Landsat-8 (L8), has an improved instrument aboard, the Operational Land Imager (OLI), whose spatial (30 m) and temporal (16 days at the equator) resolutions show some potential for the characterization of port water quality (Pahlevan et al., 2017a). A more advanced opportunity is now offered by the Copernicus Sentinel-2 (S2) mission, that included the launch of two twin satellites (S2A/B), bearing onboard the MultiSpectral Instrument (MSI). The S2 MSI, in fact, routinely collects multispectral optical images with higher spatial resolution (10 m) and a revisiting time of 5 days at the equator (Pahlevan et al., 2017b).

Some investigations have been recently conducted on the use of medium-high spatial resolution optical satellite data to assess the trophic conditions of both marine and inland waters in various regions of the globe. Papoutsa et al. (2014) used Landsat TM/ETM data to estimate the Trophic State Index of Case-2 waters in the Mediterranean region. Shi et al. (2019) proposed and tested a semi-analytical approach to predict the same index in inland waters based on L8 OLI data. Zhou et al. (2019) predicted the Trophic Level Index of some lakes in China by means of L8 OLI imagery. To date, however, no research has specifically concerned the utilization of medium-high spatial resolution satellite imagery for the estimation of TRIX in port waters. The current paper investigates this subject by exploring the possibility of driving the previously proposed TRIX estimation method with satellite images in place of in situ observations. As noted by Gholizadeh et al. (2016), this operation introduces some relevant issues, which concern in particular:

(1) The spectral configuration of the images; the original (in situ) method for spectral TRIX estimation was developed using 12 optical channels, whose degradation to the fewer OLI and MSI bands implies an inevitable information loss.
(2) The spatial resolution of the images; OLI and MSI provide multispectral reflectance measurements referred to pixels of different sizes (30 and 10 m, respectively), which is obviously influential in areas where water bodies are often small and spatially fragmented, such as ports.
(3) The actual revisit time of the images; as previously noted, the revisit cycle of L8 is much lower than that of S2 satellites. Moreover, in both cases, the real usability of the images is constrained by atmospheric disturbances (cloud cover, haze, etc.) or by the presence of sun glint, the specular reflection of light from water surfaces.
(4) The atmospheric corrections applied to the images; since about 90% of the radiance received by satellite sensors from marine waters is due to the atmosphere, the errors brought by routine atmospheric correction algorithms can significantly affect the accuracy of the reflectance and, consequently, TRIX estimates obtained.

These four issues were investigated using two datasets collected in situ. The first one in large measure coincides with that already used in Massi et al. (2019) and consists of sets of sea samples taken in five Mediterranean ports during the period 2012–2014. The second dataset was instead collected purposely for the present research and included sea samples taken quasi-contemporaneously with L8 OLI and S2 MSI satellites overpasses within two ports in Central Italy (Civitavecchia and Viareggio). The analysis of these datasets was specifically aimed at assessing the potential and limits of both satellite data types for the determination of TRIX in port waters.

TRIX estimation based on spectral observations

The trophic index TRIX is commonly defined by a linear combination of the logarithms of four environmental variables: Chlorophyll *a* concentration (Chl-

a) in μg L^{-1}, Oxygen as absolute percent deviation from saturation (aDO%) and, as nutritional factors, Nitrogen (N) and Phosphorus (P), in different combinations between the available (DIN = NO_3 + NO_2 + NH_3; DIP = PO_4) and total (N; P) forms, in μg L^{-1} (Vollenweider et al., 1998). TRIX can therefore be calculated using the following equation:

$$\mathrm{TRIX} = (\log(\mathrm{Chl}\text{-}a\text{-}|\ \mathrm{aDO\%}\ | * \mathrm{N} * \mathrm{P}) - (-1.5))/1.2 \tag{1}$$

The scalars −1.5 and 1.2 were introduced to fix the lower limit of TRIX, on the basis of the long-term dataset from the northern Adriatic Sea, and to extend the trophic scale to 10 TRIX units (Vollenweider et al., 1998). Thus, TRIX ranges from 0 to 10 covering four trophic states: 0–4 high quality and low trophic status (High); 4–5 good quality and moderate trophic status (Good); 5–6 moderate quality and high trophic status (Moderate), and 6–10 poor quality and very high trophic status (Poor).

The optical method to estimate the TRIX of port waters, which was proposed and tested by Massi et al. (2019), utilizes the relationships between some components of the index (mainly Chl-*a*) and water spectral responses. The same study, in fact, demonstrated that the spatio-temporal TRIX variability within five Mediterranean ports was strictly associated to variations of Chl-*a*, which is a major optically active seawater constituent. Consequently, an unsupervised clustering algorithm could be applied to representative spectral observations for identifying four water categories having levels of Chl-*a* and TRIX roughly corresponding to the mentioned four trophic states. The Spectral Angle (SA) metric was then used to attribute each new sample spectrum to one of these categories and predict the respective TRIX value. As fully specified in the same article, the SA metric is sensitive to the shape of the observed spectra, while it is insensitive to their amplitude variations; this property is decisive to reduce the influence of factors which can disturb the estimation of Chl-*a* and, consequently, TRIX.

Although the use of in situ spectral measurements presents relevant advantages over the collection and analysis of water samples, the operational application of the optical TRIX estimation method would greatly benefit from the availability of observations taken by medium-high spatial resolution satellite sensors, such as L8 OLI and S2 MSI, respectively. Both sensors, in fact, acquire radiation in few reflective bands, which are potentially useful for the spectral characterization of port waters. Moreover, the acquired images are freely provided in a preprocessed format (i.e. geometrically and atmospherically corrected), which is decisive in sight of their use for water quality monitoring applications. As a matter of fact, the launch of L8 and S2A/B, to which, in 2021, the new Landsat-9 will be added (Wulder et al., 2019) has allowed a more effective monitoring of aquatic ecosystems, and this can be expected to be the case also for port waters.

Study areas

The study conducted by Massi et al. (2019) concerned five Mediterranean ports (Cagliari and Viareggio, Italy; El Kantaoui, Tunisia; Porto Marina-Alexandria, Egypt; Heraklion, Greece); a full description of these ports and relevant sea measurements is provided in the same paper.

Four additional sea campaigns were carried out from November 2017 to June 2019 in the Italian ports of Civitavecchia and Viareggio (Figure 1). The main features of these ports are described below, while a summary of the four campaigns is reported in Table 1.

Port of civitavecchia

The port of Civitavecchia, located on the northern coast of Lazio, was founded in 108 AD as the port of Rome and is a major Italian hub for maritime transport, goods and passengers. The port is a multifunctional structure divided into two sectors. The first, to the south, dedicated to tourism, pleasure boating and cruises, and the second, to the north, aimed at commercial traffic, fishing and cabotage. The port includes many kilometers of piers and may host big cruise ships. The Laboratory of Experimental Oceanology and Marine Ecology (LOSEM), in collaboration with the Port Authority of Civitavecchia, has recently developed an integrated monitoring system for the study of water quality, with the aim of assessing the possible impact of the continuously expanding port activities on the marine ecosystem (Bonamano et al., 2016; Bonamano et al., 2017; Zappalà et al., 2016).

Port of viareggio

The port of Viareggio, located on the northern coast of Tuscany, was built in 1819 close to the last stretch of the Burlamacca Channel, which connects the Massaciuccoli Lake with the Ligurian Sea. The port is worldwide known for its old fishing and touristic vocation and mega-yacht shipyards mainly located in the large southern and inner docks. The outer harbour is dedicated to tourist docking and the inner smaller docks, located in the Burlamacca Channel and its mouth, accommodate numerous berths for fishing and leisure boats. The trophic conditions of the port waters are strongly affected by the eutrophic load from the Massaciuccoli Lake through the Burlamacca Channel and the inland network of channels carrying farming and urban waste waters (Cabassi et al., 2017).

Figure 1. Geographical position of Civitavecchia (42.09°N, 11.79°E) and Viareggio (43.86°N, 10.24°E) in Central Italy. Map coordinates system: WGS84/UTM 32 N.

Table 1. Ports, dates and numbers of sea samplings for the four campaigns contemporaneous with the Landsat-8 OLI and Sentinel-2 MSI acquisitions (the dates coincident with those of sea samplings are in bold) .

Port	*Sampling date* (dd/mm/yyyy)	*Number of samples*	*OLI date* (dd/mm/yyyy)	*MSI date* (dd/mm/yyyy)
Civitavecchia	**17/11/2017**	3	18/11/2017	**17/11/2017**
Viareggio	**21/06/2018**	6	**21/06/2018**	23/06/2018
Viareggio	**28/02/2019**	6	25/02/2019	**28/02/2019**
Viareggio	**03/06/2019**	6	01/06/2019	**03/06/2019**

Study data

Water samplings and analyses

One campaign was conducted in the port of Civitavecchia (Table 1), sampling a station (C1, depth 15 m) outside and two inside (C2 and C3, depth 5–6 m) the port (Figure 2). Three campaigns were carried out in the port of Viareggio (Table 1), sampling six stations (Figure 2): one in the innermost dock (P5, depth 3–4 m), one in the Burlamacca channel (P6, depth 2 m), two in the outer harbour (P3 and P4, depth 5–6 m) and two in the adjacent marine waters (P1 and P2, depth 10–15 m). The distance from land was small for the first two stations of Viareggio (10–20 m), while was relatively large for all other stations (more than 30–40 m).

At each station, profiles of temperature, salinity, pH, Dissolved Oxygen concentration and percentage of saturation (DO), were measured with a Hydrolab HL4 Multiprobe, and hyperspectral downwelling (Ed) and upwelling (Eu) irradiances (380–710 nm, 1 nm interval) were measured (AvaSoft 6.1) at 30 cm and 80 cm depth by a portable radiometric system (PUMS, Portable Underwater Mini-Spectroradiometer), composed of a diode-array spectrometer (AvaSpec-2048 Avantes), with a 350–900 nm grating and 50–600 µm optical fibres and a cosine collector (CC-UV/VIS), as detailed in Massi et al. (2019).

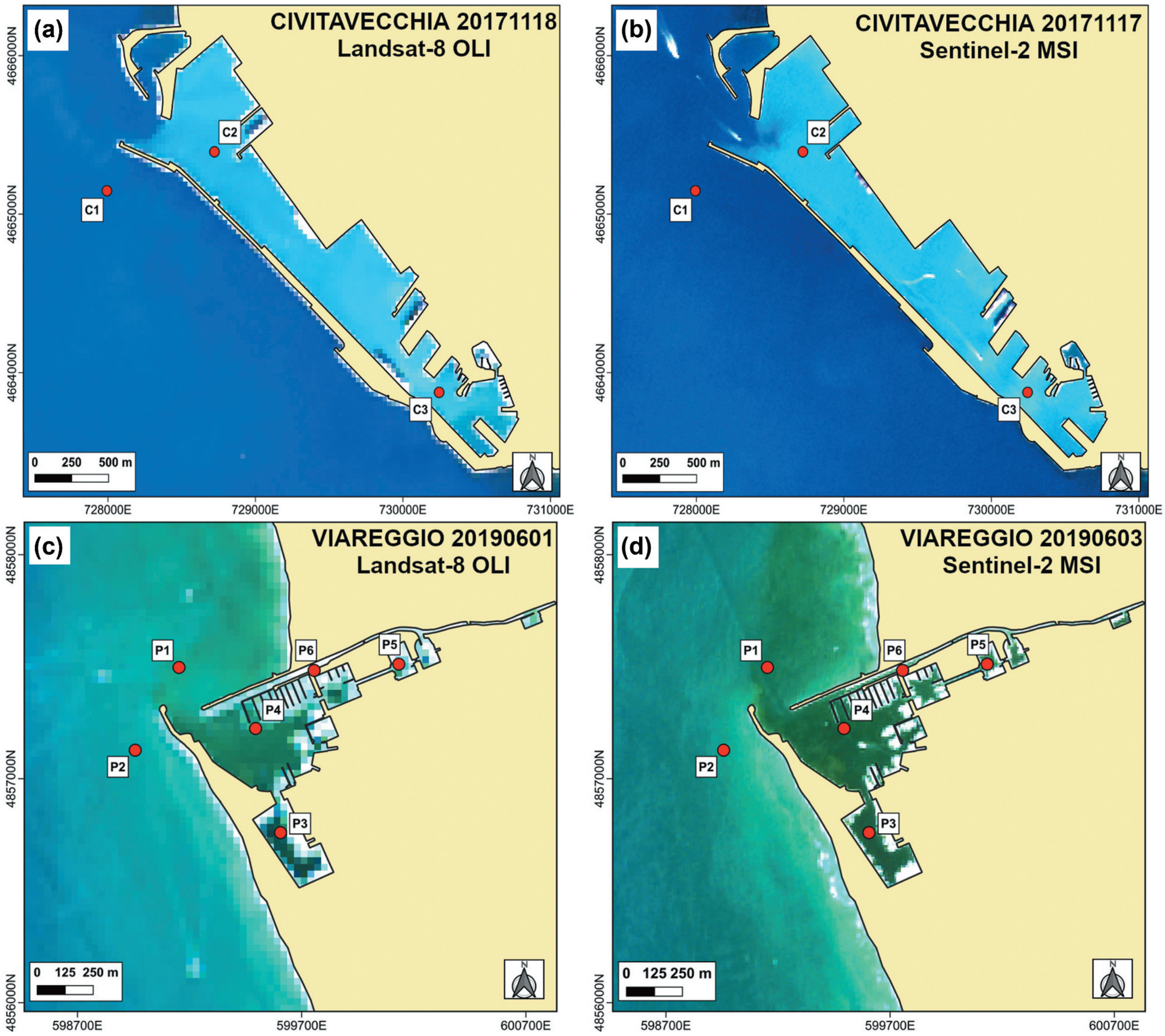

Figure 2. Landsat-8 OLI and Sentinel-2 MSI true color composites (RGB = bands 4,3,2) of the study scenes taken at Civitavecchia (a-b) and Viareggio (c-d), with position of the sampling points (all land surfaces are masked). Maps coordinates system: WGS84/UTM 32 N.

Irradiance measurements were taken in port areas free from the presence of shading ships or other structures, around noon, with calm waters in the absence of white caps and reduced cloudiness conditions, to avoid strong fluctuations of the underwater radiant flux (Kirk, 2011). The PUMS was always used on the side of the boat facing the sun, to minimize shade effects by the boat. From these measurements, irradiance reflectance (R) spectra were calculated as the ratio between Eu and Ed at 30 cm, together with attenuation coefficient spectra (Kd) between Ed at 30 and 80 cm.

R is not the first choice optical property to be used for sea colour remote-sensing applications, which are preferably based on radiance observations. In particular, the surface reflectance (SR) can be estimated by optical satellite systems, i.e. the top of atmosphere reflectance corrected for the scattering and absorbing effects of atmospheric gases and aerosols (Vermote et al., 2016). Although the comparison between R and SR is not straightforward for water bodies due to the non Lambertian properties of the water surface and the dependence of R on measurement conditions (height of the sun, cloud cover, weather, etc.), under optimal solar lighting and surface conditions R is very similar to SR, and, specifically, R and SR spectra differ only marginally in shape (Mobley, 2020).

Mean values of Kd in the PAR (Photosynthetic Available Radiation) band range from about 1.5 m^{-1} at P6 station, 0.4–0.5 m^{-1} at P4 and P5, 0.2–0.3 m^{-1} at C2 and C3, 0.15 m^{-1} at P1, P2 and C1. The optical properties derived from ocean color imagery represent vertically-integrated values from roughly the first attenuation length in the water column (1/Kd). On this basis, the influence of the bottom on the reflectance spectra can be neglected in all stations considered.

Five liters of waters were sampled at 30 cm depth of each station and stored in plastic opaque carboys until splitting for the different laboratory analysis. Variable volumes of waters (300–1000 mL) were filtered on GF/F filters (47 mm) for Chlorophyll *a* spectrophotometric analysis, according to Lazzara et al. (2010). Analyses of inorganic nutrients (NO_2 + NO_3 = DIN; PO_4) were performed on filtered waters with Autoanalyzer Bran-Luebbe, according to Strickland and Parsons (1972).

The concentrations of the main optically active substances [Chl-*a*, Total Suspended Matter (TSM), Chromophoric Dissolved Organic Matter (CDOM) absorption coefficient at 400 nm (aCDOM(400))] measured at each station during the four measurement campaigns contemporaneous with the L8 OLI and S2 MSI acquisitions are given in Table 2. Notable differences existed in the water conditions between ports and, within the port of Viareggio, among stations and seasons. Most samples collected in the port of Viareggio were quite turbid and, in particular, contained high levels of Chl-*a*.

Landsat-8 OLI images

L8 is a near-polar orbit satellite launched in 2013 and provides scenes of about 185 km with a revisit time of 16 days on the same area at the equator. L8 carries onboard the Operational Land Imager (OLI), a sensor which collects image data in 8 multispectral bands in the visible, near-infrared, and shortwave infrared portions of the spectrum (433–2300 nm), with 30 m of spatial resolution, and a panchromatic band (500–680) at 15 m.

In this work, the L8 SR product provided by United States Geological Service (USGS) and included in the Collection 1 (C1), Level 2, was used (USGS, 2020). The product provides atmospherically corrected data in which the orthorectified surface reflectance is generated using the Land Surface Reflectance Code (LaSRC version 1.4.1), originally developed at National Aeronautics and Space Administration (NASA) by Dr. Eric Vermote and continuously update by the staff at USGS Earth Resources Observation and Science (EROS) Center (Vermote et al., 2016). All scenes held in the USGS archive are freely distributed and can be downloaded from the USGS Earth Explorer website (https://earthexplorer.usgs.gov).

The investigation focused on four OLI cloud-free scenes temporally close to the described sea campaigns, one for Civitavecchia and the others for Viareggio (Table 1). In particular, the first five bands of the sensor were considered, centred at 443, 482, 562, 655 and 865 nm. Two true color composites of these images are shown in Figure 2(A,C).

Sentinel-2 MSI images

The two twin polar satellites, S2A/B, which are part of the European Union's Earth Observation Programme Copernicus, were launched in 2015 and 2017, respectively, and are placed on the same orbit with a phase delay of 180 degrees to each other. The MultiSpectral Instrument (MSI) sensor installed aboard both satellites detects the Earth's surface reflectance in 13 bands, from 443 to 2190 nm and with different spatial

Table 2. Values of the main optically active substances [Chl-*a*, Total Suspended Matter (TSM), Chromophoric Dissolved Organic Matter (CDOM) absorption coefficient at 400 nm (aCDOM(400))] and TRIX measured at each station during the four measurement campaigns contemporaneous with the Landsat-8 OLI and Sentinel-2 MSI acquisitions.

Port	*Station*	*date* (dd/mm/yyyy)	*Chl-a* (mg/m^3)	*TSM* (mg/L)	*aCDOM (400)* (m^{-1})	*TRIX*
Civitavecchia	C1	17/11/2017	0.33	3.19	0.046	2.58
Civitavecchia	C2	17/11/2017	0.98	4.43	0.383	5.15
Civitavecchia	C3	17/11/2017	0.94	4.56	0.075	5.18
Viareggio	P1	21/06/2018	0.46	1.60	0.094	4.72
Viareggio	P2	21/06/2018	0.25	2.76	0.045	2.98
Viareggio	P3	21/06/2018	16.02	5.59	0.565	4.86
Viareggio	P4	21/06/2018	22.32	5.28	0.759	6.84
Viareggio	P5	21/06/2018	20.21	6.18	1.717	7.44
Viareggio	P6	21/06/2018	10.54	12.21	0.840	7.03
Viareggio	P1	28/02/2019	2.01	3.29	0.684	4.62
Viareggio	P2	28/02/2019	3.83	2.57	0.223	5.06
Viareggio	P3	28/02/2019	2.57	3.24	1.373	5.44
Viareggio	P4	28/02/2019	2.10	3.77	0.913	5.39
Viareggio	P5	28/02/2019	4.80	4.85	4.269	7.60
Viareggio	P6	28/02/2019	2.68	7.82	2.131	7.39
Viareggio	P1	03/06/2019	7.43	19.69	1.350	5.09
Viareggio	P2	03/06/2019	4.05	16.68	0.431	4.28
Viareggio	P3	03/06/2019	183.17	24.15	4.947	6.65
Viareggio	P4	03/06/2019	27.23	6.66	1.925	5.69
Viareggio	P5	03/06/2019	10.80	10.33	6.247	7.15
Viareggio	P6	03/06/2019	14.33	12.78	5.224	7.12

resolution (10, 20 and 60 m). MSI provides scenes with about 290 km of swath and, considering both satellites, a revisit time of 5 days at the equator.

S2 MSI data are freely distributed by some portals, such as the Copernicus Open Access Hub (https://scihub.copernicus.eu), with several processing levels. Starting from 26 March 2018, for the Euro-Mediterranean region, Level-2A products (atmospheric and geometrically corrected surface reflectance) derived from Level-1 C products are available (ESA, 2020a; 2020b). The atmospheric correction was performed by the Sen2Cor (vers. 2.8) standard processor (Main-Knorn et al., 2017), which produces Bottom-Of-Atmosphere (BOA) SR estimates.

The current study utilized four MSI cloud-free scenes temporally close to the described sea campaigns, one for Civitavecchia and the others for Viareggio (Table 1). For each scene, only images with the highest spatial resolution (10 m) were considered, corresponding to four MSI bands centered at 490, 560, 665 and 842 nm. Two true color composites of these images are shown in Figure 2(B,D).

Data analysis and results

This section is divided into four sub-sections, which are aimed at assessing the impact of the mentioned issues on the determination of TRIX in port seawaters; a final sub-section describes the overall evaluation of OLI and MSI imageries for the same purpose.

Spectral configurations of OLI and MSI imagery

The analysis of this issue was based on all available analytical and spectral measurements collected in the old and new sea campaigns. Following the same procedure described in Massi et al. (2019), TRIX was determined by analyzing all in situ water samples. The TRIX values obtained for the samples of the four new sea campaigns in the ports of Civitavecchia and Viareggio are reported in Table 2.

Next, OLI and MSI four-band spectra were simulated as previously done for 12-band spectra by averaging the original in situ spectra collected in 60 bands with 5 nm interval. Due to the lack of spectral measurements above 710 nm, the near infrared band of both sensors was simulated as coincident to this upper bound. The three spectral datasets (i.e. original twelve bands, OLI five bands and MSI four bands) were then used for discriminating the four TRIX levels previously mentioned. The accuracies obtained from these experiments were assessed versus the respective analytical TRIX measurements and summarized through common statistics, i.e. the coefficient of determination (r^2), the root mean square error (RMSE) and the mean bias error (MBE).

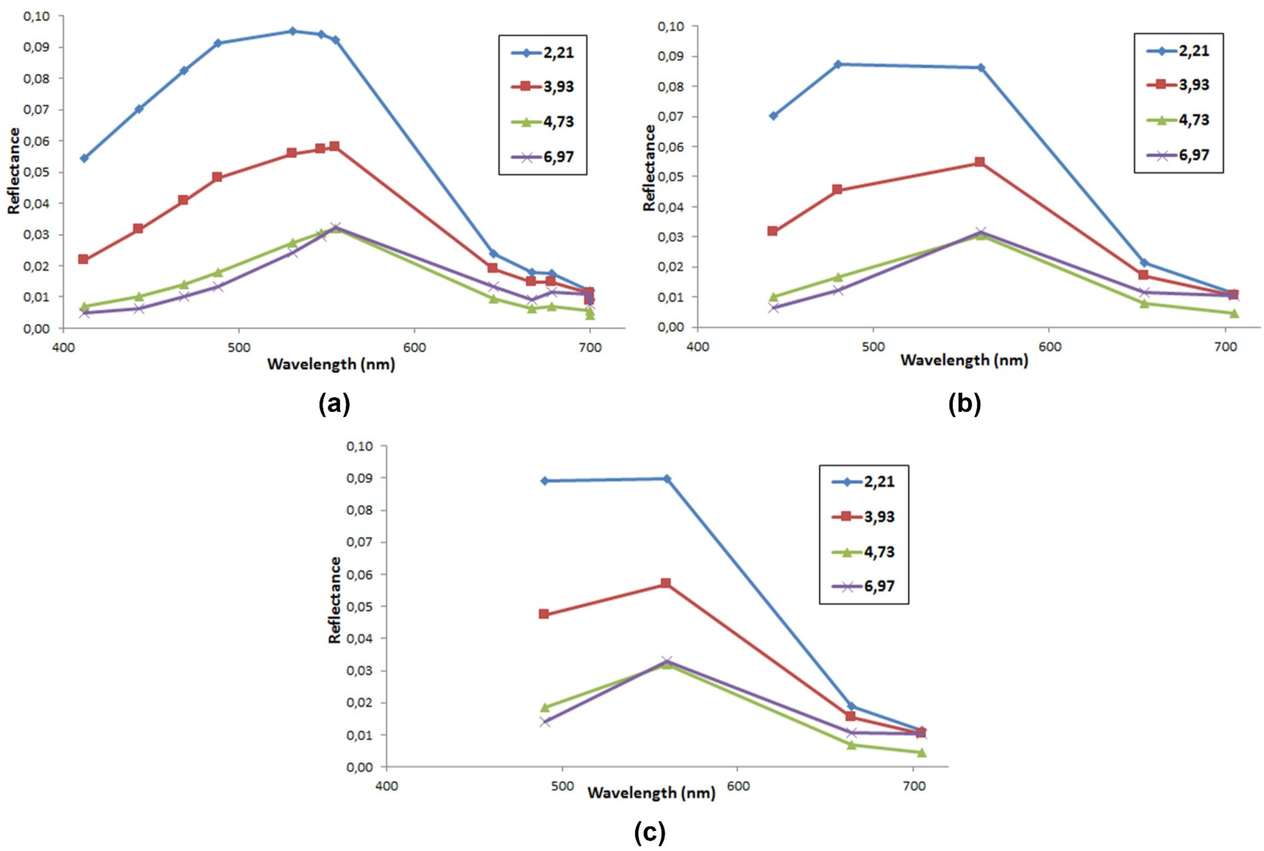

Figure 3. Mean reflectance spectra of the four categories defined in Massi et al. (2019) with corresponding TRIX values; (a) originals (12 bands) and degraded to the five OLI bands (b) and to the four MSI bands (c) .

The information loss caused by the spectral degradation from 12 (in situ) to five and four satellite bands can be visually appreciated in Figure 3, where the mean spectra of the four categories identified by Massi et al. (2019) are shown in the three formats together with the corresponding TRIX values.

Both five and four band formats maintain a good spectral separation of the four categories, both in magnitude and in shape.

The analysis of the 78 samples available from all campaigns confirms that TRIX can be estimated with reasonable accuracy when the 12 band spectral configuration is considered (Table 3). The degradation of this configuration to the five OLI bands leads to only a marginal deterioration of the estimation accuracy; the same degradation to the four MSI bands implies a slightly greater reduction in accuracy, i.e. around 6%.

Spatial resolution of OLI and MSI imagery

This subject was investigated by creating land buffers of different sizes in the two examined ports (Civitavecchia and Viareggio). The fractions of port seawaters covered by the different buffers were then analyzed in relation to the spatial resolution of the OLI and MSI images, i.e. 30 and 10 m, respectively.

Figure 4 shows the fractions of port waters covered by the different land buffers in the two ports. In the first port the cumulative fractions comprised in the 10 and 30 m buffers are relatively small (0.09 and 0.26, respectively) while the same fractions are much larger for Viareggio (0.27 and 0.57, respectively).

This obviously implies that very different port fractions can be monitored by the two satellite data types; in the latter case (Viareggio) the use of the higher spatial resolution data is virtually mandatory, while this is less the case for the port of Civitavecchia.

Table 3. Accuracy statistics of the 78 TRIX estimates obtained by the optical method of Massi et al. (2019) using the in situ spectral measurements taken in the original 12 bands, in the five bands of OLI and in the four bands of MSI (** = highly significant correlation, $P < 0.01$) .

Spectral configuration	r^2	RMSE	MBE
12 bands	0.616**	1.35	−0.08
5 OLI bands	0.615**	1.37	−0.25
4 MSI bands	0.549**	1.47	−0.20

Temporal resolution of OLI and MSI imagery

This analysis was focused on the port of Viareggio and consisted in the visual examination of all OLI and MSI images acquired during 2018 and 2019. The L8 revisit time of 16 days at the equator is halved in the Viareggio area due to the overlap of two orbits. The orbital configuration is instead typical of mid-latitudes for S2, leading to an actual revisit time of 2–3 days.

Figure 5 shows the numbers of good quality (i.e. clear sky and no sun glint) OLI and MSI images obtained in the Viareggio area during the two study years, divided by season. As expected, these images are more numerous in summer, when clear sky conditions more frequently occur, while are few in fall and winter. Despite the fortunate position of Viareggio with respect to L8 orbits, the number of good quality MSI images is notably higher than that of OLI images for all seasons. On average, MSI images are about three times more numerous than OLI images.

Radiometric difference between OLI and MSI imagery

The impact of the different reflectance types measured in situ and from satellite platforms was evaluated together with that of the routine atmospheric corrections applied to the OLI and MSI images by comparing the mean reflectance values obtained from the two

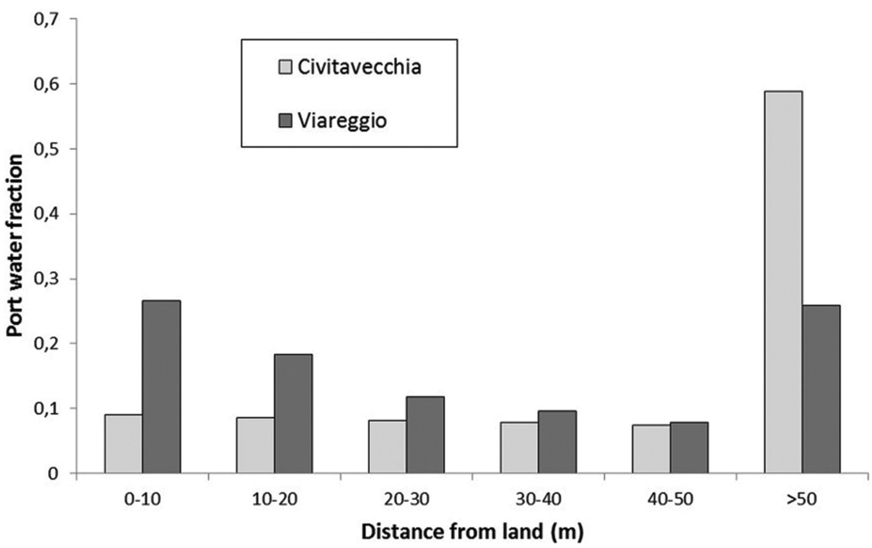

Figure 4. Fractions of seawaters covered by the land buffers in the ports of Civitavecchia and Viareggio.

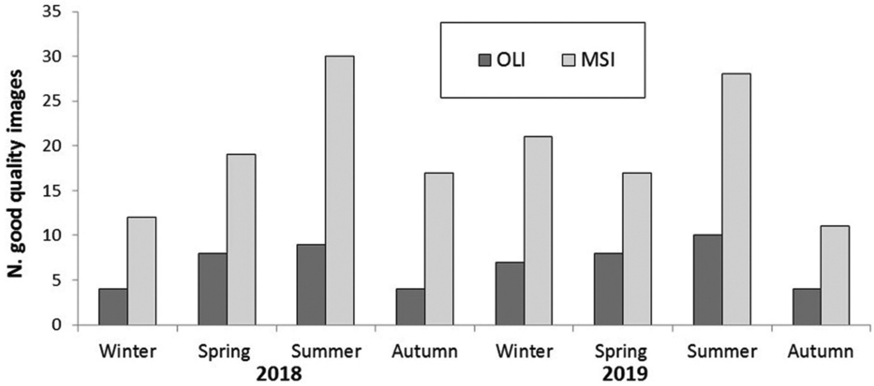

Figure 5. Numbers of good quality OLI and MSI images found for the Viareggio area during the seasons of 2018 and 2019.

sources. This analysis was focused on the most reliable observations, which implied the selection of sea samples taken more than 30 m far from land and in the same day of the satellite overpasses (Table 1 and Figure 2).

The application of these criteria led to select only four samples for OLI and eleven for MSI; the averages and standard errors of the measured and estimated multispectral reflectance derived from these samples are shown in Figure 6. A significant reflectance overestimation is visible for OLI, while a minor underestimation can be observed for MSI. In both cases, the spectra measured in situ and observed from satellite are almost coincident in shape (r = 0.982 for OLI and r = 0.968 for MSI), but the latter are somewhat flattened and show a less pronounced green peak. This modification obstructs the identification of the spectral classes associated to high TRIX values (see Figure 3), thus inducing a general tendency to TRIX underestimation.

Overall assessment of OLI and MSI imagery

The assessment of the overall TRIX estimation capacity obtainable from OLI and MSI data was performed using all available spectral observations taken in the respective five and four bands. Accordingly, also samples relatively close to the land boundary were considered, and the same was for the satellite acquisitions not coincident with the respective sea samplings (Table 1).

The accuracy of the TRIX estimates was quantified through comparison with the in situ analytical measurements and was summarized by means of the same statistics used previously (i.e. r^2, RMSE and MBE).

Overall, the estimation capacity of the two satellite sensors is very different. Figure 7 shows that the use of OLI data leads to a notable inaccuracy, mostly due to a marked underestimation of high TRIX values. Such phenomenon can be partly ascribed to the previously noted flattening of the estimated spectra, which is most evident for some samples taken in Viareggio during the second campaign (28/02/2019, Table 1). An even greater effect is exerted by the lower spatial resolution of OLI with respect to MSI, which, as seen above, induces a higher contamination of seawater pixels with the spectral signal coming from land.

These problems are partially fixed by the use of MSI observations, which yields relatively accurate TRIX estimates, significantly correlated with the sea measurements. Also in this case, however, a minor tendency to TRIX underestimation persists.

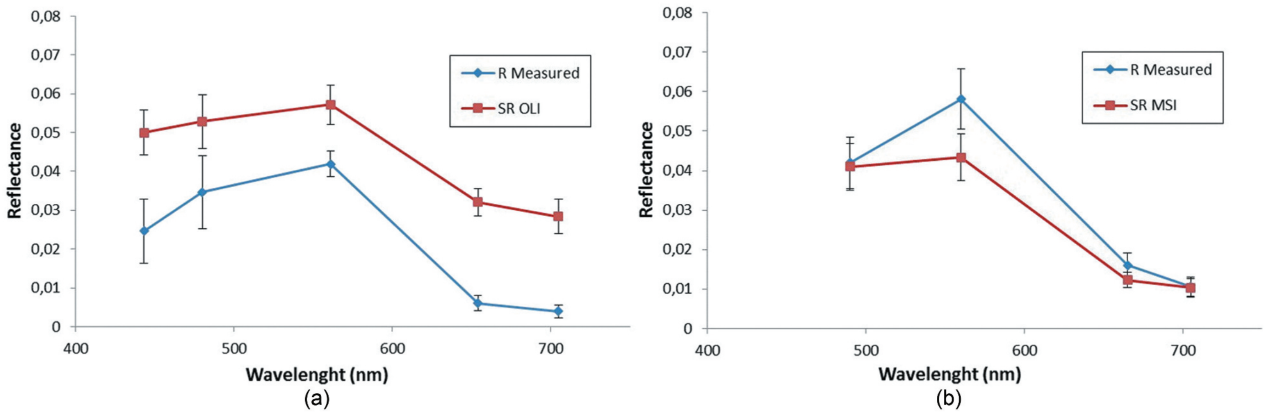

Figure 6. Mean reflectance spectra measured in situ and estimated from OLI images (a, four samples) and from MSI images (b, eleven samples) (the bars indicate the standard errors).

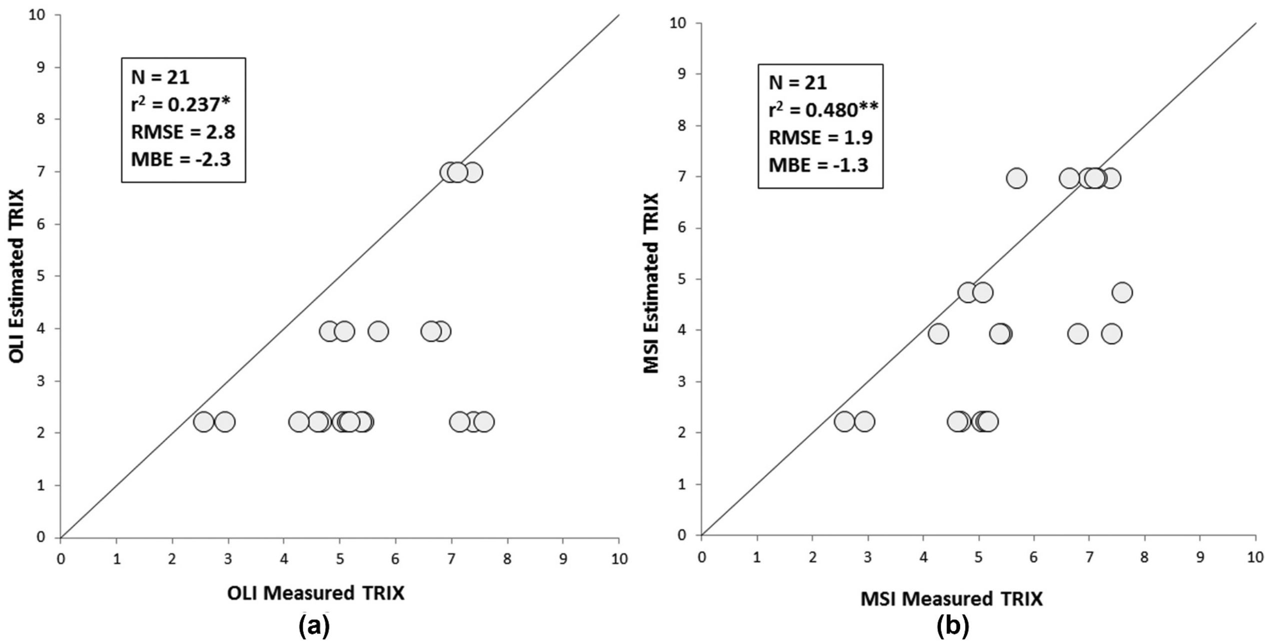

Figure 7. Comparison of TRIX measured and estimated from OLI (a) and MSI images (b) (* = significant correlation, $P < 0.05$; ** = highly significant correlation, $P < 0.01$).

An example of TRIX map obtained from the latter images is displayed in Figure 8 for the port of Viareggio; as expected, the lowest TRIX values were found in the open sea, while the highest values were observed in the inner docks of the port.

Discussion

TRIX represents an effective means to characterize the ecological quality of port waters, which, as previously noted, require continuous monitoring on suitable spatial and temporal scales. The pros and cons brought by an

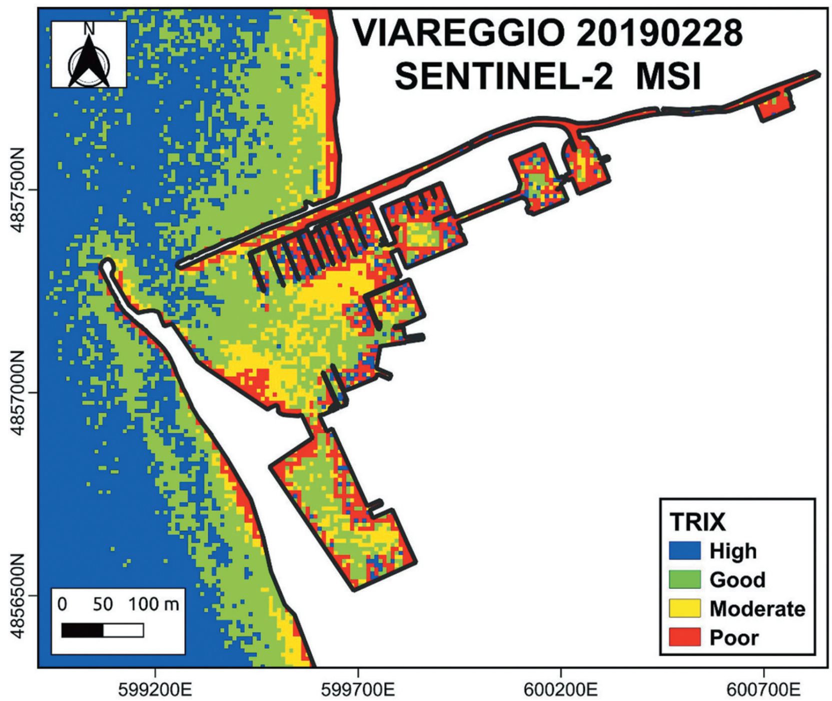

Figure 8. TRIX map of Viareggio obtained from the MSI images of 28 February 2019; the four TRIX values actually correspond to those defined in Massi et al. (2019), i.e. 2.21 (High), 3.93 (Good), 4.73 (Moderate), and 6.97 (Poor) (all land surfaces are masked). Map coordinates system: WGS84/UTM 32 N.

optical classification of TRIX levels over the conventional assessment based on the collection and analysis of seawater samples are discussed in Massi et al. (2019). The optical categorization of port seawaters proposed in that article was effective in discriminating four levels of ecological quality, explaining more than 60% of the TRIX variance contained in a large number of samples collected in five Mediterranean ports.

Such efficiency was partly attributed to the use of the SA metric, which removes the differences due to amplitude variations of the sample spectra, thus emphasizing spectral shape variations. According to Maselli et al. (2009) in fact, SA variations are mainly related to differences in concentration of Chl-*a*. This is also the case in Case-2 waters such as those of ports, which are generally characterized by high concentrations of complexly interacting Light Attenuating Substance (LAS) (Gordon & Morel, 1983; IOCCG, 2000). Most of the samples collected in the ports of Civitavecchia and Viareggio actually confirm this expectation. In fact, Chl-*a* showed a variation in concentration much greater than CDOM and TSM and therefore dominated the optical variability of the examined port waters. The direct effect of Chl-*a* in the determination of TRIX, as well as the indirect effect due to the statistical association of Chl-*a* and CDOM with the other components of the index (DIP, DIN; Table 4 in Massi et al. (2019)) explain the observed efficiency of the SA metric in discriminating categories informative on seawater ecological quality.

The choice of a limited number of bio-optical categories (four) was made in accordance with the four states under which TRIX is usually interpreted (Vollenweider et al., 1998). The four spectral categories that emerged from the applied optical classification showed increasing concentrations of Chl-*a*, nutrients (especially DIP) and consequently TRIX, and also agreed with the features highlighted in the phytoplankton communities (Massi et al., 2019). Consequently, four diversified levels of ecological quality were associated with spectra that were clearly separable in shape. This last property is expected to be decisive particularly when these spectra are degraded to a reduced number of bands, such as the five of L8 OLI and the four of S2 MSI.

These considerations are supported by the current experimental results, which are similar to those obtained by Massi et al. (2019), which used only a part of the currently available in situ measurements (47 out of 78 samples). The use of the full spectral configuration (12 bands), in fact, led to a satisfactory TRIX estimation accuracy ($r^2 > 0.61$), which was only marginally reduced when degrading the spectral configuration to the five bands of OLI ($r^2 > 0.61$); a greater but still limited reduction was obtained using the four band configuration of MSI ($r^2 > 0.54$). Both these assessments are affected by the consideration of a different spectral range for simulating the near infrared bands of the two sensors (i.e. OLI band 5 and MSI band 8), which, however, should have a minor impact due to the very low reflectance of water bodies at these wavelengths.

Satellite images provide gridded spectral observations referred to pixels of various sizes. This is a relevant issue for the monitoring of artificial water bodies, such as ports, which generally have a complex and irregular spatial arrangement. The current study has shown that the pixel size of OLI images may be sufficient to observe the waters of medium-large ports such as that of Civitavecchia, but are suboptimal to pursue the same objective in smaller, more spatially fragmented ports such as that of Viareggio. In the latter case, the use of higher spatial resolution images is therefore fundamental, and MSI actually provides a good tradeoff between this requirement and the operational availability of the acquired imagery.

The same advancement of MSI over OLI has been highlighted for the temporal acquisition frequency, since the actually usable images taken by MSI are much more numerous than those taken by OLI. This obviously represents a decisive advantage in sight of operational monitoring applications, particularly for seasons, such as spring and fall, which are more affected by atmospheric disturbances but are fundamental for evaluating the ecological status of port waters.

The consistency of remote sensing reflectance and derived products by OLI and MSI sensors in ideal atmospheric conditions and for turbid/eutrophic coastal waters has been demonstrated by Pahlevan et al. (2019). The operational use of satellite data, however, requires also the simulation of more complex atmospheric situations, which is generally a critical issue. The various problems related to atmospheric corrections (sun glint, aerosol type, adjacent effect, etc.) are, in fact, difficult to solve completely in an operational mode, when specific measurements of atmospheric conditions contemporaneous to the satellite overpass are not available. This often introduces under or over-correction issues which can be particularly relevant for lowly reflecting surfaces, such as those of water bodies (Warren et al., 2019). The problem can be exacerbated by the adjacency effect, which influences the observations of dark water pixels close to the land/water boundary; these pixels, in fact, are contaminated by the light reflected from adjacent bright land surfaces, and the same is the case for highly reflecting clouds (Franz et al., 2015; Vanhellemont, 2019).

The current experimental results confirm the existence of these drawbacks, showing over and underestimation patterns, which affect the seawater reflectance derived from OLI and MSI images, respectively. Such patterns have a relatively minor impact on the TRIX estimates currently obtained, due to the mentioned insensitivity of the SA metric to spectral amplitude variations. The use of satellite data, however, seems to induce a flattening of the observed spectra, which implies a tendency to TRIX underestimation. This issue is particularly evident when using OLI images, likely due to an inaccurate correction of the atmospheric effect in the first two bands, which has already been noted by previous studies (Ilori et al., 2019). Similar results can be expected from the use of atmospheric correction algorithms alternative to the standards ones currently applied, such as those described in De Keukelaere et al. (2018), Vanhellemont (2019) and Warren et al. (2019); assessing the efficiency of these algorithms, however, is beyond the scope of the present study, which is focused on two methods (L8-LaSRC and S2-Sen2Cor) applied routinely.

Our analysis has not been focused on the impact of the different reflectance types measured by Massi et al. (2019) and derived from satellite observations, i.e. R and SR, respectively. As previously noted, however, under the above-mentioned measurement conditions, R and SR spectra are expected to be very similar and, specifically, almost identical in shape, which should make their alternative use nearly uninfluential on the current TRIX estimation method. In particular, the impact of this factor should be marginal with respect to that of the atmospheric correction applied to the satellite images and is anyway not assessable separately from the latter using the current experimental datasets.

Similarly, no analysis has been conducted on the spectral contribution of the sea bottom, which can be relevant where shallow sea areas are associated with high water clarity, as typically occurs in coral reefs (Dattola et al., 2018; Hedley et al., 2018). This is not, however, the case in the ports of Civitavecchia and Viareggio, where, due to the high seawater turbidity, the light absorption occurs in the very first meters of the water column and the bottom contribution is negligible (Massi et al., 2019). The situation is presumably similar for other ports, due to the common concomitance of relatively high bottom depths and water turbidities.

Another issue is connected to the possible presence of boats in the port areas, which can alter the water spectral signatures observed by the satellite sensors, presumably leading to reflectance overestimation particularly for high wavelengths. As can be easily understood, the impact of this issue is intrinsically very variable and almost impossible to predict/correct, and must therefore be considered as an unavoidable source of noise for the application of the current method.

Overall, the main issues which affect the potential of the examined satellite datasets for estimating the ecological quality of port seawaters are related to the relevant spatial and temporal features. The different spatial resolutions of the two sensors examined, in fact, are very influential, implying a higher contamination of the OLI reflectance with undesired signal, particularly for samples close to the land boundary. A minor contribution to the different accuracies found is presumably also brought by the lower mean temporal proximity of the OLI satellite overpasses with the sea samplings. The superior spatial and temporal characteristics of MSI over OLI are therefore reflected in a decidedly higher accuracy in the prediction of TRIX, which is obtained by the use of the former sensor. In both cases, however, the atmospheric corrections applied induce a flattening of the estimated spectra, which implies a certain tendency to TRIX underestimation.

Summary and conclusions

The current research line stems from the need for monitoring the environmental condition of port waters, which are subjected to intense physical-chemical and biological pollution phenomena sometimes leading to the formation of harmful algal blooms that can contaminate the port area and surrounding ecosystems. The trophic index TRIX is highly informative of the ecological quality of seawaters and has been successfully applied in various coastal marine environments, particularly in the Mediterranean basin (Fiori et al., 2016; Pettine et al., 2007).

The optical method proposed by Massi et al. (2019), allows a rapid and cost-effective estimation of TRIX in port waters, thus representing a notable improvement over the conventional bio-chemical analysis of seawater samples. The present study is a direct extension of that methodological research which concerns the possibility of predicting TRIX from the data taken by two satellite sensors, L8 OLI and S2 MSI.

The main conclusions that can be drawn from the investigation are:

- The spectral degradation induced by the use of OLI and MSI images has relatively minor impact on TRIX estimation.
- The spatial resolution of OLI images is sufficient to characterize the ecological quality of waters within large ports, but the higher resolution of MSI is decisive for achieving the same results in medium-small ports.
- The same is the case for the temporal frequency of the acquired images; as expected, the actually usable images are much more numerous for MSI than for OLI, which guarantees more frequent monitoring possibilities.
- A moderate decrease in TRIX estimation accuracy is caused by the use of surface reflectance

obtained from the application of routine atmospheric correction algorithms to both image types. In the examined cases, in fact, such use tends to only marginally flatten the shape of water reflectance spectra, generally inducing variable TRIX underestimation.

Globally, MSI is much more efficient than OLI in providing accurate TRIX predictions for port waters. The images acquired by the former sensor, in fact, produce TRIX estimates which express about half of the total TRIX variability measurable in the ports of Civitavecchia and Viareggio. This satisfactory result is mostly due to the high spectral differentiation of the four TRIX categories defined in Massi et al. (2019) and to the use of the SA metric, which implies a high robustness of the optical TRIX estimation method against various disturbing factors.

It can consequently be concluded that the use of MSI images allows the operational estimation of the ecological quality of port seawaters, at least in the examined Mediterranean reality. In particular, such activity could be aimed at detecting a deterioration of water ecological conditions, which could alert local maritime authorities and promote in situ checks of possible emergency situations. In sight of exporting the method to other port areas, however, further studies should be conducted to assess both the utility of TRIX and the possibility of deriving this index from spectral observations in different environmental situations.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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