Unmixing and mapping components of Northern Ireland's geochemical composition using FastICA and random forests

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Abstract

There is an increasing trend for the collection of multi-sensory quantitative data to support the mapping of geology and environment. In the United Kingdom and Ireland this trend has been led by the Tellus mapping programmes; large scale multidisciplinary surveys which have collected quantitative data by a combination of geophysical survey from the air and geochemical survey on the ground. Such datasets contain a huge amount of geological and environmental information. However, these datasets have tended to be analysed on a variable--by--variable basis rather than as an integrated representation of a single geoenvironmental system. Using the example of Northern Ireland, this paper presents a demonstration of the quality of information that can be extracted through an integrated approach using modern data analytics. Two tools are used: FastICA independent component analysis to unmix the full composition of Northern Ireland's soil geochemistry into meaningful components, and the random forest machine learning algorithm to map these components in high-resolution according to their relationships with geophysical parameters.

We find that when unmixed to eight independent components, each explaining different aspects of geological and surficial processes, the geochemical features of Northern Ireland can be interpreted concisely. High resolution mapping aids this interpretation, with the random forest approach providing more accurate maps than traditional IDW interpolation for all but one of the components. In addition, by recombining the high resolution maps of independent components into a ternary colour image, a highly detailed output is produced in which all the features of the region's traditional geological map (and more) can be seen, all as a continuous and accurate fully quantitative representation of Northern Ireland's geochemical composition.

Keywords:
Compositional data analysis
Independent component analysis
Machine learning
Geology
Geophysics
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1. Introduction

Surficial geochemical data contains a wealth of geo-environmental information (e.g. Darnley, 1990; Grunsky et al., 2009; McKinley et al., 2016) and therefore has the potential to improve our understanding of both underlying geology (e.g. Kirkwood et al., 2016b) and the surface environment (e.g. Filzmoser et al., 2009b). Historic barriers to the full utilisation of soil geochemical data have included its relative complexity (high dimensionality and compositional nature; Pawlowsky-Glahn and Egozcue, 2006) and the typically coarse spatial sampling density, which when mapped by traditional spatial interpolation lacks resolution, therefore limiting useful interpretation.

Developments in the field of compositional data analysis (CoDA) have provided a set of transformations (Aitchison, 1986; Egozcue et al., 2003) to allow classical dimension reduction techniques such as principal component analysis, factor analysis, and independent component analysis to be non--spuriously applied to compositional data, allowing useful unbiased information to be extracted from bulk geochemical data in the form of compositional components (Filzmoser et al., 2009a; Filzmoser et al., 2009b; McKinley et al., 2016).

Meanwhile, developments in the field of machine learning (and the increasing acceptance of geoscientists towards them; e.g Cracknell et al., 2014; Cracknell and Reading, 2014; Carranza and Laborte, 2015; Harris et al., 2015; Rodriguez-Galiano et al., 2015; Kirkwood et al., 2016a) have provided solutions to the problem of low resolution geochemical maps by modelling geochemistry from high resolution geophysical and remotely sensed data where it is available, with the ability to provide improved prediction accuracy to boot (Kirkwood et al., 2016a).

In this paper independent component analysis (FastICA; Hyvarinen, 1999) is applied to the geochemical composition of Northern Ireland's soils after a log-ratio transformation procedure as previously described by Filzmoser et al. (2009a) for compositional principal component analysis. The use of independent component analysis allows the complex mixture of signals within Northern Ireland's soil composition to be unmixed, providing independent and denoised compositional components, each representing a 'latent variable' attributable to a particular process. These components are subsequently mapped using the random forest regression tree ensemble approach (Breiman, 2001) supported by high -resolution geophysical survey data to provide maps with greater detail and accuracy than their traditionally interpolated equivalents. The work is presented as a demonstration and visualisation of the quality of information that can be extracted by applying modern methods of data analysis to integrated multi-source survey data.

2. Materials

2.1 Study area

The study area, Northern Ireland, is a constituent unit of the United Kingdom of Great Britain and Northern Ireland and is situated in the northeast of the island of Ireland. The geology of Northern Ireland can be considered in four main domains (Fig. 1; Cooper, 2004). Firstly, in the north west are the oldest rocks of Northern Ireland; the Proterozoic basement of the Central Highland or Grampian Terrane. Secondly, in the south east are Ordovician-Silurian sedimentary rocks of the Southern Uplands-Down-Longford Terrane, intruded by Late Caledonian and Palaeogene granitoids. Thirdly, in the south west are Devonian-Carboniferous sedimentary rocks, and finally, in the north east, are the Cenozoic (Permian-Cretaceous) rocks that most notably include the early Paleogene Antrim Lava Group. In addition to this impressive and variable bedrock history, Northern Ireland has experienced repeated glaciations during the Quaternary that have resulted in the formation of a range of glacial deposits that mantle the landscape. For some of these deposits their geochemical composition reflects the underlying bedrock source (Dempster et al., 2013), whilst for others there is a disparity because of transport or processes of deposition. Each of these various various domains and their constituent lithologies (bedrock and superficial deposits) can be expected to impose a unique geochemical signature on the composition of the soils that overlie them.

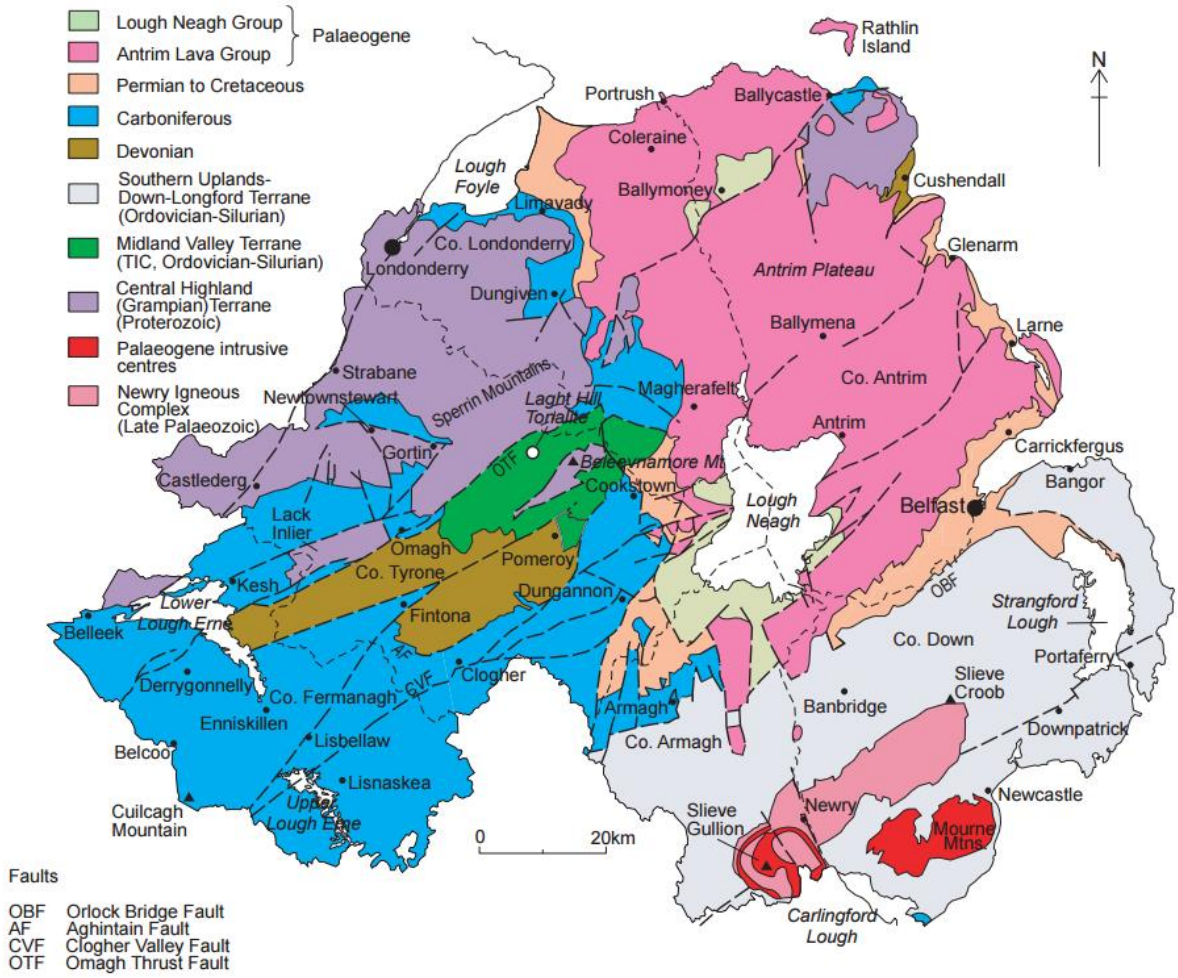

Fig. 1. Simplified bedrock geology of Northern Ireland, from Cooper (2004).

2.2 Soil geochemical data

The soil geochemical data used in this study comes from the analysis of 6862 shallow soil samples (Fig. 2) collected for the Tellus Northern Ireland project between the years of 2004 and 2006 (Young and Donald, 2013). Samples were collected in accordance with standardised methods developed by the British Geological Survey for the Geochemical Baseline Survey of the Environment (G-BASE) project (Johnson et al., 2005). Each sample represents material collected at 5-20cm depth at a randomly positioned locality within each 1km grid square of the Irish National Grid, subject to the avoidance of immediate anthropogenic influence where possible. This study uses the data from XRF analysis, which provided concentration data for the following 52 elements (with major elements as oxides): Ag, Cd, In, Sn, Sb, Te, I, Cs, Ba, La, Ce, Na_2O, MgO, Al_2O_3, SiO_2, P_2O_5, SO_3, K_2O, CaO, TiO_2, MnO, Fe2O3, Cl, Sc, V, Cr, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Rb, Sr, Y, Zr, Nb, Mo, Nd, Sm, Yb, Hf, Ta, W, Tl, Pb, Bi, Th, U, and R – the unmeasured remainder of the full composition. The elemental analyses were conducted by the British Geological Survey.

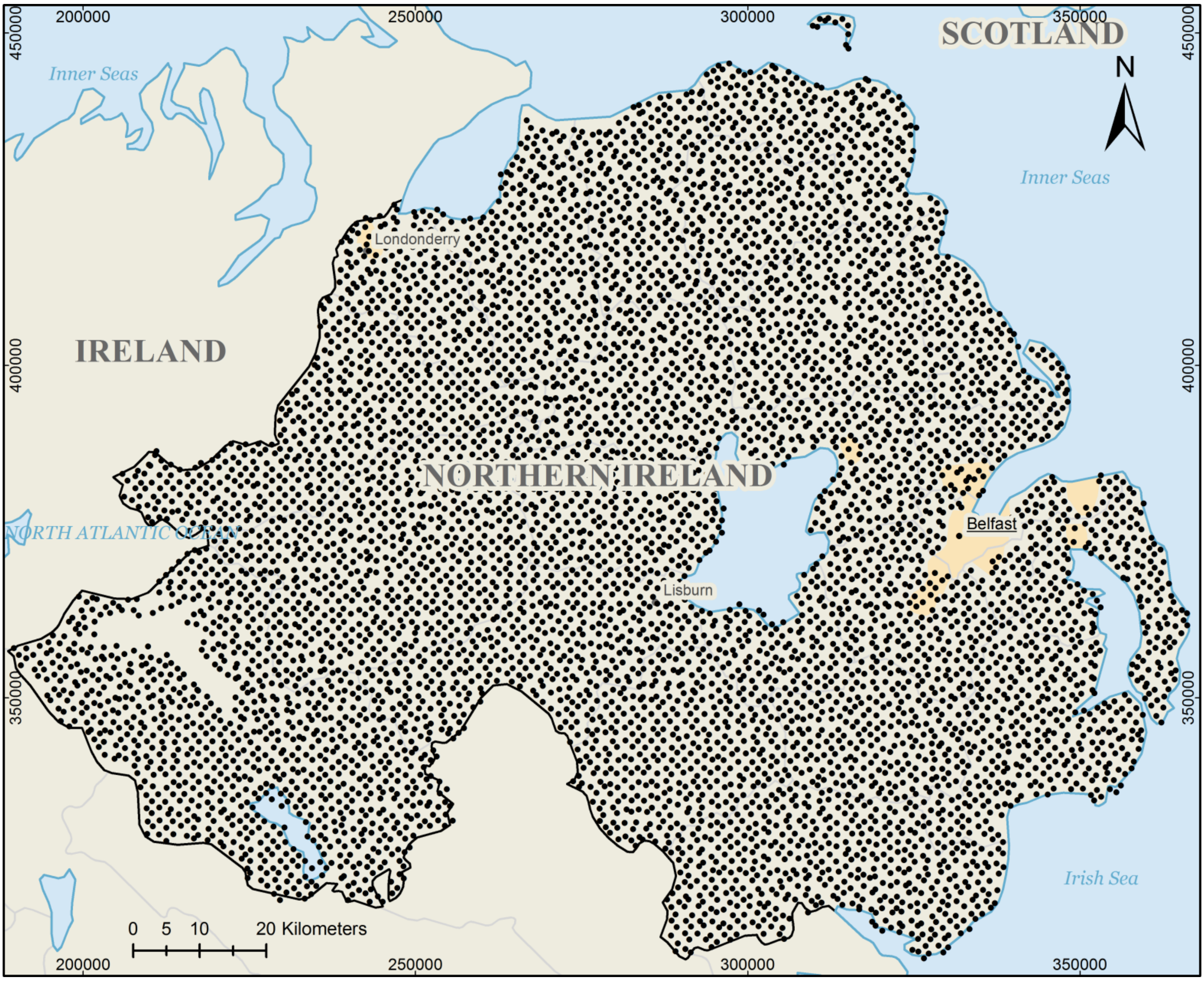

Fig. 2. Locations of 6862 shallow soil samples collected and chemically analysed for the Tellus Northern Ireland project.

2.3 Geophysical data

In addition to providing a comprehensive geochemical survey of the ground, the Tellus Northern Ireland project also flew a high resolution geophysical survey from the air (Beamish and Young, 2009; Young and Donald, 2013). The airborne geophysical survey acquired magnetic, radiometric, and frequency-domain electromagnetic data (Hodgson and Young, 2016), and is supplemented in this study by pre-existing elevation and gravity data. Each measured geophysical variable (Table 1) was interpolated to a 100m grid prior to use in this study. Magnetics data was interpolated using a bicubic spline, while all other variables were interpolated using a minimum curvature method, as is common practice for geophysical data (Hinze et al., 2013).

Table 1
Explanations of the geophysical and remotely sensed predictor variables used in the high resolution mapping.

Variable name	Explanation
Elevation	Digital Terrain Model
Regional Bouguer Anomaly	Gravity survey bouguer anomaly
Residual Bouguer Anomaly	Gravity survey high pass filtered bouguer anomaly
MAG_RTP	Total magnetic intensity, reduced to pole
MAG_RTP_HGM	Horizontal gradient of MAG_RTP
MAG_RTP_1VD	1st vertical derivative of MAG_RTP
MAG_AS	Analytical signal of total magnetic intensity
Radiometrics_uranium	Uranium counts from gamma ray spectrometry
Radiometrics_thorium	Thorium counts from gamma ray spectrometry
Radiometrics_potassium	Potassium counts from gamma ray spectrometry
Radiometrics_total_count	Total count of unmixed gamma ray signal
COND_3K	Ground conductivity – 3Khz band
COND_14K	Ground conductivity – 14Khz band

3. Methods

3.1 compositional independent component analysis (ICA)

All data analysis and modelling was conducted in R (R Core Team, 2016). In order to extract meaningful components of soil composition from the geochemical data, compositional independent component analysis was used. The kind of geochemical data used in this study should be treated compositionally because the variables (element concentrations) are not truly independent of each other, but are confined to sum to the total of the closed composition, i.e. 100% or 1 000 000 mg/kg (Pawlowsky-Glahn et al., 2007). The variables therefore have an imposed tendency to negatively correlate; as one increases, others must decrease and vice versa. The values of a single variable are therefore entirely dependent on the degree of dilution by other variables. Each variable is therefore said to carry only relative information (Aitchison, 1986): what matters are the ratios between variables rather than their individual values. Applying classical correlation-based statistical methods directly to such data is therefore bound to produce spurious and misleading results (Pearson, 1896;

Chayes, 1960). Instead, the data must first be transformed into a more appropriate mathematical space, where correlation measures are replaced with measures of the stability of ratios between variables. The isometric log-ratio- transformation (ilr; Egozcue et al., 2003) provides this, and is the first step of the compositional ICA procedure.

ICA was conducted using the FastICA algorithm (Hyvarinen, 1999). ICA was chosen over principal component analysis for its ability to unmix (make orthogonal and independent) trends which are not necessarily orthogonal in the original feature space. It does this by separating components according to the shapes of their distributions (their non-Gaussianity) assuming that they are not perfectly normal distributions but differ in skewness and kurtosis. This makes it more powerful than principal component analysis, which can only rotate the input data to maximise variance along the principal axes, and so may well not align with the true 'latent variables' within the data. As a result of its power, ICA has become a preferred technique for making sense of complex mixtures, for example in neuroscience it is used to unmix electroencephalographic (EEG) data (e.g. Makeig et al., 1996; Delorme and Makeig, 2004) and it has had some recent uptake in geochemical applications (Liu et al., 2014; Yang and Cheng, 2015).

The ICA parameters for this study were selected manually with the aim of maximising the orthogonality (independence) of the output components. This was assessed subjectively by viewing output components as pairwise scatter plots. It was found that unmixing to eight components using deflation and an exponential G function (Hyvärinen and Oja, 2000) provided the best results: trends within the output data became most strongly aligned with the component axes, indicating that the ICA algorithm had been successful in unmixing the data into independent components. By applying FastICA to ilr transformed data, the process is unaffected by the spurious correlations within the original closed-composition geochemical data, and can be expected to produce valid and meaningful results (Filzmoser et al., 2009a).

A complication of the ilr transformation is that the dimensionality of the data is reduced by one in the process, i.e. in this case 53 concentration variables are transformed into 52 log-ratio variables, losing their names (and their immediate meaning) in the process. To allow interpretable visualisations of element loadings to be made after ICA the results were subsequently transformed from isometric log-ratio-s to centred log-ratios (CLR; Aitchison, 1986). Through CLR transformation, the original number of variables is restored, and each can be referred to by its original name, though in fact as CLRs they represent log-ratios of the original element concentrations against the geometric mean of the whole measured composition.

3.2 Mapping soil compositional components in high resolution

The output soil compositional components were mapped in high resolution using the random forest (Breiman, 2001) algorithm to learn the physio-chemical relationships present between the high resolution geophysical survey data and the coarsely sampled geochemical data. The same technique has provided improved prediction accuracy and insight into the concentrations of the majority of elements in south west England (Kirkwood et al., 2016a), and has been gaining momentum in recent years for predictive mapping applications in general (e.g. Henderson et al., 2005; Gislason et al., 2006; Lawrence et al., 2006; Evans et al., 2011; Wiesmeier et al., 2011; Rodriguez-Galiano et al., 2012; Cracknell et al., 2014; Cracknell and Reading, 2014; Carranza and Laborte, 2015; Harris et al., 2015; Rodriguez-Galiano et al., 2015). In this study the R package 'Rborist' is used (Seligman, 2016), with 1001 trees, and a minimum node size of 1. To assess the accuracy of each map, 10-fold cross validation is used, and metrics are compared to the equivalent map produced by Inverse Distance Weighted (IDW) interpolation, the method that has historically been used to produce geochemical maps in the UK.

4. Results

4.1 Compositional ICA overview

The variance explained by each of the eight independent components of the ilr -transformed soil geochemical data (Fig. 3) reveals that 39% of the total variance is explained by the first component alone, with components two, three, and four providing an additional 10.6, 10.5 and 9.5% of explanation respectively. The eight components together explain 86% of the total variance in Northern Irelands' soil composition and are highly independent (Fig. 4). Component eight itself explains just 2.6% of the variance, but can be assumed to have some importance, as the ICA was less successful (outputs appeared increasingly co-dependent) when run with seven components or less. The 14% of variance that is not captured within the eight independent components can be assumed to be unstructured noise, as again the ICA produced correlated outputs when run with more than eight components. The eight independent components used in this study can therefore be taken as a 'subjectively optimal' summary of Northern Ireland's soil chemistry, with only minimal loss.

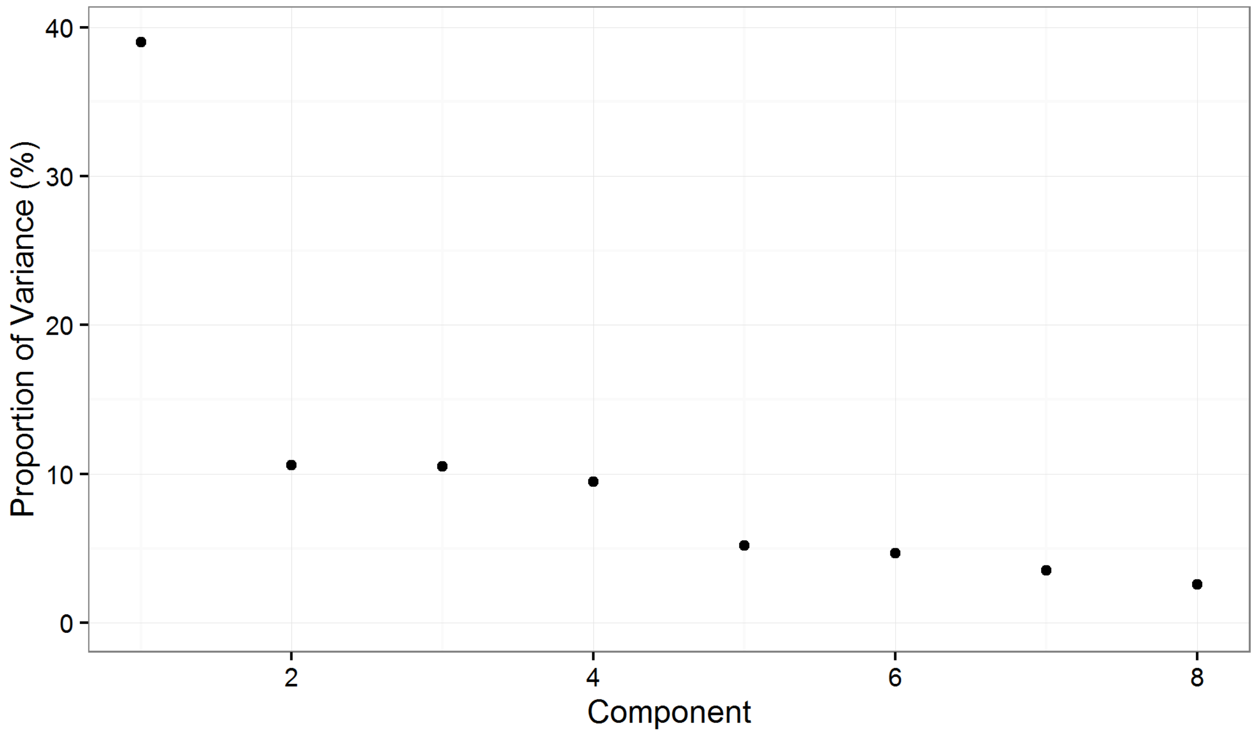

Fig. 3. Proportion of variance explained by each independent compositional component of Northern Ireland's soil geochemical data. The explanations sum to 86%, indicating that 14% of the original variance has been discarded as 'noise'.

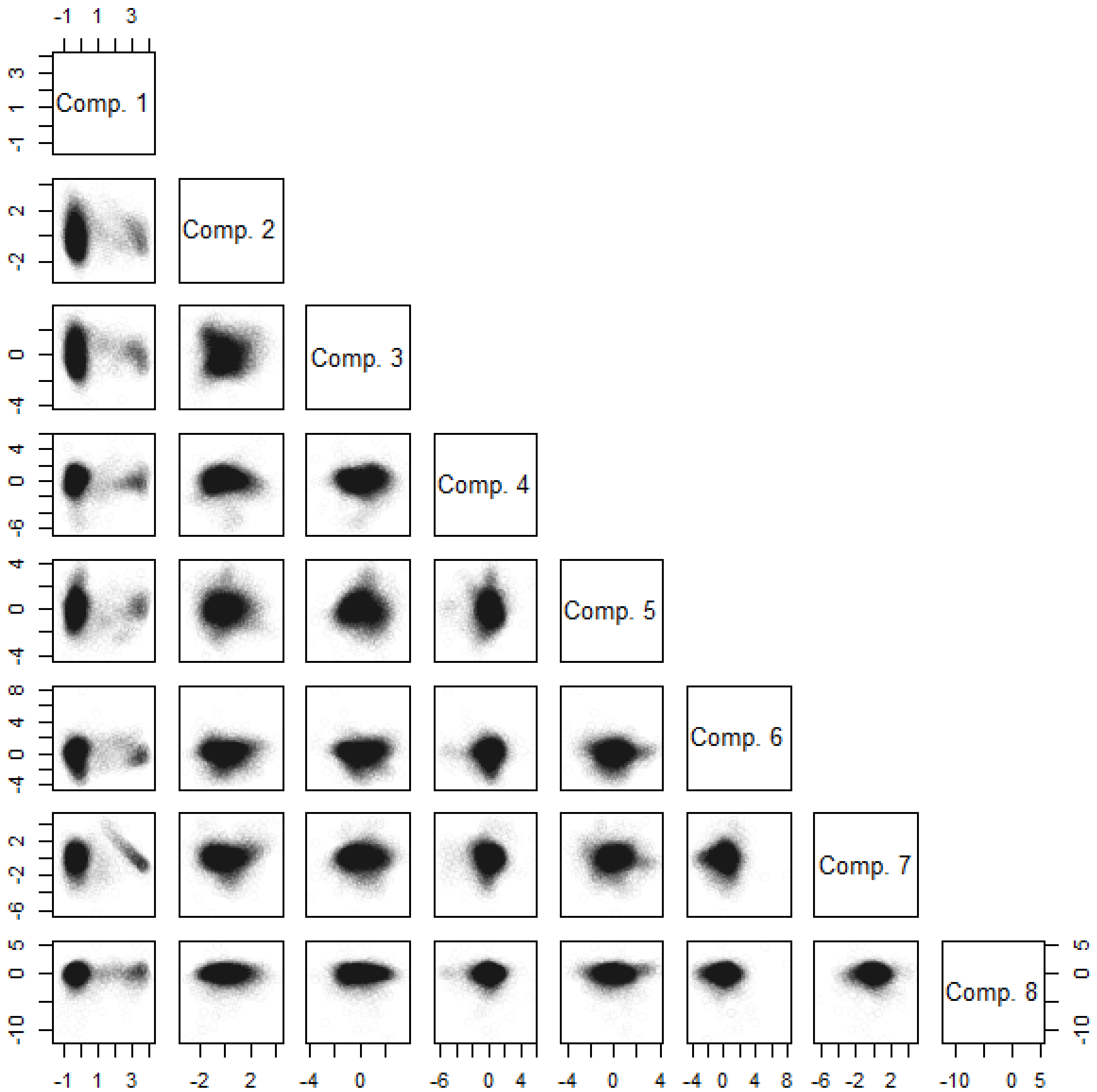

Fig. 4. Pairwise scatter plots of the eight independent components of Northern Ireland's soil chemistry. The success of the ICA procedure is evident in the general absence of correlation between components: trends within the point clouds tend to be aligned with the component axes i.e. either horizontally or vertically, thus indicating their independence.

4.2 Random forest independent component maps, with component loadings

The use of random forests to map the eight independent components of Northern Ireland's soil chemistry was successful in producing more accurate maps than IDW interpolation for all but one component (for which the difference is negligible), as evaluated by 10-fold cross-validation (Table 2). In every case, the random forest maps offer a detailed format from which to visualise the relationships between geochemistry and environment. The component maps have been visualised using the perceptually uniform Viridis colour scale (Garnier, 2015).

Table 2

Root-mean---square errors (RMSEs) of predictions made by random forest and IDW interpolation in mapping the eight independent components. Lower is better. This error was measured through 10-fold cross-validation.

	Comp. 1	**Comp. 2**	**Comp. 3**	**Comp. 4**	**Comp. 5**	**Comp. 6**	**Comp. 7**	**Comp. 8**
Random forest	0.60	0.68	0.61	0.59	0.65	0.79	0.88	0.89
IDW interpolation	0.85	0.74	0.70	0.67	0.72	0.78	0.91	0.90

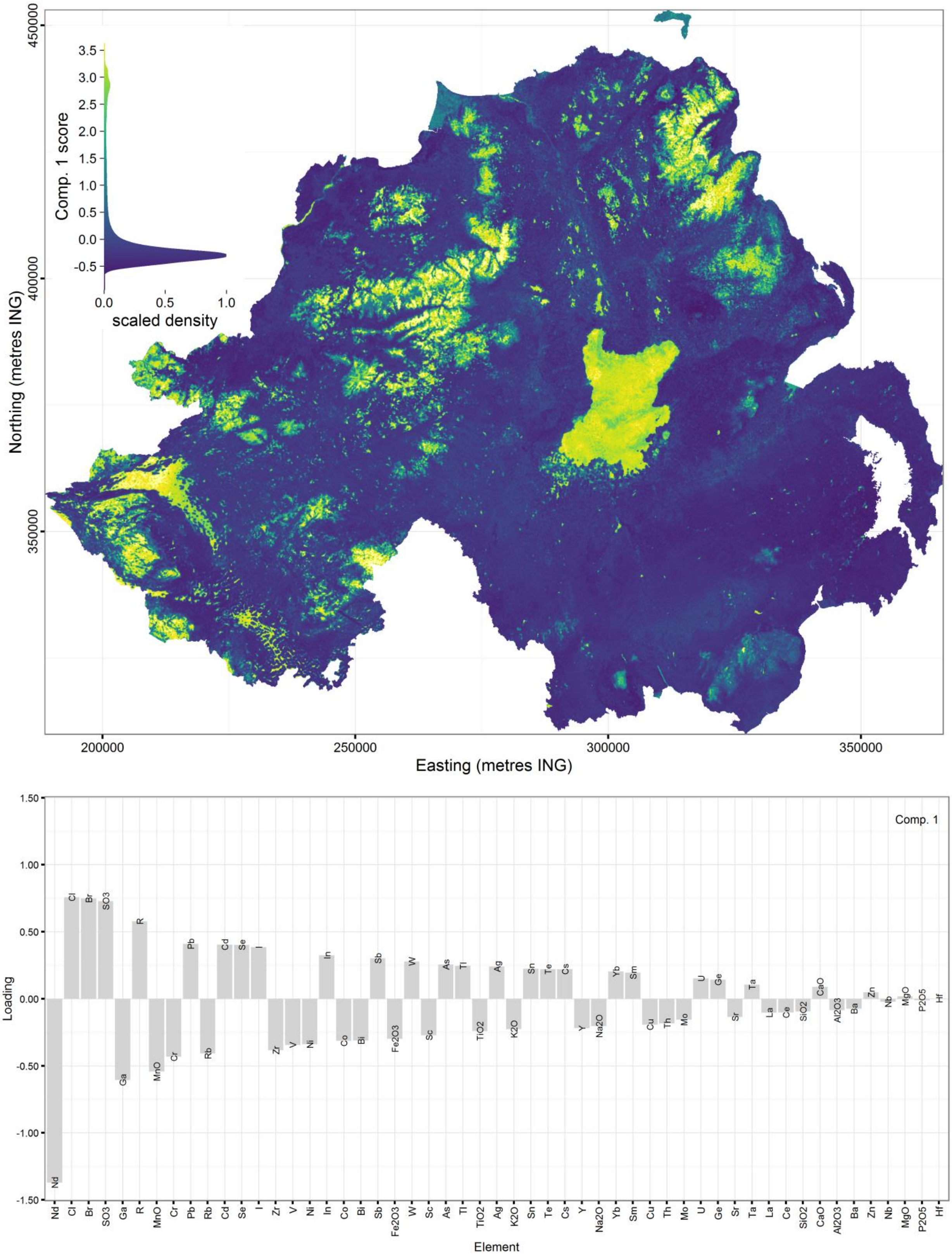

Fig. 5. Top) Map of independent component 1 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 1, as centred log-ratios (relative enrichments/depletions).

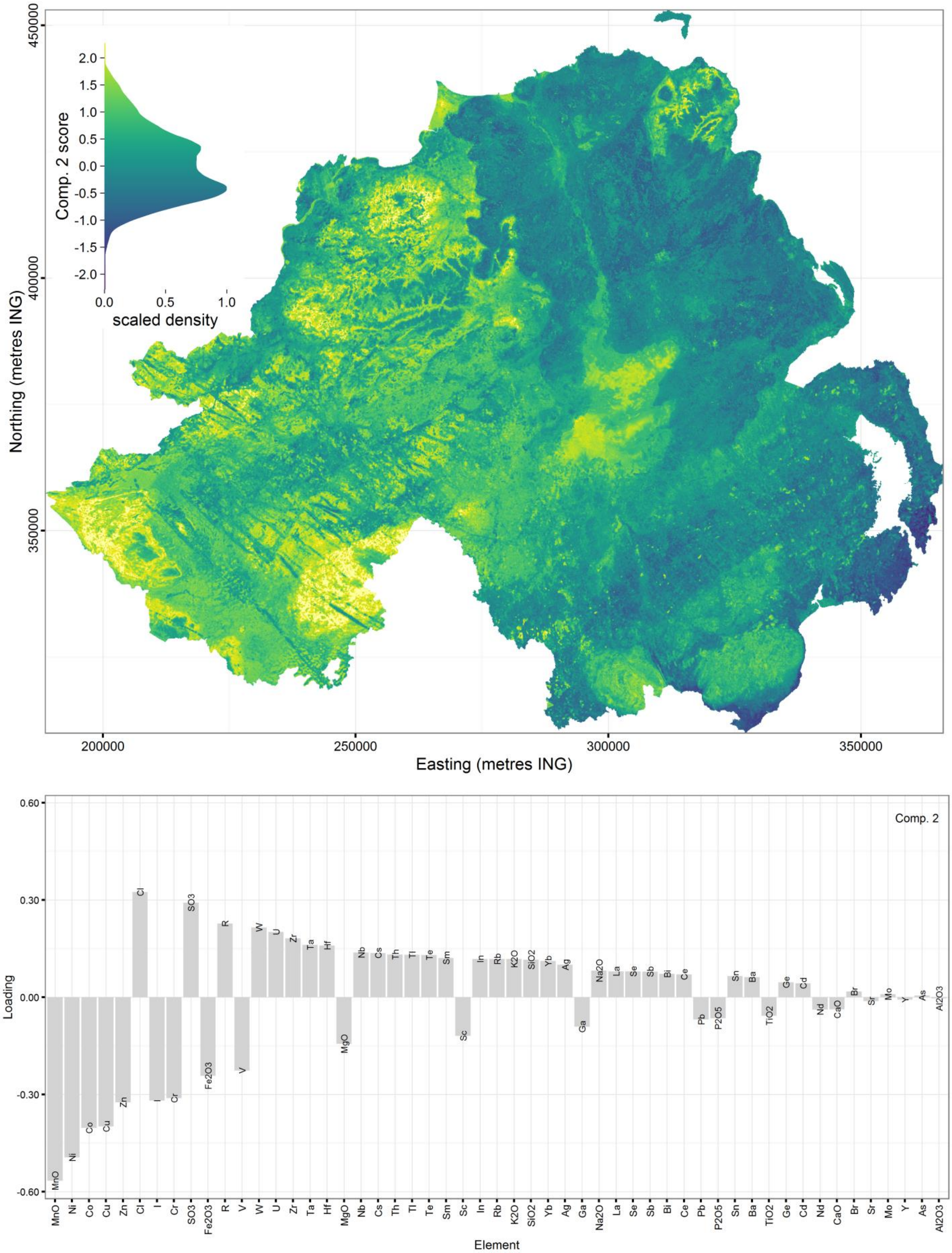

Fig. 6. Top) Map of independent component 2 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 2, as centred log-ratios (relative enrichments/depletions).

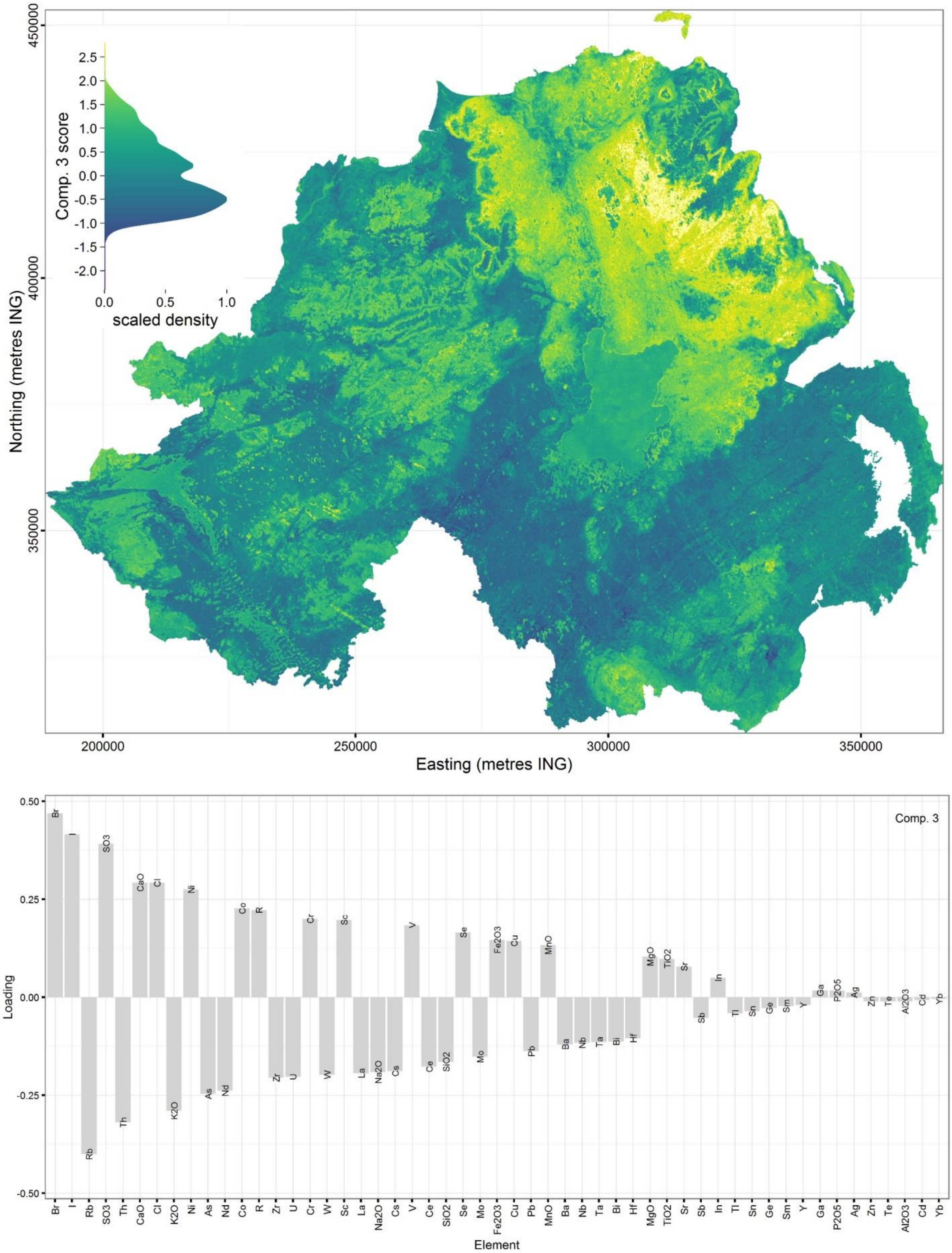

Fig. 7. Top) Map of independent component 3 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 3, as centred log-ratios (relative enrichments/depletions).

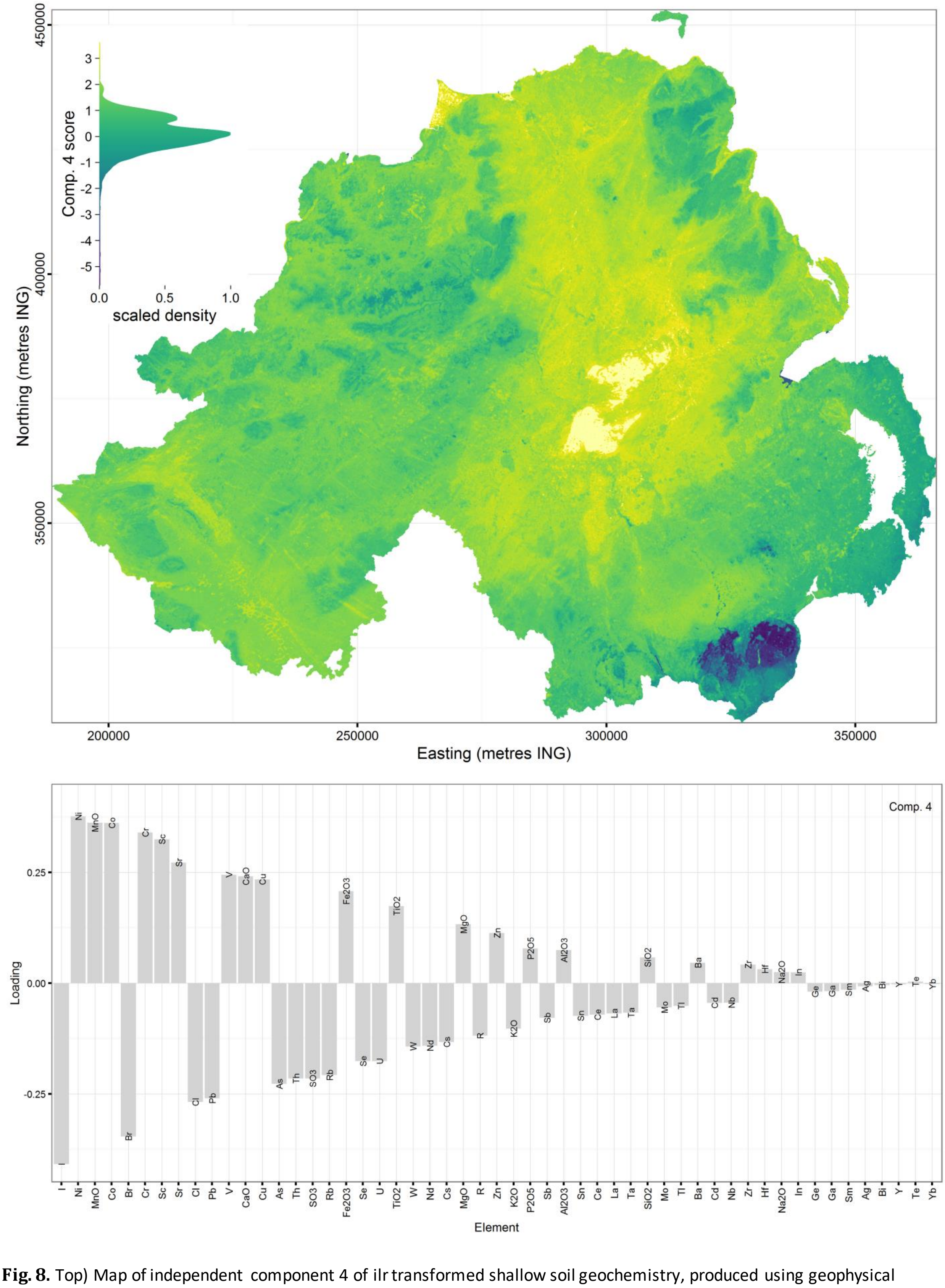

Fig. 8. Top) Map of independent component 4 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 4, as centred log-ratios (relative enrichments/depletions).

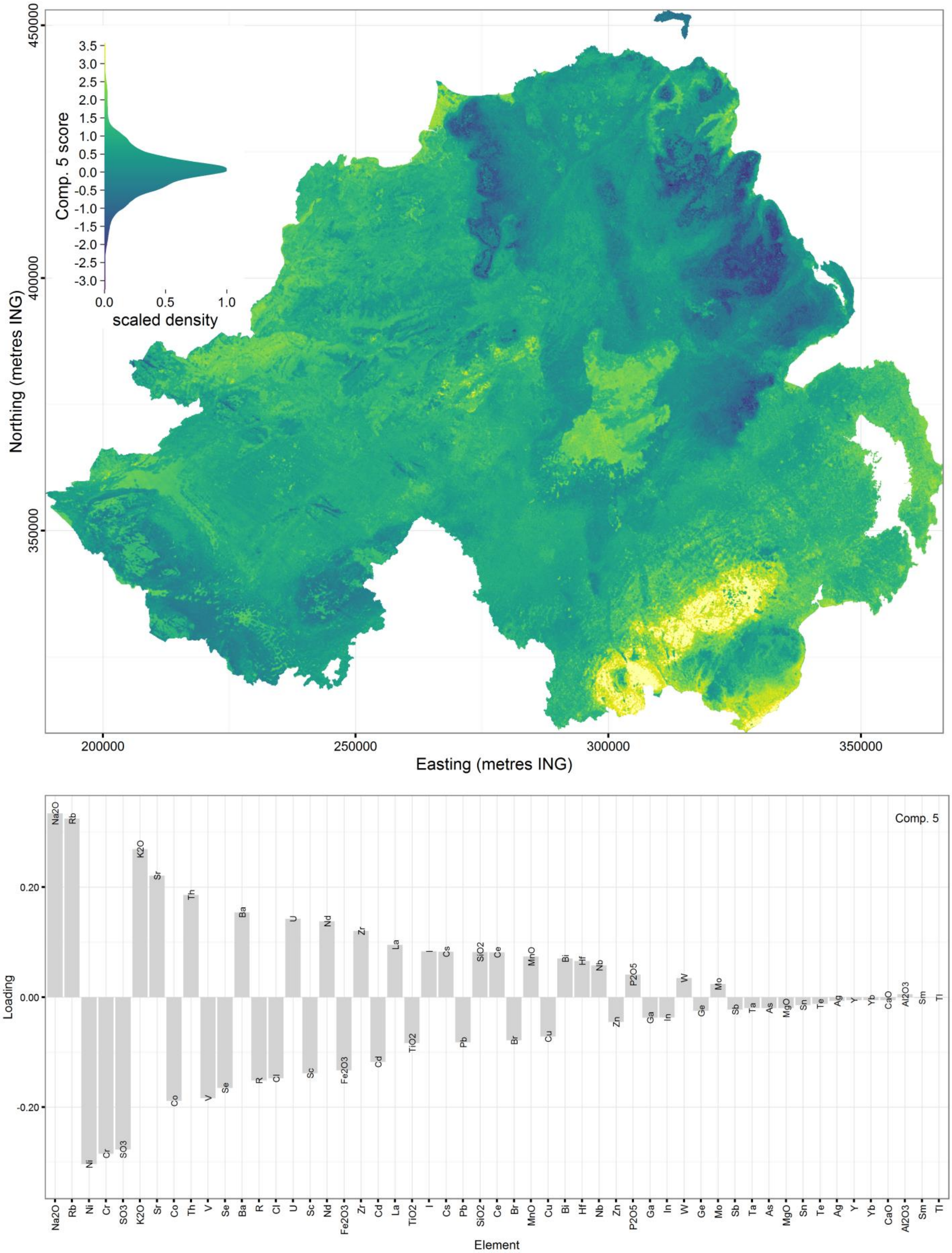

Fig. 9. Top) Map of independent component 5 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 5, as centred log-ratios (relative enrichments/depletions).

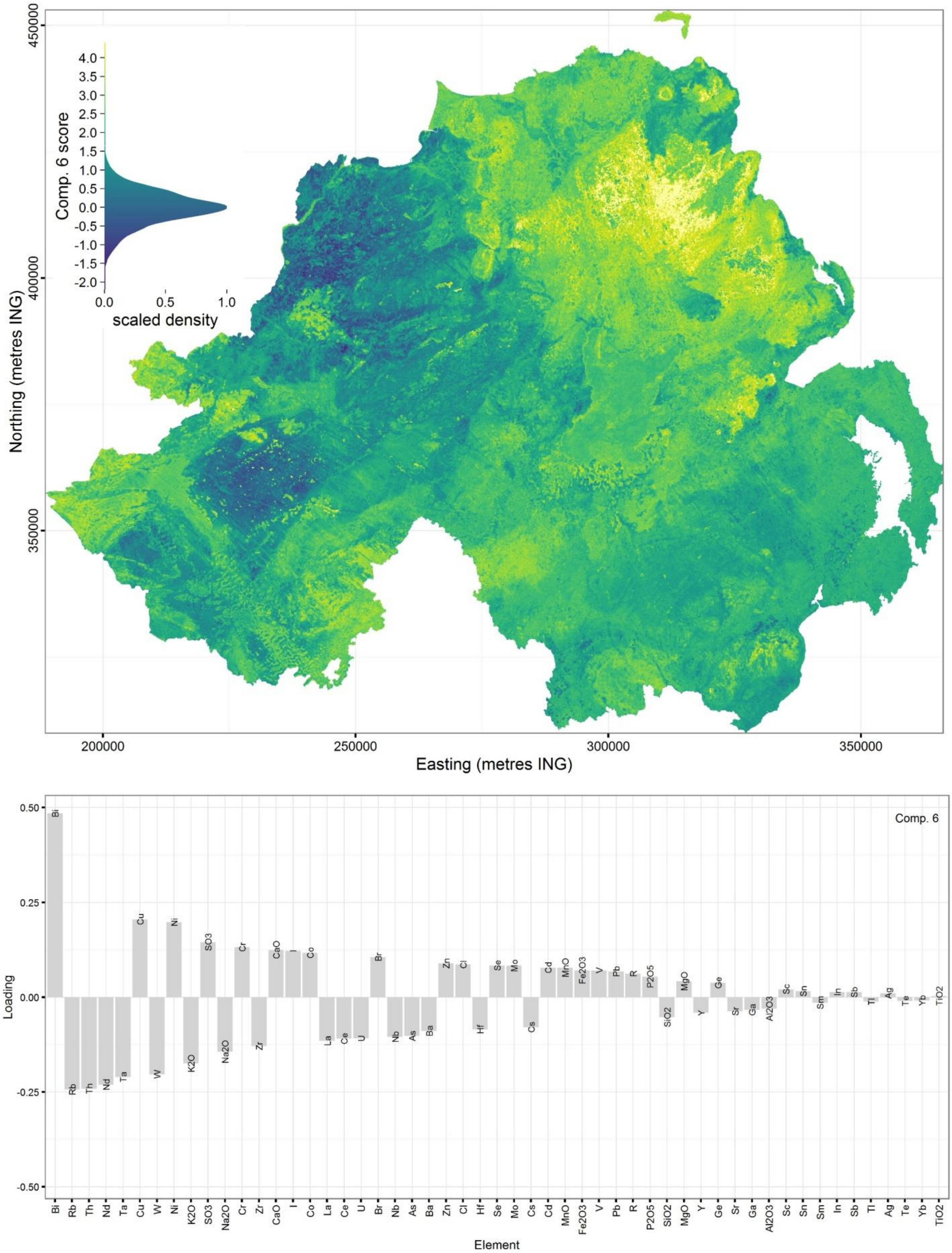

Fig. 10. Top) Map of independent component 6 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 6, as centred log-ratios (relative enrichments/depletions).

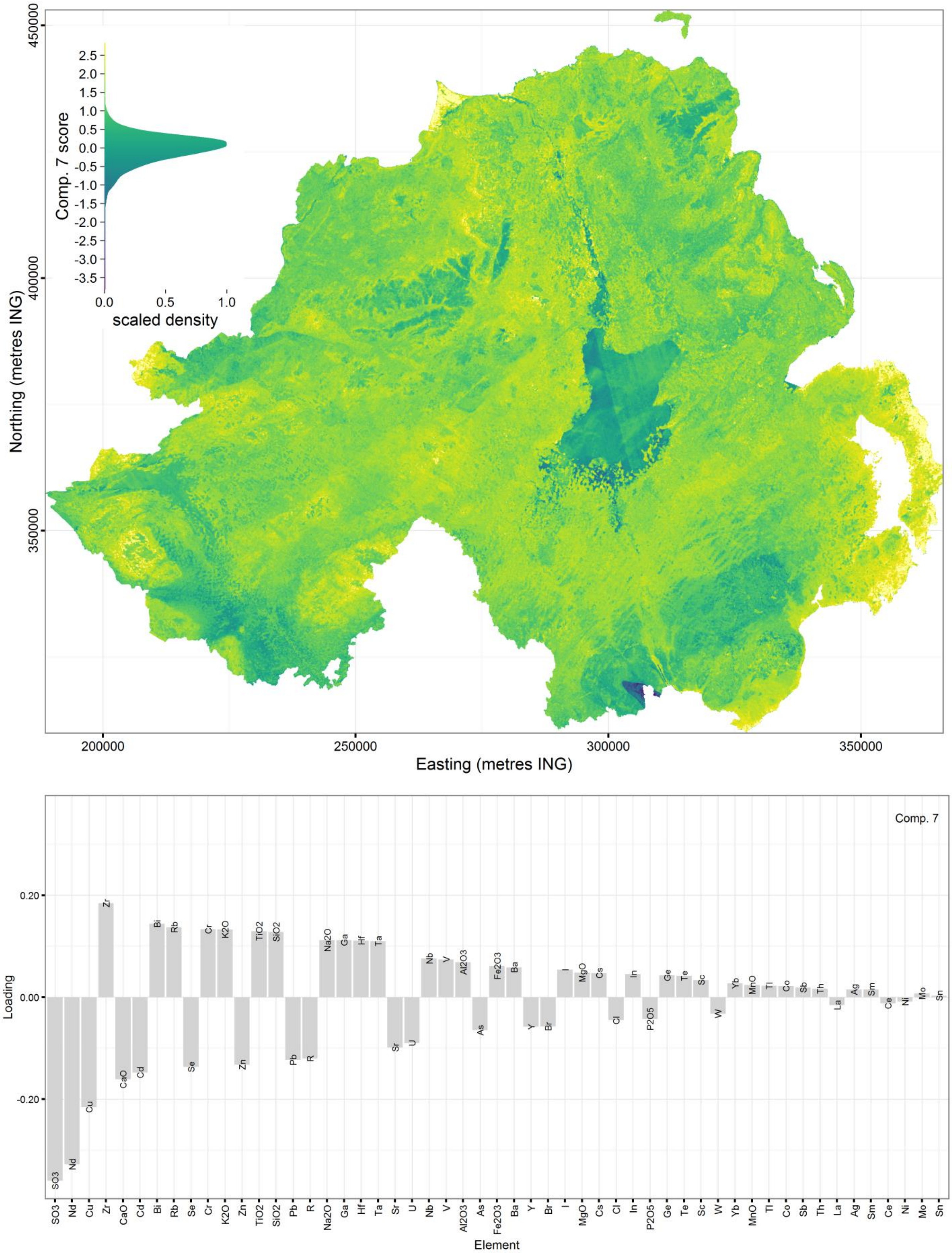

Fig. 11. Top) Map of independent component 7 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 7, as centred log-ratios (relative enrichments/depletions).

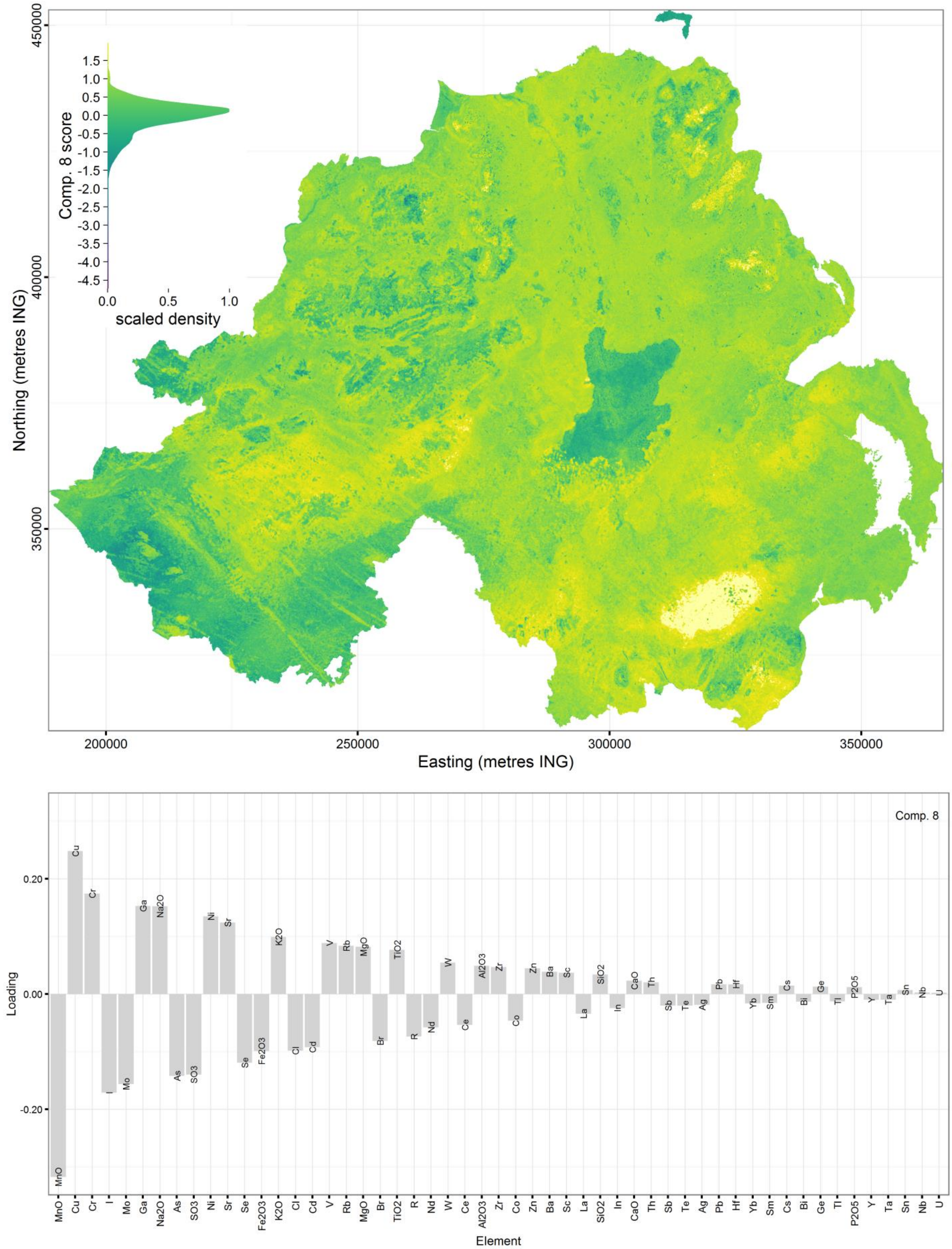

Fig. 12. Top) Map of independent component 8 of ilr transformed shallow soil geochemistry, produced using geophysical covariates and the random forest machine learning algorithm. Bottom) Element loadings on independent component 8, as centred log-ratios (relative enrichments/depletions).

5. Discussion

5.1 Independent Component 1

Component 1 is the largest component of the chemical composition of Northern Ireland's soils, accounting for 39% of the total variance. The component is positively skewed, with a second mode in the long tail of the data. With background knowledge it is clear from the map (Fig. 5) that this component represents the separation of peat (high values) from all other soils (low values). The Random Forest algorithm has also predicted high values for this component in water bodies, which is likely to be in recognition of the relationship between peat and gamma attenuation due to water content (Beamish, 2013). There are no soil samples within the water bodies and so this is an untestable extrapolation of logic by the Random Forest, but it is likely to hold some truth.

In terms of element loadings (Fig. 5), Component 1 represents a depletion of neodymium, gallium, and manganese and an enrichment of chlorine, bromine, sulphur and unmeasured remainder 'R' (a proxy for loss on ignition; Kirkwood et al., 2016a). These loadings confirm the identity of Component 1 as a separator of peat from non-peat soils; at high positive scores Component 1 is enriched in volatile elements that often associate with organic material, and depleted in elements which are associated with lithic material i.e. rock forming minerals.

5.2 Independent Component 2

Component 2 accounts for 10.6% of the variance in Northern Ireland's soil composition. As can be seen from the map (Fig. 6), Component 2 is not entirely invariant to peat, and this is captured in the element loadings; with chlorine, sulphur and the unmeasured remainder 'R' the top three enrichments. However, Component 2 has successfully separated the basalts of the early Paleogene Antrim Lava Group (Cooper and Johnston, 2004c) in the north east from surrounding sedimentary rocks. It also captures, with the same negative scores, the dyke swarms in the west (Cooper et al., 2012), indicating their mafic composition (with loadings of nickel, chromium, iron and magnesium). In the south east Component 2 has separated the Late Caledonian Newry Igneous Complex (Cooper and Johnston, 2004a) and Palaeogene Slieve Gullion and Mourne Mountains complexes (Cooper and Johnston, 2004a) from their surrounding Silurian and Ordovician Country rocks (Anderson, 2004). Overall the component seems to have provided power to distinguish between felsic and mafic compositions.

5.3 Independent Component 3

Component 3 accounts for 10.5% of the variance in Northern Ireland's soil composition. Again, Component 3 has been influenced by the peat, with enrichments of bromine, iodine and sulphur. However, where the ground is not covered by peat, Component 3 captures some subtle bedrock variations across the entire region (Fig. 7). In the north east the extent of the Antrim Lava Group is well constrained although there is some blurring of the contact between it and underlying Cretaceous rocks most likely due to down slope movement of basalt talus (scree). Also in this part of Northern Ireland the rhyolitic Tardree Complex (Cooper and Johnston, 2004c) is differentiated from the surrounding Antrim Lava Group and it would appear, based on known outcrop of bedrock, that there has been significant north west transport of material by ice during the Quaternary which is consistent with the findings of previous studies (Dempster et al., 2013).

To the south east Component 3 separates the Newry Igneous, Slieve Gullion and Mourne Mountains complexes from their surrounding Silurian and Ordovician country rocks. Whilst in the west clear differences are observed between Proterozoic basement rocks (Cooper and Johnston, 2004b) of the Lough Derg Inlier, Tyrone Central Inier, Dalradian Supergroup (including the Lack Inlier) and younger Devonian and Carboniferous rocks of this area. In addition, rocks of the predominantly mafic Tyrone Igneous Complex (Cooper et al., 2011; Hollis et al., 2012) are also picked out and share similar character to the similarly mafic Antrim Lava Group to the east. This component picks out faults and dykes in the south west and east of the region. Of all the components, Component 3 may provide the single best 'summary' of Northern Ireland's geology at a glance.

5.4 Independent Component 4

Component 4 accounts for 9.5% of the variance in Northern Ireland's soil composition. The strongest feature on the map (Fig. 8) is the stark lowlighting of the Paleogene granitoid of the Mourne Mountains relative to surrounding rocks, including other granitoids, of the Southern-Uplands-Down-Longford Terrane in the south. For the Mourne Mountains (negative scores on Component 4) compared to the other granitoids, the element loadings (Fig. 8) suggest a lower calcium, higher thorium and higher rubidium composition, with additional enrichments of lead and arsenic. Movement of Mourne granite debris is apparent in superficial deposits including southward and south-easterly transport by glacial processes onto the Mourne Plain, and northward fluvial transport by the Lagan River. On the north coast, blown sand is apparent at Magilligan Point, the Bann Estuary, Portrush Strand and Bushfoot dune complexes.

5.5 Independent Component 5

Component 5 accounts for 5.2% of the variance in Northern Ireland's soil composition. The most striking feature on the map (Fig. 9) is the Newry Igneous Complex relative to surrounding country rocks of the Southern Uplands-Down-Longford Terrane. To the south east on the Mourne Plain, this signal is repeated and may represent the presence of Newry Igneous Complex detritus in the glacial deposits of this area (Fig. 21). Negative scores are observed in peripheral areas of the Antrim Plateau and are related to the presence of Antrim Lava Group basalt at or close to surface, whilst, more positive score in this area are due mainly to the presence of glacial deposits (Geological Survey of Northern Ireland, 1991).

The northern part of mostly mafic Tyrone Igneous Complex has negative scores, whilst the positive scores in southern part are associated with bedrock of the Tyrone Central Inlier (Chew et al., 2008) and the Slieve Gullion granite (Hollis et al., 2013) both of which are essentially felsic in composition. Some parts of the southern area have positive scores because of superficial deposits of glaciofluvial sand and gravel (Geological Survey of Northern Ireland, 1991). In the south east of Northern Ireland to the south west of Lough Erne, component 5 successfully differentiates the Carboniferous limestone and shale dominated Meenymore, Glencar Limestone, Dartry Limestone (inc Knockmore Member) and Benbulben Shale formations (which have negative scores) from the sandstone dominated Glenade Sandstone Formation (Mitchell, 2004).

The element loadings (Fig. 9) indicate that the Antrim Lava Group basalts are relatively enriched in nickel, chromium and sulphur, and that the Newry Igneous Complex is more enriched in sodium than the surrounding country rock.

5.6 Independent Component 6

Component 6 accounts for 4.7% of the variance in Northern Ireland's soil composition. The most striking feature on the map (Fig. 10) is the negative scoring Proterozoic Dalradian Supergroup of the Sperrin Mountains and the NE Antrim Inlier compared to the positive scoring basalts of the Antrim Plateau and the low positive scoring of Lower Carboniferous (red bed) sequences in the Rathlin, Newtownstewart and Omagh Basins (Fig. 24). Devonian and Carboniferous rocks of the Fintona Block are like the Dalradian Supergroup negative scoring. The element loadings (Fig. 10) suggest that the low scoring terranes are depleted in bismuth, copper and nickel, and enriched in rubidium, thorium and neodymium relative to their Carboniferous surroundings. It is an interesting point that a component which captures only 4.7% of the variance in the data may actually provide the most effective separation of terranes from different geological periods. Traditional geological mapping differentiates rocks according to criteria beyond chemical composition, but there is rarely a boundary between established units that is not also captured by some aspect of chemical composition.

5.7 Independent Component 7

Component 7 (Fig. 11) accounts for 3.5% of the variance in Northern Ireland's soil composition. Most notably, Component 7 reveals the low to negative scoring Newry Igneous Complex compared to its surrounding Ordovician-Silurian country rock of the Southern Uplands-Down-Longford terrane.

Within the latter, positive scoring north east – southwest trending packages of Moffat Shale Group rocks are apparent on tract boundaries and although they don't match well with the regional scale bedrock map (Geological Survey of Northern Ireland, 1997) they do correspond closely with recently published interpretations of the Tellus electromagnetic imagery (Beamish et al., 2010; Cooper et al., 2016b). Glacial transport of positive scoring Ordovician-Silurian bedrock detritus is also apparent along the north-northwest orientated Camlough and Newry Faults. Similar to Component 5, Component 7 in the southeast of Northern Ireland successfully differentiates Carboniferous sandstone, limestone and shale formations. Some diagonal striations are visible across Lough Neagh, these are artefacts in the geophysical survey data which have become apparent as the random forest algorithm is forced to use such minor subtleties of the data in order to model such minor components as this one.

The element loadings for Component 7 (Fig. 11) indicate that the central portion of the Newry Igneous Complex is relatively enriched in neodymium, and to a lesser extent copper, zinc and lead. In the terranes of the north west, the loadings would suggest a higher concentration of zirconium, potassium, and silicon in the Carboniferous compared to the Proterozoic.

5.8 Independent Component 8

Component 8 accounts for 2.6% of the variance in Northern Ireland's soil composition, and in terms of element loadings is characterised by relative depletion of manganese and enrichment of copper (Fig. 12). The map of Component 8 (Fig. 12) most notably highlights the positive scoring southwestern part of the Rathfriland Pluton of the Newry Igneous Complex (Cooper et al., 2016a), as well as contrasting between different fault blocks in the sedimentary terrains of the west and highlighting the dykes within them. The central part of the Slieve Gullion Complex is also apparent as a negative scoring area, which corresponds to granophyric rocks (felsic).

5.9 Beyond single components

While separating the geochemical composition of Northern Ireland into constituent independent components provides a solid framework from which to interpret geochemical variations, the best overall impression of Northern Ireland's geochemistry can be obtained by recombining the independent components in ternary colour images (i.e. with a different component representing each of the three channels of human vision; red, green and blue). With only three channels it is not possible to capture all of the geochemical variation at once, but, for whichever three components are chosen, ternary visualisation provides maximal conveyance of information to the viewer. For example, a ternary red-green-blue image of independent components six, three and five (Fig. 13) provides sufficient bedrock detail to reveal all of the features that are present in the geological map (Fig. 1) and more. As the image provides information in a continuous fully-quantitative manner, variation within units can be seen, which is something that a traditional classified map cannot provide, and is likely to be very useful to any geoenvironmental stakeholders.

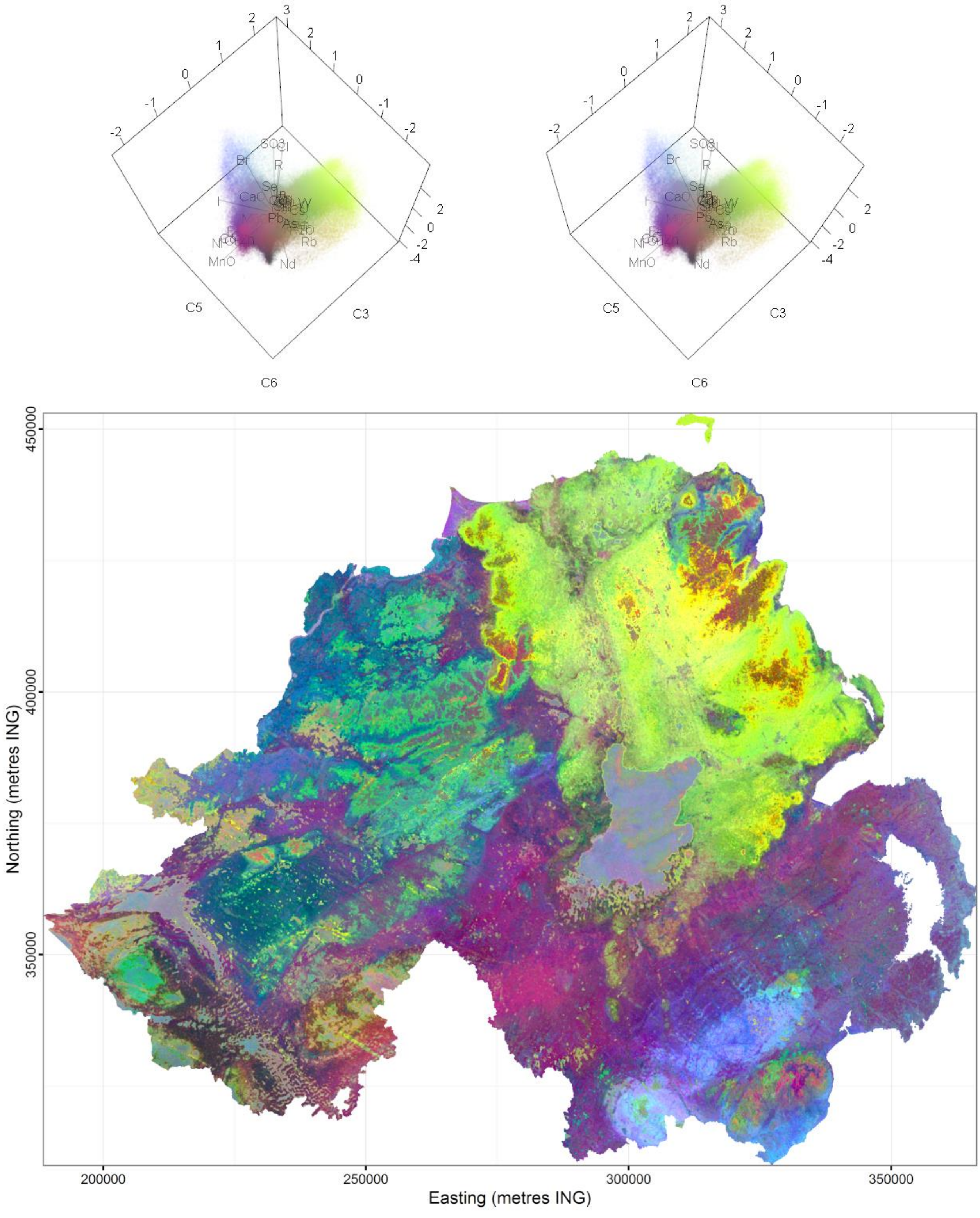

Fig. 13. Ternary red-green-blue map of independent components six, three and five, each quantile clipped within 0.1 and 99.9%. Above the map, two 3D triplots provide a legend for the meaning of the colours in terms of geochemical composition, this is best viewed in 3D by crossing the eyes. The components were selected for their abilities to differentiate bedrock. The appearance may be psychedelic, but in fact by revealing subtle variations in chemical composition the map captures all the features of the geological map (Fig. 1) and more, all in a fully-quantitative format.

6. Conclusion

Compositional FastICA was successful in unmixing the complex geochemistry of Northern Ireland into eight independent and interpretable components, each with distinct elemental loadings to differentiate separate aspects of Northern Ireland's geochemical composition. The use of random forest to map these components on the basis of their relationships with geophysical parameters has provided high-resolution maps of geochemical composition (with all but one more accurate than their IDW interpolated counterparts). By combining these machine learned geochemical component maps into full-colour ternary images, we are presented with a rich visualisation of the geochemical composition of Northern Ireland's soils, with both the chemical resolution of laboratory XRF analysis and the spatial resolution of high-resolution geophysics.

By translating geophysical survey data into chemical composition in this way, we are able to capture all of the features of a traditional geological map and more, with the significant benefit that the continuous fully-quantitative format reveals intra-unit variation and is derived from a transparent, reproducible, data-driven workflow. This approach would be particularly useful in reconnaissance mapping of unexplored terrains, as well as in providing quantitative evidence, consistent across the entire region, from which to update and unify legacy maps.

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References

Aitchison, J., 1986. The statistical analysis of compositional data. Chapman & Hall, London.

Anderson, T., 2004. Southern Uplands - Down Longford Terrane, in: Mitchell, W.I. (Ed.), The Geology of Northern Ireland: Our Natural Foundation, Second edition ed. Geological Survey of Northern Ireland, Belfast, pp. 41-60.

Beamish, D., 2013. Gamma ray attenuation in the soils of Northern Ireland, with special reference to peat. Journal of environmental radioactivity 115, 13-27.

Beamish, D., Kimbell, G., Stone, P., Anderson, T., 2010. Regional conductivity data used to reassess Early Palaeozoic structure in the Northern Ireland sector of the Southern Uplands–Down–Longford terrane. Journal of the Geological Society 167, 649-657.

Beamish, D., Young, M., 2009. Geophysics of Northern Ireland: the Tellus effect. First Break 27.

Breiman, L., 2001. Random forests. Machine learning 45, 5-32.

Carranza, E.J.M., Laborte, A.G., 2015. Random forest predictive modeling of mineral prospectivity with small number of prospects and data with missing values in Abra (Philippines). Computers & Geosciences 74, 60-70.

Chayes, F., 1960. On correlation between variables of constant sum. Journal of Geophysical research 65, 4185-4193.

Chew, D., Flowerdew, M., Page, L., Crowley, Q., Daly, J., Cooper, M., Whitehouse, M., 2008. The tectonothermal evolution and provenance of the Tyrone Central Inlier, Ireland: Grampian imbrication of an outboard Laurentian microcontinent? Journal of the Geological Society 165, 675-685.

Cooper, M., 2004. The geology of Northern Ireland: our natural foundation, Second edition ed. Geological Survey of Northern Ireland.

Cooper, M., Anderson, H., Walsh, J., Van Dam, C., Young, M., Earls, G., Walker, A., 2012. Palaeogene Alpine tectonics and Icelandic plume-related magmatism and deformation in Northern Ireland. Journal of the Geological Society 169, 29-36.

Cooper, M., Crowley, Q., Hollis, S., Noble, S., Roberts, S., Chew, D., Earls, G., Herrington, R., Merriman, R., 2011. Age constraints and geochemistry of the Ordovician Tyrone Igneous Complex, Northern Ireland: implications for the Grampian orogeny. Journal of the Geological Society 168, 837-850.

Cooper, M., Johnston, T., 2004a. Palaeogene intrusive igneous rocks, in: Mitchell, W.I. (Ed.), The Geology of Northern Ireland: Our Natural Foundation, Second edition ed. Geological Survey of Northern Ireland, Belfast, pp. 179-198.

Cooper, M.R., Anderson, P.C.D.J., Stevenson, C.T.E., Ellam, R.M., Meighan, I.G., Crowley, Q.G., 2016a. Shape and intrusion history of the Late Caledonian, Newry Igenous Complex, Northern Ireland, in: Young, M.E. (Ed.), Unearthed: impacts of the Tellus surveys of the north of Ireland. Royal Irish Academy.

Cooper, M.R., Floyd, J.D., Barker, G.J., Ture, M.D., Hodgson, J.A., McConnell, B.J., Warke, M.R., 2016b. The geological significance of electrical conductivity anomalies of the Ordovician-Silurian Moffat Shale Group, Northern Ireland., in: Young, M.E. (Ed.), Unearthed: impacts of the Tellus surveys of the north of Ireland. Royal Irish Academy.

Cooper, M.R., Johnston, T., 2004b. Central Highlands (Grampian) Terrane - Metamorphic Basement, in: Mitchell, W.I. (Ed.), The Geology of Northern Ireland: Our Natural Foundation, Second edition ed. Geological Survey of Northern Ireland, Belfast, pp. 9-24.

Cooper, M.R., Johnston, T., 2004c. Palaeogene extrusive igneous rocks, in: Mitchell, W.I. (Ed.), The Geology of Northern Ireland: Our Natural Foundation, Second edition ed. Geological Survey of Northern Ireland, Belfast, pp. 167-178.

Cracknell, M., Reading, A., McNeill, A., 2014. Mapping geology and volcanic-hosted massive sulfide alteration in the Hellyer–Mt Charter region, Tasmania, using Random Forests™ and Self-Organising Maps. Australian Journal of Earth Sciences 61, 287-304.

Cracknell, M.J., Reading, A.M., 2014. Geological mapping using remote sensing data: A comparison of five machine learning algorithms, their response to variations in the spatial distribution of training data and the use of explicit spatial information. Computers & Geosciences 63, 22-33.
Darnley, A.G., 1990. International geochemical mapping: a new global project. Journal of Geochemical Exploration 39, 1-13.
Delorme, A., Makeig, S., 2004. EEGLAB: an open source toolbox for analysis of single-trial EEG dynamics including independent component analysis. Journal of neuroscience methods 134, 9-21.
Dempster, M., Dunlop, P., Scheib, A., Cooper, M., 2013. Principal component analysis of the geochemistry of soil developed on till in Northern Ireland. Journal of Maps 9, 373-389.
Egozcue, J.J., Pawlowsky-Glahn, V., Mateu-Figueras, G., Barcelo-Vidal, C., 2003. Isometric logratio transformations for compositional data analysis. Mathematical Geology 35, 279-300.
Evans, J.S., Murphy, M.A., Holden, Z.A., Cushman, S.A., 2011. Modeling species distribution and change using random forest, Predictive Species and Habitat Modeling in Landscape Ecology. Springer, pp. 139-159.
Filzmoser, P., Hron, K., Reimann, C., 2009a. Principal component analysis for compositional data with outliers. Environmetrics 20, 621-632.
Filzmoser, P., Hron, K., Reimann, C., Garrett, R., 2009b. Robust factor analysis for compositional data. Computers & Geosciences 35, 1854-1861.
Garnier, S., 2015. viridis: Matplotlib Default Color Map. R package version 0.2.
Geological Survey of Northern Ireland, G., 1991. Geological Map of Northern Ireland (Quaternary). Geological Survey of Northern Ireland, Belfast.
Geological Survey of Northern Ireland, G., 1997. Geological Map of Northern Ireland (Solid). Geological Survey of Northern Ireland, Belfast.
Gislason, P.O., Benediktsson, J.A., Sveinsson, J.R., 2006. Random forests for land cover classification. Pattern Recognition Letters 27, 294-300.
Grunsky, E.C., Drew, L.J., Sutphin, D.M., 2009. Process recognition in multi-element soil and stream-sediment geochemical data. Applied Geochemistry 24, 1602-1616.
Harris, J., Grunsky, E., Behnia, P., Corrigan, D., 2015. Data-and knowledge-driven mineral prospectivity maps for Canada's North. Ore Geology Reviews.
Henderson, B.L., Bui, E.N., Moran, C.J., Simon, D., 2005. Australia-wide predictions of soil properties using decision trees. Geoderma 124, 383-398.
Hinze, W.J., Von Frese, R.R., Saad, A.H., 2013. Gravity and magnetic exploration: Principles, practices, and applications. Cambridge University Press.
Hodgson, J., Young, M., 2016. The Tellus airborne geophysical data and results, in: Young, M. (Ed.), Unearthed: impacts of the Tellus surveys of the north of Ireland. Royal Irish Academy, Dublin.
Hollis, S.P., Cooper, M.R., Roberts, S., Earls, G., Herrington, R., Condon, D.J., 2013. Stratigraphic, geochemical and U–Pb zircon constraints from Slieve Gallion, Northern Ireland: a correlation of the Irish Caledonian arcs. Journal of the Geological Society 170, 737-752.
Hollis, S.P., Roberts, S., Cooper, M.R., Earls, G., Herrington, R., Condon, D.J., Cooper, M.J., Archibald, S.M., Piercey, S.J., 2012. Episodic arc-ophiolite emplacement and the growth of continental margins: Late accretion in the Northern Irish sector of the Grampian-Taconic orogeny. Geological Society of America Bulletin 124, 1702-1723.
Hyvarinen, A., 1999. Fast and robust fixed-point algorithms for independent component analysis. IEEE transactions on Neural Networks 10, 626-634.
Hyvärinen, A., Oja, E., 2000. Independent component analysis: algorithms and applications. Neural networks 13, 411-430.
Johnson, C., Breward, N., Ander, E., Ault, L., 2005. G-BASE: baseline geochemical mapping of Great Britain and Northern Ireland. Geochemistry: Exploration, Environment, Analysis 5, 347-357.
Kirkwood, C., Cave, M., Beamish, D., Grebby, S., Ferreira, A., 2016a. A machine learning approach to geochemical mapping. Journal of Geochemical Exploration 167, 49-61.

Kirkwood, C., Everett, P., Ferreira, A., Lister, B., 2016b. Stream sediment geochemistry as a tool for enhancing geological understanding: An overview of new data from south west England. Journal of Geochemical Exploration 163, 28-40.

Lawrence, R.L., Wood, S.D., Sheley, R.L., 2006. Mapping invasive plants using hyperspectral imagery and Breiman Cutler classifications (RandomForest). Remote Sensing of Environment 100, 356-362.

Liu, B., Guo, S., Wei, Y., Zhan, Z., 2014. A Fast Independent Component Analysis Algorithm for Geochemical Anomaly Detection and Its Application to Soil Geochemistry Data Processing. Journal of Applied Mathematics 2014.

Makeig, S., Bell, A.J., Jung, T.-P., Sejnowski, T.J., 1996. Independent component analysis of electroencephalographic data. Advances in neural information processing systems, 145-151.

McKinley, J.M., Hron, K., Grunsky, E.C., Reimann, C., de Caritat, P., Filzmoser, P., van den Boogaart, K.G., Tolosana-Delgado, R., 2016. The single component geochemical map: Fact or fiction? Journal of Geochemical Exploration 162, 16-28.

Mitchell, W.I., 2004. Carboniferous, in: Mitchell, W.I. (Ed.), The Geology of Northern Ireland: Our Natural Foundation, Second edition ed. Geological Survey of Northern Ireland, Belfast, pp. 79-116.

Pawlowsky-Glahn, V., Egozcue, J., 2006. Compositional data and their analysis: an introduction. Geological Society, London, Special Publications 264, 1-10.

Pawlowsky-Glahn, V., Egozcue, J.J., Tolosana Delgado, R., 2007. Lecture notes on compositional data analysis.

Pearson, K., 1896. Mathematical Contributions to the Theory of Evolution.--On a Form of Spurious Correlation Which May Arise When Indices Are Used in the Measurement of Organs. Proceedings of the royal society of london 60, 489-498.

R Core Team, 2016. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria.

Rodriguez-Galiano, V., Sanchez-Castillo, M., Chica-Olmo, M., Chica-Rivas, M., 2015. Machine learning predictive models for mineral prospectivity: An evaluation of neural networks, random forest, regression trees and support vector machines. Ore Geology Reviews.

Rodriguez-Galiano, V.F., Ghimire, B., Rogan, J., Chica-Olmo, M., Rigol-Sanchez, J.P., 2012. An assessment of the effectiveness of a random forest classifier for land-cover classification. ISPRS Journal of Photogrammetry and Remote Sensing 67, 93-104.

Seligman, M., 2016. Rborist: Extensible, Parallelizable Implementation of the Random Forest, R package version 0.1-1 ed.

Wiesmeier, M., Barthold, F., Blank, B., Kögel-Knabner, I., 2011. Digital mapping of soil organic matter stocks using Random Forest modeling in a semi-arid steppe ecosystem. Plant and soil 340, 7-24.

Yang, J., Cheng, Q., 2015. A comparative study of independent component analysis with principal component analysis in geological objects identification, Part I: Simulations. Journal of Geochemical Exploration 149, 127-135.

Young, M., Donald, A., 2013. A guide to the Tellus data. Geological Survey of Northern Ireland, Belfast.