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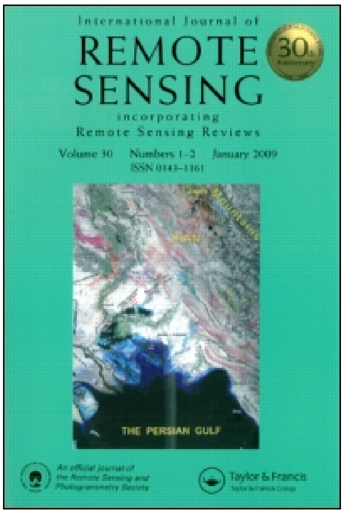

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What is up? Testing spectral heterogeneity versus NDVI relationship using quantile regression

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What is up? Testing spectral heterogeneity versus NDVI relationship using quantile regression

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Environmental diversity and net primary productivity (NPP) are powerful indicators of local plant species richness (α-diversity). Remote sensing proxies of environmental diversity, such as spectral heterogeneity and NPP, are often used in modelling species richness variability, usually through regression analysis. As multicollinearity may affect analysis of species diversity, the interdependence of such proxies should be a major concern in their use. However, few attempts have been made to examine the interdependence between spectral heterogeneity and NPP proxies such as the Normalized Difference Vegetation Index (NDVI), in most cases using Ordinary Least Square (OLS) regression or Pearson correlations. We test the possible dependence of Landsat Enhanced Thematic Mapper (ETM+) local spectral heterogeneity versus NDVI using quantile regression and rejecting the main assumption of OLS regression, i.e. the symmetry of model residuals. A second-order polynomial function was fitted to the data and both OLS and quantile regression led to a humped-back relationship between spectral heterogeneity and biomass. Nonetheless while for most of the quantiles the humped-back curve was significant (with a negative and significant quadratic slope), for quantiles higher than 0.90, the parabola opened up until it reached an almost linear shape, showing that, at very low values of biomass, pixels may show high levels of local heterogeneity. Hence, patterns of spectral heterogeneity versus NDVI are possible when considering maximum potential spectral variability. We show that the investigation of all possible subsets within a scatter plot may lead to identification of patterns that remain hidden in OLS regression.

1. Introduction

The determination of biodiversity hotspots and species richness is often based on the measurement of environmental heterogeneity and net primary productivity (NPP) (Fairbanks and McGwire 2004). The use of these two variables is linked to two basic relationships between species richness and the environment. On the one hand, ecological variability in environmental properties should increase heterogeneity in habitat characteristics by allowing higher local species richness (Palmer and White 1994). On the other hand, energy availability, i.e. the availability of resources such as nutrient and water (strictly related to NPP), should shape richness gradients (Hawkins *et al.* 2003).

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Remote sensing has long been used to predict species-rich sites at a local scale (α-diversity) based on environmental diversity as derived from spectral heterogeneity (Gould 2000, Palmer *et al.* 2002, Foody and Cutler 2003, Rocchini *et al.* 2004) and NPP as derived from the Normalized Difference Vegetation Index (NDVI) (Whittaker and Heegaard 2003, Fairbanks and McGwire 2004, Gillespie 2006).

However, a major issue in such analyses is the interdependence between these potential explanatory variables, since problems of multicollinearity can affect the prediction of species diversity (Graham 2003, Meynard and Quinn 2007, Rocchini 2007b). To date, few attempts have been made to model the interdependence between spectral heterogeneity and NDVI (e.g. Gillespie 2006). Most attempts have been limited to Pearson coefficients or Ordinary Least Square (OLS) regression, considering the whole set of input data (hereafter referred to as the universe of points *U*). On the other hand, regression functions based on *U* could hide patterns that may be present for grouped data (Koenker and Hallock 2001).

In regression analysis, a parametric class of models is generally expected to describe a phenomenon by considering the whole distribution of input data within a regression model (Koenker and Bassett 1978). The best model is fitted by minimizing the residual sum of squares within a regression model for the mean of the dependent-variable distribution (Sokal and Rohlf 1995). However, many datasets are characterized by high variability within the scatter plot (Schröder *et al.* 2005, Rocchini 2007a), which can add noise to the regression model. This is particularly true if we consider the potentially very large number of available pixel values, which is a function of the grain (spatial resolution) and the extent (e.g. in terms of number of rows and columns) of the image being considered. In these cases, quantile regressions can be used to evaluate trends at different quantiles, rather than the whole distribution of input points, by constraining the regression model on a given quantile threshold τ (Koenker and Bassett 1978, Cade and Guo 2000, Cade and Noon 2003). Quantile regression may allow for a more comprehensive description of response patterns across a range of regression quantiles (Cade *et al.* 1999).

The present study examines the possible interdependence between local spectral heterogeneity and NDVI by rejecting one of the basic assumptions of OLS regression, i.e. the symmetry of model residuals (Koenker and Hallock 2001). We apply a quantile regression to investigate all possible trends of data considering different subsets *S*.

2. Methods

2.1 *Study area*

The Tuscany Region, in central Italy, is located between 9° and 12° E and between 42° and 44° N (WGS84). The region is characterized by a complex physical geography covering about 21 000 km^2 (figure 1). Following CORINE Land Cover data, 44% of the total area is covered by forests (broad-leaved forests), while crops cover about 46% (Bossard *et al.* 2000). Forested areas are characterized by different plant communities, varying from coastline evergreen Mediterranean forests dominated by *Quercus ilex*, to mountain beech and fir forests dominated by *Fagus sylvatica* and *Abies alba*. The climate ranges from typically Mediterranean to temperate warm and temperate cool in relation to altitudinal and latitudinal gradients (Rapetti and Vittorini 1995).

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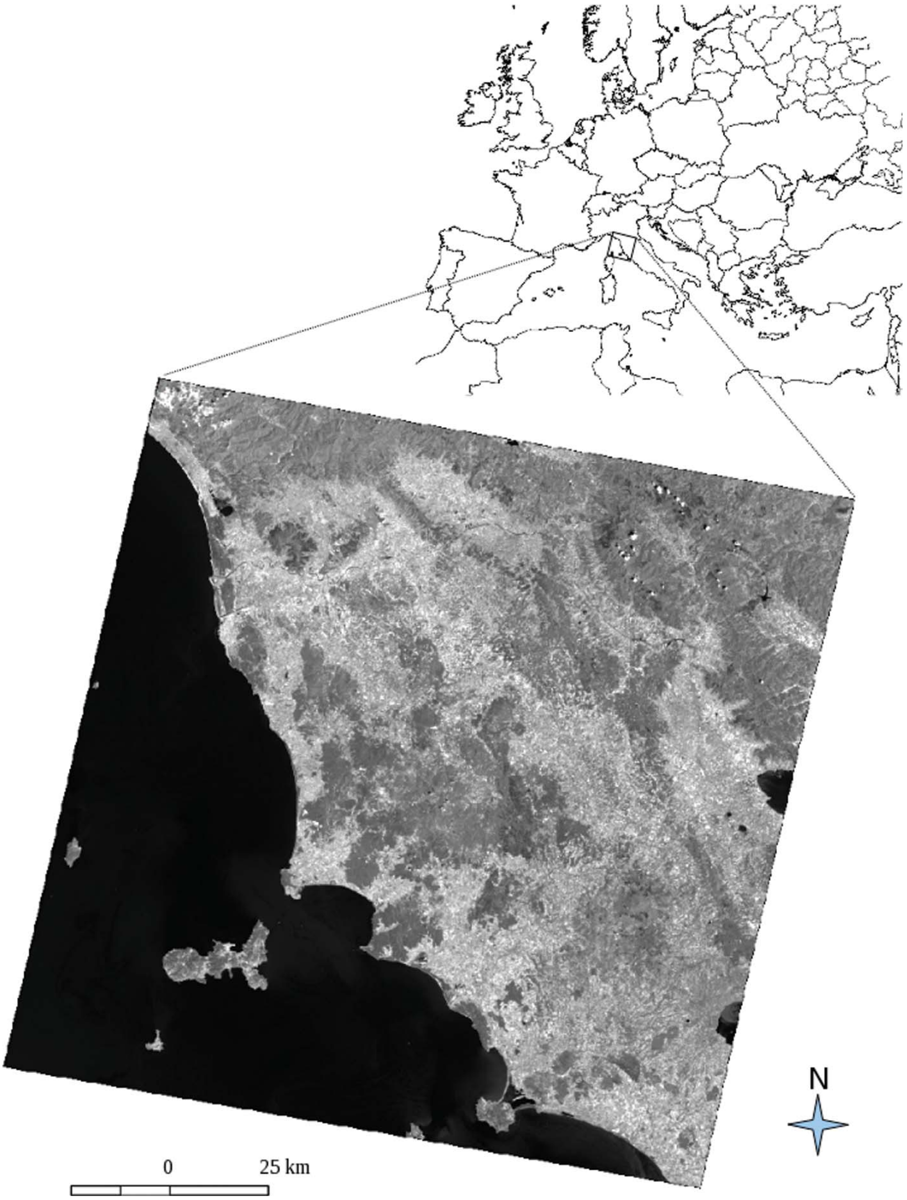

Figure 1. The ortho-Landsat ETM+ image (path 192, row 030) of Tuscany, Italy. PC1, explaining 86.53% of the total variance, is shown.

2.2 *Image acquisition and calculation of spectral variables*

An ortho-Landsat Enhanced Thematic Mapper (ETM+) image (path 192, row 030, acquisition date 20 June 2000; bands 1–5 and 7 spatial resolution 28.5 m) was acquired from the Global Land Cover Facility site hosted by the University of Maryland (htpp://glcfapp.umiacs.umd.edu, figure 1). We refer to Tucker *et al.* (2004) for complete information about image pre-processing.

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Spectral heterogeneity was derived as the spectral standard deviation within a moving window of 3 × 3 cells (Albani *et al.* 2004). Rather than directly using the whole multispectral dataset, an unstandardized Principal Component Analysis (PCA) was applied. PCA has long been used as a data compression tool that reduces the number of dimensions to be analysed, (see Jensen (1996) or Duda *et al.* (2001)). In this paper, the first PCA component (PC1), explaining 86.53%, was retained for the local (3 × 3 cells) spectral standard-deviation calculation.

In order to calculate the NDVI, band 4 (0.76–0.90 μm, near-infrared (NIR)) and band 3 (0.63–0.69 μm, red) were linearly combined as

$$\mathrm{NDVI} = \frac{\lambda_{\mathrm{NIR}} - \lambda_{\mathrm{R}}}{\lambda_{\mathrm{NIR}} + \lambda_{\mathrm{R}}}, \tag{1}$$

where λ_{NIR} is the reflectance in the NIR part of the spectrum and λ_{R} is the reflectance in the red part of the spectrum. The NDVI can vary from a theoretical minimum of –1 (minimum reflectance in the NIR and maximum in the red, low biomass) and a theoretical maximum of 1 (maximum reflectance in the NIR and minimum in the red, high biomass). Strictly speaking, the NDVI increases at high biomass due to (i) the high reflectance by vegetation in the NIR, which is linked to scattering processes at the leaf scale, and (ii) the low reflectance in the red spectrum due to the absorption by chloroplasts for photosynthesis.

In order to maintain the same scale of analysis with respect to the previously described PC1, mean NDVI within 3 × 3 cells was calculated and will be referred to as NDVI.

2.3 *Quantile regression fitting procedure*

Figure 2 shows a scatter plot of two variables ϖ_x and ϖ_y that appear to be related by a positive exponential model. However, when fitting an OLS-based model, the best fit is found to be a linear model (adjusted coefficient of determination $R^2 = 0.046$, slope = 0.37, probability threshold of regression models $p < 0.05$), rather than an exponential one (adjusted $R^2 = 0.010$, slope = 0.006, $p = 0.16$). Conclusions from the use of the 'mean' of the input data would therefore be that: (i) variables are weakly related to each other with a very low slope and (ii) variables are related to each other by a linear rather than an exponential function.

However, when considering the upper trend of values, the exponential relation between ϖ_x and ϖ_y becomes apparent (slope = 0.013, $p < 0.05$, $\tau = 0.75$), reaching higher values at $\tau = 0.90$ and 0.95, with slopes equalling 0.025 and 0.030 ($p < 0.01$), respectively. The linear pattern found by OLS regression, which obscures other possible patterns, is seen when the quantiles approach 0.5 (not shown in figure 2). The quantile at 0.5 (i.e. $\tau = 0.5$) represents the median of the input data.

Thus, a variable ϖ_y may show different response patterns with respect to ϖ_x when considering different subsets $s_{\omega y}$. A method considering different responses with respect to each $s_{\omega y}$ is strongly recommended to fully understand the phenomenon under study. Obviously, the same reasoning may be applied by considering lower trends in the data.

Formally, let $\{\varpi_{y1}, \varpi_{y2}, \ldots, \varpi_{yn}\}$ denote the n values of a set of points of the variable ϖ_y. OLS regression minimizes residuals by solving

$$\text{residual} = \min \sum \left(\varpi_{yi} - \hat{\varpi}_{yi}\right)^2, \tag{2}$$

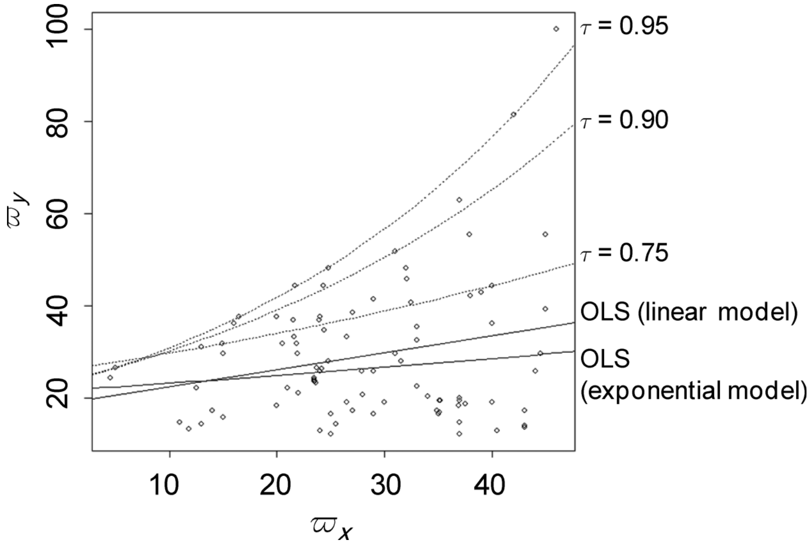

Figure 2. Worked example of OLS versus quantile regression. A linear pattern is found by fitting an OLS-based model. On the contrary, quantile regression may reveal previously hidden patterns such as an upper exponential relation (considering higher quantile values, τ) between the considered variables (ϖ_y and ϖ_x). See Cade and Noon (2003) for a similar example.

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where $\hat{\varpi}_{yi}$ is the estimated value for each *i*th point. Once the residual of each ϖ_{yi} value with its corresponding $\hat{\varpi}_{yi}$ value is calculated, the model is fitted using a symmetrical minimization of the achieved residuals.

Giving different weights to positive and negative residuals leads to an asymmetric minimization of residuals such that

$$\text{residual} = \min \sum \left|\varpi_{yi} - \hat{\varpi}_{yi}\right| T, \qquad (3)$$

where T is a multiplier term equalling τ (the quantile value) for positive deviations $\left(\varpi_{yi} - \hat{\varpi}_{yi}\right)$ and $(1 - \tau)$ for negative deviations. This asymmetric minimization fits a regression model through the upper data for high τ and through the lower data for small τ.

It should be noted that the quantile minimization of residuals (equation (3)) is based on absolute values rather than on squared deviations as in OLS regression, thus reducing outlier effects. For a more detailed description of quantile-based fitting, see Koenker and Hallock (2001), Cade and Noon (2003) and Gotelli and Ellison (2004).

2.4 *Building the model: OLS and quantile regression of local spectral variability versus NDVI*

We considered a subset of 1000 cloud-free random pixels. Pixels located in the sea were removed from the analysis, leaving a total number of 604 pixels for the analysis. The variability of local spectral heterogeneity (PC1 standard deviation within 3 × 3 cells) with respect to the NDVI (mean NDVI within 3 × 3 cells) was then tested using regression analysis.

The NDVI is expected to increase with increasing vegetation cover up to about 80–100%. Local spatial heterogeneity of NDVI, or any spectral measure, is expected to increase up to about 40–60% cover and then begin to decrease towards 100% (Woodcock and Strahler 1987). Consequently, a second-order polynomial function is expected to give the best fit. Second-order polynomial models at various quantile thresholds ($0.10 \leq \tau \leq 0.99$) were fitted to the data by the quantreg package (Koenker 2007) within R software (R Development Core Team 2007) following

$$h = \beta_1(\mathrm{NDVI})^2 + \beta_2(\mathrm{NDVI}) + h_0, \tag{4}$$

where h is the spectral heterogeneity, β_1 is the slope of the two sides of the parabola and β_2 is the coefficient basically regulating the coordinates of the centre of the parabola (together with β_1 and intercept h_0).

The comparison with the OLS linear regression was made by only considering the quadratic slope term β_1, which is expected to highly impact the slope of the parabola. In this paper $\beta_1 < 0$, i.e. as expected from the theoretical assumptions discussed above, a humped-back parabola fits the data.

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3. Results and discussion

OLS regression based on a parabola model led to a significant negative slope ($\beta_1 = -52$, $p < 0.01$, figures 3 and 4), indicating that a humped-back curve fits the relationship between spectral heterogeneity versus NDVI.

Considering quantile regression, β_1 showed low but significant values at lower quantiles. For quantiles approaching 0.65, β_1 reached its minimum ($\beta_1 = -70$), thus

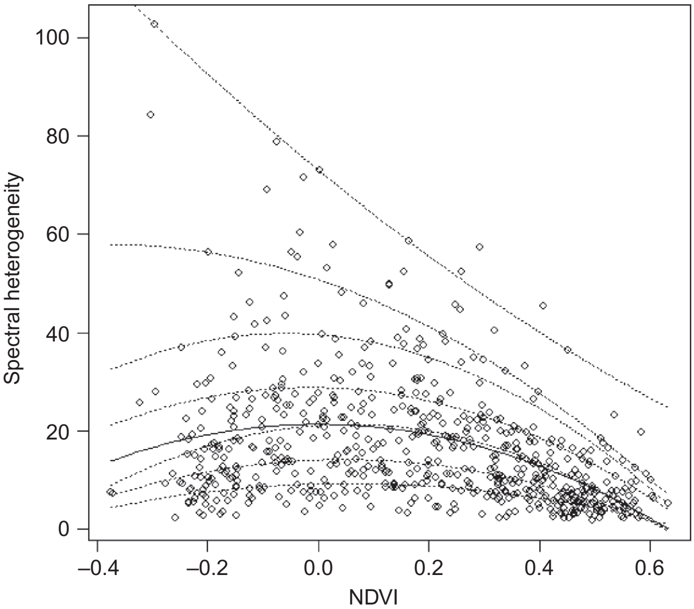

Figure 3. Scatter plot of spectral heterogeneity as measured by PC1 standard deviation (3 × 3 cells) versus NDVI (mean NDVI within 3 x 3 cells). Dotted lines: regression curves derived from quantile regression at different thresholds τ, The following quantiles are shown, from the top to the bottom: 0.99, 0.95, 0.90, 0.80, 0.60, 0.40, 0.20. Solid line: regression curve derived from OLS regression.

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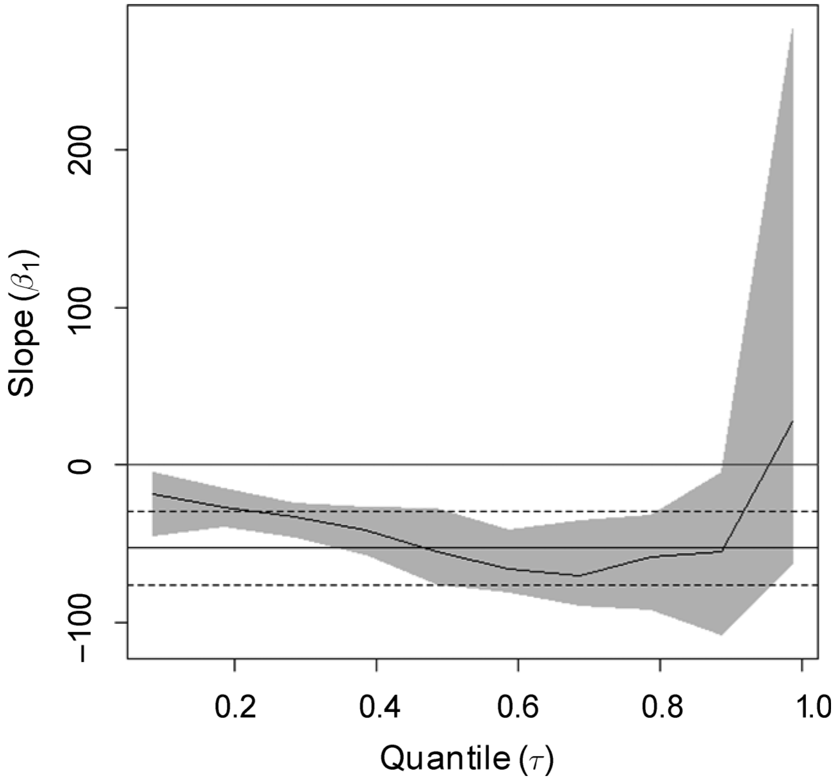

Figure 4. Variation (solid black line) of the quadratic slope coefficient (β_1) of the considered second-order polynomial models (equation (4)). The grey area represents 99% confidence intervals; thus, when they include zero (solid grey line) the coefficient is not significant at $p < 0.01$. The horizontal solid black line represents the slope (β_1) value with 99% confidence intervals (dashed black lines) obtained by OLS regression. A similar representation of quantile and OLS parameters is provided by Koenker and Hallock (2001).

increasing once again until its non-significance at $\tau \geq 0.90$. While, for most of the quantiles, the humped-back curve was significant (β_1 being negative and different from zero at $p < 0.01$), as τ equalled *ca* 0.90, the parabola opened up, reaching an almost linear shape (figures 3 and 4). In fact, fitting linear models (not shown in figure 3) at higher quantiles led to significant negative slopes (e.g. the slope was –48 at $\tau = 0.9$, –68 at $\tau = 0.95$ and –80 at $\tau = 0.99$, $p < 0.01$).

Of course, both OLS and quantile regression models carry the same conceptual information, i.e. a humped-back relationship between spectral (and thus spatial) heterogeneity and biomass. From a statistical point of view, Woodcock and Strahler (1987) found that the local variability depends on the match between the dimension of the scene objects and that of the pixels. In particular, local spectral variability should reach its maximum when the pixel spatial resolution is approximately the same as the scene objects being considered. Local spectral variability should decrease as the pixel dimension becomes larger or smaller (Woodcock and Strahler 1987, Song and Woodcock 2002), as the correlation among the nearest pixels decreases and the local variability rises (Ricotta *et al.* 1999). In this paper, the scene objects are considerably larger than the pixel size at the two extremes of the humped-back curve model (low and high NDVI), mostly related to bare soil and dense-canopy cover, respectively.

From an ecological point of view, the chief source of variation within the dataset is caused by differences among different land-use classes (Woodcock and Strahler 1987, Ricotta *et al.* 1999). In fact, considering points falling in ecosystems with a high degree of canopy cover (right-hand side of figure 3), it is expected that a denser canopy cover will lead to lower variability of spectral reflectance. When dense canopy occurs in forested environments, the spatial heterogeneity perceived by the remote sensor should be low (Nagendra 2001). On the other hand, when the canopy opens up (central part of figure 3), understorey vegetation and bare soil should increase spectral contrast between isolated tree crowns, shrubs and herbaceous/soil background. Finally, completely bare soil or water (left-hand side of figure 3) is expected to show a very low amount of variability for medium-spatial-resolution images. The spectral consequences of such reduced variability on high and low NDVI values results in the humped-back relationship shown here.

The pattern reported in this paper is not novel and has been reported elsewhere in the Mediterranean biogeographical region. A number of studies have found high levels of heterogeneity, even at very low NDVI values in a range of ecosystems, including wetland areas (Rocchini *et al.* 2005, Laba *et al.* 2008), urban areas (Small 2005, Nichol and Wong 2007) and bare soil areas such as the Mediterranean badlands (Phillips 1998, Marignani *et al.* 2008). Rocchini *et al.* (2007) demonstrated that wetland areas might show a high local variability due to the presence of local clearings within marshes, despite the very low NDVI values enhanced by the presence of water, which severely affects the spectral response in the NIR. More generally, Small (2005) highlighted the extremely high variability of urban reflectance at a variety of spatial scales, which is suspected to show lower values of NDVI when compared with shrubland and woodland areas. If an OLS model is used to fit the whole universe U of points, such patterns are not discernible.

The noise present in the examined scatter plots is largely due to the statistical distribution of the data and the effects of the spatial and spectral resolution of the satellite sensor. Statistical distributions of ecological data often show unequal variation due to complex interactions between the factors being accounted for (Cade and Noon 2003). In other words, most of the actual response variability is lost when only one factor is considered as an explanatory variable (Gotelli and Ellison 2004). Univariate models are expected to reach only a part of the total variance of the system (Orlóci 1978, Orlóci and Kenkel 1985, Legendre and Legendre 1998). Therefore, the NDVI cannot, by itself, explain the statistical variability in spectral heterogeneity, as the NDVI is not necessarily a limiting factor of spectral heterogeneity.

With regard to spatial resolution, ecological processes provide different information at different scales (Dungan *et al.* 2002). Therefore, inference is strictly related to the spatial scale of analysis and some patterns or processes can be recognized only at specific resolutions (Palmer and White 1994, Stohlgren *et al.* 1997a,b, Hortal and Lobo 2005, Legendre *et al.* 2005). Since pixels represent spatially explicit entities containing several objects (Fisher 1997, Cracknell 1998), mixed pixels increase as resolution decreases (Schiewe 2005, Small 2005). A medium-resolution sensor, such as Landsat ETM+, may fail in detecting NDVI and spectral heterogeneity. Rocchini (2007b) demonstrated that spectral resolution can compensate where spatial resolution is limiting. In fact, high spectral resolution should bring higher information content by minimizing low spatial-resolution effects (see Nagendra and Rocchini (2008) for

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a review on the matter). Here, the spectral information content of the whole multispectral dataset was reduced to PC1. This may partially account for the noise found in the presented scatterplot. However, it should be stressed that the main aim of this paper was not to test for absolute models of spectral heterogeneity versus NDVI, but to examine relative differences among regression models applied to the same input variables.

4. Conclusion

As stressed by Woodcock *et al.* (1988a,b), understanding the causes of spatial variation in images can provide a basis for developing new streamlined image analysis procedures. Here, we demonstrate that quantile regression may represent a powerful technique for the analysis of remotely sensed data, as it may reveal patterns that OLS regression may hide. On the one hand, regression-based analysis represents an important tool in the first stages of any ecological study, where little is known *a priori* about the ecosystem being studied and researchers are limited to unstructured surveys based on correlative patterns between variables (Anderson and Gribble 1998). On the other hand, OLS regression has both statistical (e.g. Schröder *et al.* 2005, Cade and Richards 2006, Cade *et al.* 2006) and ecological limitations (e.g. Cade *et al.* 2005, Griffith and Peres-Neto 2006, Buhk *et al.* 2007, Cho *et al.* 2007). Such drawbacks are reviewed by Koenker and Hallock (2001, p. 154), where the authors state:

> 'what the regression curve does is give a grand summary for the averages of the distributions corresponding to the set of *x*'s. We could go further and compute several different regression curves corresponding to the various percentage points of the distributions and thus get a more complete picture of the set. Ordinarily this is not done and so regression often gives a rather incomplete picture. Just as the mean gives an incomplete picture of a single distribution, so the regression curve gives a corresponding incomplete picture for a set of distributions.'

In this paper, we argue that caution needs to be taken with this 'mean concept' (Schröder *et al.* 2005) when performing regression analysis on reflectance data, while a more detailed examination of all possible subsets within a scatter plot may increase the understanding of patterns that are otherwise lost by commonly used regression techniques.

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