



Uncovering which elements drive timber and soybean traceability models

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Abstract. Independent verification of commodity origin is increasingly needed to support deforestation-free and legality-based supply-chain regulation. Multi-element chemical fingerprints are a promising tool for this purpose as plant and wood chemistry integrates information about soil conditions, which carries a spatially distinct signal. However, machine-learning provenance models are often difficult to scrutinize and interpret. The goal of this work is to evaluate whether elemental fingerprints can predict geographic harvest location and produce interpretable and environmentally plausible evidence for commodity tracing. Its novelty lies in combining continuous coordinate prediction with multiple explainable-machine-learning tools to compare predictive performance, robust feature importance, local explanations and reduced element panels across both soybean and timber. The source data comprised 398 soybean (*Glycine max*) samples from Argentina, Bolivia, Brazil and Paraguay, and 1253 East-European and West-Asian timber samples from *Betula*, *Fagus*, *Pinus* and *Quercus*. We trained Random Forest, XGBoost and support-vector regression models to predict longitude and latitude and evaluated the models with a Haversine skill score (HSS) relative to a centroid baseline. Feature importance was assessed with permutation importance, conditional permutation importance, SHapley Additive exPlanations (SHAP) values and cumulative feature-addition analyses. Soybean models achieved the strongest coordinate-prediction performance (mean HSS 0.596–0.628), while timber genera showed lower but consistently positive skill scores. Attribution analyses identified relatively small element suites: soybean predictions were driven mainly by Co, Ba, Cu, Mg, Ni, Se, Ca and Cs. Timber markers were genus-specific, with Sr, Pb and Fe being ranked the highest for *Betula*; Cl, Fe and Bi for *Fagus*; Rb, Br and Zn for *Pinus*; and Fe, Sr and Ni for *Quercus*. The results show that explainable machine learning can provide a more transparent and auditable basis for elemental-based commodity-origin prediction.

Keywords. commodity traceability, deforestation-free supply chains, elemental fingerprinting, explainable machine learning, soybean, timber



1 Introduction

Global trade in forest-risk commodities creates a persistent verification problem as documentary records may be incomplete or erroneous, supply chains may obscure provenance and origin declarations may be falsified (Fripp et al., 2023; Mortier et al., 2024; Maor et al., 2026). Timber and soy are especially relevant because both are associated with high-value international trade and with land-use pressures in regions where deforestation, illegal harvesting and supply-chain mixing are difficult to monitor solely through paperwork (Fripp et al., 2023). Together, legality requirements, sanctions on restricted timber flows and deforestation-free supply-chain rules, including the European Deforestation Regulation, increase the need for independent tools capable of testing whether a declared origin is compatible with the material itself (European Parliament and Council of the European Union, 2023). Scientific origin verification is not intended to replace documentary traceability, but to provide an independent line of evidence when supply chains are opaque or high risk.

Intrinsic material-based tracing methods exploit properties that are embedded in the commodity during growth. For timber, these include DNA markers, stable isotopes, near-infrared or other spectroscopic fingerprints and elemental composition (Deguilloux et al., 2004; Hung et al., 2017; Mortier et al., 2024; Boeschoten et al., 2025). For agricultural commodities such as soybean, elemental and isotope fingerprints have similarly been used to distinguish countries, biomes or production regions (Zhou et al., 2023; Maor et al., 2026; Soni et al., 2026). Elemental analysis is an attractive tool because elemental profiles can be generated at relatively high throughput. At the same time, many measured elements reflect spatially structured environmental processes. Soil parent material, weathering, pH, hydrology, atmospheric deposition, fertiliser use and anthropogenic contamination can all leave chemical signatures in plant tissues such as seeds and wood (Galán et al., 2008; Alloway, 2013; Liu et al., 2021). However, these signatures are not simple maps of soil chemistry. Species physiology, tissue type, element mobility, and analytical constraints filter them, producing high-dimensional, correlated datasets.

Early origin studies often used univariate comparison or classical multivariate discrimination to identify elements that differed between regions (Krivan et al., 1993). More recent work has increasingly used machine learning because provenance data are heterogeneous and can exhibit nonlinear patterns between measurements and geographic origin location (Mortier et al., 2024; Soni et al., 2026). Tree-based ensemble models such as Random Forest and gradient boosting can represent interactions and non-monotonic responses, while kernel-based support-vector machines can model complex decision surfaces (Menze et al., 2011; Chen and Guestrin, 2016). In commodity tracing, these architectures have mainly been applied to classification among predefined origins. Continuous coordinate prediction remains less common, and recent timber and soybean applications have instead used probabilistic Gaussian-process models (Mortier et al., 2024; Maor et al., 2026). This leaves an open question as to how established Random Forest, XGBoost and support-vector architectures perform when adapted directly to coordinate regression.

Predictive performance alone is insufficient when provenance estimates may support regulatory or environmental decisions. Analysts must also understand which chemical signals drive a prediction, whether conclusions remain stable across models and whether the identified signals are environmentally and biologically plausible. This is particularly important for legal and governmental uses of algorithmic outputs, where opacity can undermine accountability (Janssen et al., 2022). Explainable-



machine-learning methods provide complementary global and sample-level views of model behaviour and can reveal both robust signals and model-specific dependencies (Lundberg and Lee, 2017; Molnar et al., 2020). Furthermore, key explanatory variables could be used to further develop more targeted downstream traceability tools.

The goal of this work is to determine whether multi-element fingerprints can support interpretable geographic harvest location prediction for soybean and timber, two commodities with direct relevance to deforestation-risk supply chains. The novelty is methodological and applied: instead of choosing a black box classifier, we combine continuous coordinate regression with (conditional) permutation-based feature importance, SHAP-based spatial explanations and feature-set reduction to identify which elemental signals are predictive, robust and environmentally interpretable. The analysis focuses on supervised coordinate-regression models and their interpretation, rather than country-level or province-level classification models. Specifically, we ask whether elemental profiles contain enough spatial signal to predict sample coordinates, how consistent or model-dependent feature-importance conclusions are across architectures and attribution methods, whether a subset of the full feature sets can retain most predictive skill, and how feature-attribution methods can make commodity tracing models more transparent for environmental applications.

2 Material and methods

2.1 Multi-element commodity datasets

The analysis used coordinate-referenced multi-element datasets for soybean and timber. Samples were collected from the field following World Forest ID protocols (learn.worldforestid.org/). The soybean dataset contained 398 *Glycine max* samples from Argentina (38), Bolivia (25), Brazil (245) and Paraguay (90). Samples were collected during the February–June 2022 harvest period by pooling beans from two to five plants at each location (Maor et al., 2026). Additional samples were collected and analysed between July 2023 and June 2025 following the same methodology. Element concentrations were measured in mg kg⁻¹ using collision-cell inductively coupled plasma mass spectrometry (ICP-MS). Elements for which more than 40% of measurements were below the detection limit were excluded. The final 32-element soy panel comprised B, Mg, Al, Si, P, S, K, Ca, Ti, Mn, Fe, Co, Ni, Cu, Zn, As, Se, Rb, Sr, Y, Mo, Pd, Cd, Cs, Ba, La, Ce, Pr, Nd, Eu, Gd and Dy. For a full description of field and analysis methodology, we refer to Maor et al. (2026).

The timber analyses included 1253 samples from the four principal genera: *Betula* (387), *Fagus* (366), *Pinus* (209) and *Quercus* (291). Samples originated mainly from Eastern Europe, with additional West-Asian material, and were collected between June and December 2022 following standardised World Forest ID protocols (Mortier et al., 2024). Additional samples were collected and analysed between January 2023 and December 2025 following the same methodology. Pith-to-bark wood was ball-milled, oven dried and analysed using a SPECTRO XEPOS X-ray fluorescence (XRF) instrument. Elemental intensities were normalised to a Compton scatter region. For a full description of field and analysis methodology, we refer to Mortier et al. (2024).

Timber filtering comprised the removal of duplicate or unusable records, sparsely represented geographic outliers and one extreme analytical outlier, together with elements affected by extensive missingness or reliability concerns. The final 23-

element timber panel comprised P, S, Cl, K, Ca, Mn, Fe, Ni, Cu, Zn, Br, Rb, Sr, Ba, Pb, Ga, Y, Zr, Nb, Mo, Bi, Th and U for all genera.

- 90 Figures 1 and 2 show the geographic coverage of the soybean and timber datasets, respectively. Coordinates were randomly jittered in these maps to protect location confidentiality and collector privacy. The soybean dataset covers a broad region of South America, spanning from the equator down to 35°S latitude (encompassing Brazil, Paraguay, Uruguay, and northern Argentina) and from 65°W to 40°W longitude. Across this area, one degree of latitude consistently represents about 111 km, while one degree of longitude narrows from 111.1 km at the equator to approximately 91 km at the dataset's southern edge. The
- 95 timber samples span Europe and western Russia, mapped on axes where one degree of latitude corresponds to approximately 111 km (ranging from 110.6 km in southern Europe to 111.7 km in the north), and one degree of longitude narrows from roughly 91 km in the south to 36 km in the far north. The distributions are spatially uneven, particularly within the genus-specific timber datasets, which is relevant when interpreting coordinate-prediction performance and spatial validation: *Betula* ranges widely from eastern Scandinavia and Central Europe into western Russia and Kazakhstan, *Fagus* remains tightly concentrated in
- 100 Germany, the Balkans, and southeastern Europe, *Quercus* spans broadly across Poland, and Eastern Europe, and *Pinus* is heavily clustered around central eastern Europe, eastern Scandinavia, the Baltics, and has samples in northwestern Russia.

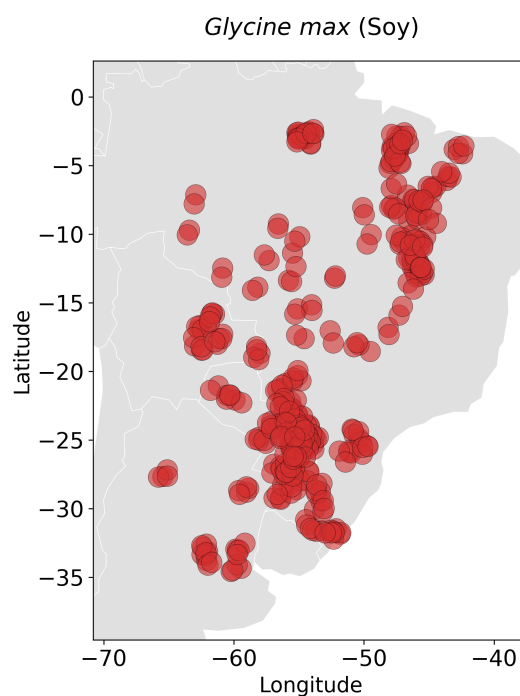


Figure 1. Geographic distribution of the soybean samples from Argentina, Bolivia, Brazil and Paraguay used for coordinate prediction.

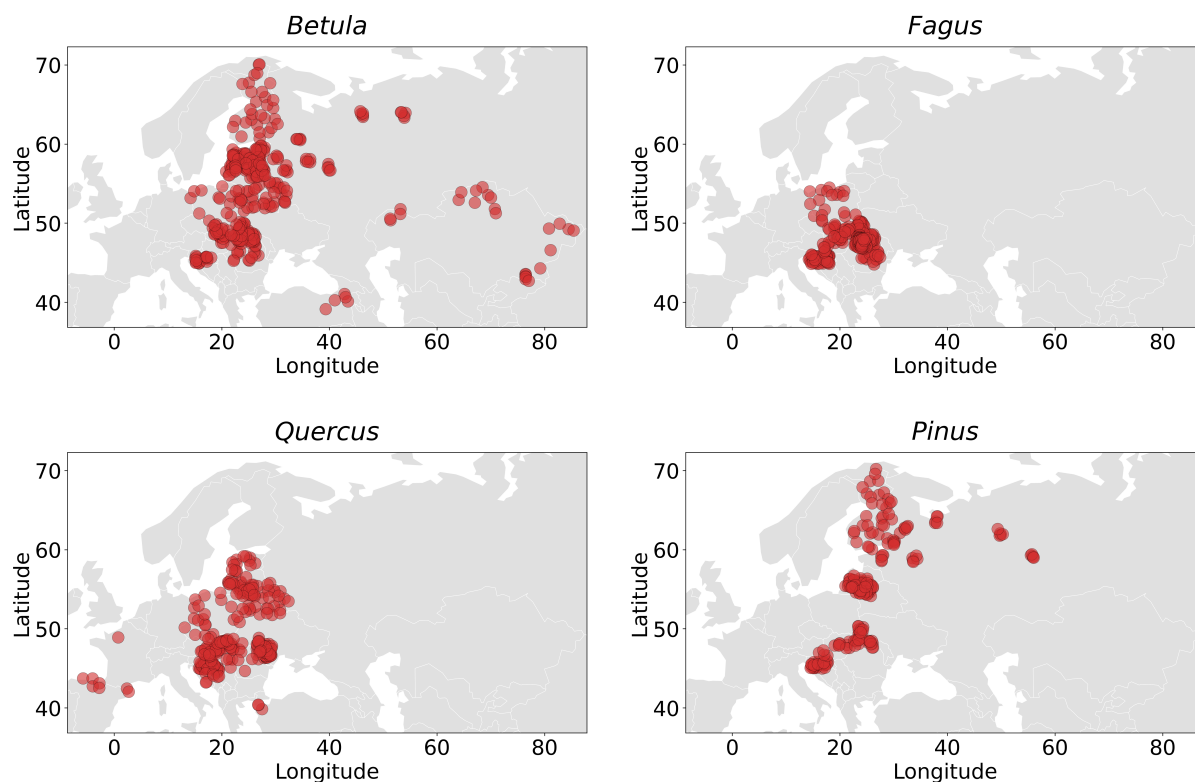


Figure 2. Geographic distribution of the timber samples for the four genera included in the genus-specific coordinate-prediction analyses.

2.2 Data preprocessing

The preprocessing workflow was designed to make elemental variables comparable while retaining the information needed for model interpretation. All corresponding code is publicly accessible in the associated repository. Unusable rows and variables were filtered as described above. Missing timber values and left-censored soybean measurements were imputed before cross-validation using multiple imputation by chained equations with predictive mean matching (van Buuren and Groothuis-Oudshoorn, 2011). Five imputations were generated and averaged. Soybean imputations were additionally constrained to the interval between zero and the element-specific detection limit using a truncated normal distribution, whereas timber missing values used unconstrained predictive-mean-matching estimates. None of the variables appearing in the reported top-ten importance rankings required imputation; the possible influence of pre-cross-validation imputation is therefore expected to be concentrated among lower-ranked variables.

Chemical concentrations (ICP-MS) and normalised intensities (XRF) were natural-log transformed to reduce right-skewness and the influence of extreme values. Features were then standardised to make variables measured on different scales comparable, especially for the distance-based SVM model. This standardisation was performed within each cross-validation split to



115 prevent data leakage: means and standard deviations were fitted on the training subset and then applied to the corresponding validation and test subset.

2.3 Coordinate prediction models

Geographic harvest location was formulated as a supervised multi-output regression problem in which the longitude and latitude of each sample formed the response vector and its elemental profile formed the predictor set. Random Forest regression provided a bagged tree ensemble capable of representing nonlinearities and interactive effects while reducing variance through aggregation (Breiman, 2001). XGBoost used sequentially fitted gradient-boosted trees to capture complex predictor structure by iteratively minimising a squared-error objective (Chen and Guestrin, 2016). Support-vector regression provided a kernel-based alternative that can model smooth nonlinear relationships in high-dimensional feature spaces (Steinwart, 2002). Support-vector regression was implemented through a multi-output wrapper that fitted separate epsilon-insensitive models for longitude and latitude. Comparing these distinct learning strategies also allowed us to assess whether predictive performance and feature-attribution patterns were consistent across model architectures.

The modelling was performed separately for soybean and for each of the four timber genera. Analysing the timber genera separately was scientifically more informative than fitting a single pooled timber model, as our preliminary analyses showed that genus is a top-ranked feature based on the permutation importance, and previous timber-tracing studies indicate that the elements carrying geographic information can differ among genera (Mortier et al., 2024; Aguzzoni et al., 2025). These differences could reflect genus-specific element uptake, internal transport and storage, and interactions between plant physiology and locally available elements (Salt et al., 2008; Liu et al., 2021). The genus-specific design therefore allowed the models and their explanations to characterise within-genus geographic fingerprints directly, without assuming that the same elemental relationships apply across taxonomically distinct groups.

135 Hyperparameter selection and performance evaluation were conducted in two separate geographically stratified cross-validation procedures. First, a randomised search used internal cross-validation to select one hyperparameter configuration for each dataset–model combination, with geographic clusters recalculated within the training data supplied to the tuning procedure. The selected hyperparameters were then saved and held fixed for a separate five-fold performance evaluation and for all subsequent feature-importance, SHAP and cumulative feature-addition analyses. Standardisation was handled within modelling pipelines in every split. Complete hyperparameter search ranges, selected values and random seeds are available in the accompanying analysis repository.

For both procedures, k-means clustering of the observed coordinates defined geographic zones, and stratified fold assignment distributed those zones proportionally across the folds. This design reduced regional imbalance while retaining broad geographic coverage in every training and validation split; it did not enforce geographic separation between training and test samples. During hyperparameter tuning, a single global centroid was used as a fixed HSS reference across candidate settings. As this reference was used only to rank tuning configurations, it did not enter the final performance estimates. During performance evaluation, the centroid baseline was recalculated using only the training coordinates of each fold.



Predictive accuracy was evaluated using the Haversine distance between observed and predicted coordinates and a Haversine skill score (HSS). Haversine distance measures great-circle geographic error in kilometres and is a standard geodetic way to quantify distance between latitude–longitude pairs on a spherical Earth approximation (Sünkel, 1983). The HSS follows the general logic of skill scores, which express predictive improvement relative to a reference or naive forecast (Murphy, 1988), using the geographic centroid of the training data as the baseline:

$$\text{HSS} = 1 - \frac{E_{\text{model}}}{E_{\text{baseline}}}, \quad (1)$$

where E_{model} is the mean Haversine error of the fitted model and E_{baseline} is the mean error obtained by predicting the training-set spatial centroid. HSS = 1 indicates perfect coordinate prediction, HSS = 0 indicates no improvement over the centroid baseline and negative values indicate worse-than-baseline performance.

2.4 Feature importance and interpretability

Feature importance was first assessed using permutation importance (PI). For each trained model, we randomly permuted each feature in the validation data and recorded the decrease in HSS. Importance scores were averaged over $R = 10$ repetitions and across geographically stratified folds, with larger decreases indicating stronger model reliance on a feature for geographic prediction. However, elemental variables are often correlated because they reflect shared geochemical processes and physiological regulation (Grunsky and Caritat, 2020; Salt et al., 2008). Standard permutation can therefore create unrealistic combinations of elements and inflate the importance of correlated variables (Strobl et al., 2008; Liu et al., 2021). Conditional permutation importance (CPI) was consequently also applied. For each target feature, a Ridge regression model was fitted on the training data to predict that feature from all remaining predictors. On the validation data, residuals between the observed and Ridge-predicted feature values were permuted ten times and added back to the conditional predictions. This procedure preserves part of the multivariate dependence structure and estimates the predictive contribution not explained by correlated variables. Ridge regression was selected as the conditional model after comparison with a shallow Random Forest because it produced more accurate feature predictions and less structured residuals. To compare rankings across models and importance definitions, the PI and CPI ranks were summarised as interval plots, with consensus order based on the median of the model-specific ranks averaged across PI and CPI 3, 4. For each variable, three horizontal intervals represent Random Forest, XGBoost and support-vector regression, and their endpoints indicate the ranks obtained with PI and CPI. Short intervals at similar positions indicate stable importance across permutation methods and model architectures, whereas long intervals indicate sensitivity to the permutation method, potentially reflecting dependence on correlated predictors.

A SHAP analysis was used to examine local feature-model interactions using the saved tuned hyperparameters. TreeSHAP was used for Random Forest and XGBoost, with 100 randomly sampled observations as the background dataset. KernelSHAP was used for support-vector regression, with the background distribution summarised by $k = 50$ k-means centroids to reduce computation time. For computational tractability and to describe the final fitted models, SHAP extraction was performed after fitting each model to the complete corresponding dataset rather than within the performance-evaluation folds. SHAP values were computed separately for longitude and latitude. Beeswarm plots summarised the distribution and direction of



latitude effects, while longitude and latitude attributions were combined in a visualisation termed a “SHAP vector map”. Each vector originates at the true sample location and indicates the direction and magnitude by which a feature shifts the predicted coordinate relative to the model baseline.

Finally, separate cumulative feature-addition (CFA) trajectories were constructed based on the PI and CPI rankings. Each ranking was calculated once and held fixed while features were added sequentially; importance was not recalculated after each addition. Every subset was evaluated through geographically stratified cross-validation using the previously selected hyperparameters and compared with the full-panel HSS. Shaded intervals in the figures 7 show variation across folds. The analysis therefore evaluates performance along a predefined importance ordering rather than searching for an independently optimal subset at every panel size. Ideally, a nested cross-validation procedure in which feature rankings are recomputed at each iteration would be used to account for the dependence of the rankings on the selected feature set.

3 Results and discussion

3.1 Spatial prediction performance

All three models (RF, XGB, SVM) extracted geographic signal from the soybean elemental profiles and outperformed the baseline prediction that assigns every validation sample to the geographic centroid of the corresponding training set. Soybean showed the strongest predictive performance among the analysed datasets, while the limited differences among model architectures suggest that its spatially structured chemical signal is robust to the choice of learning algorithm. Timber coordinate prediction was weaker than soybean prediction but remained better than the centroid baseline for every genus. This difference may partly reflect the smaller and more spatially patchy genus-specific datasets, while the models did not incorporate prior constraints on the geographic ranges of the genera. Geographic information in timber elemental profiles may also be more diffuse across correlated features or more strongly moderated by biological and local environmental variation. Nevertheless, the consistently positive skill indicates that normalised XRF profiles contain meaningful geographic information across taxonomically distinct timber groups.

The HSS results for every dataset are summarised in Table 1. The table reports the mean and standard deviation across the three model-level mean HSS values. Full model-specific summaries, including Haversine distance errors and variation across evaluation folds, are provided in Appendix A. Looking at the per-model performance for each dataset, we can conclude that no model is clearly better.

Figure B1 in Appendix B shows the spatial behaviour of the XGBoost soybean model across the five evaluation folds. The grey error vectors reveal a characteristic regression-to-the-mean pattern: samples near the edge of the sampling domain are often pulled inward toward more densely represented regions. This inward bias is consistent with the broader difficulty of regression models in predicting sparsely represented extreme response values when model fitting is dominated by more frequent central values (Ribeiro and Moniz, 2020). It means that HSS should not be interpreted as a guarantee of precise farm-level assignment; rather, it indicates improvement over a naive spatial baseline. Other model-dataset spatial behaviour plots are not shown as they show similar behaviour to the XGBoost-soybean figure.



Table 1. Coordinate-prediction performance for all analysed datasets. Values are the mean and standard deviation across the three model-level mean Haversine skill scores (HSS) and Haversine distances (km) obtained with Random Forest, XGBoost and support-vector regression. The standard deviation therefore describes between-model variation rather than variation across cross-validation folds.

Dataset	Three-model mean HSS	HSS standard deviation	Three-model mean distance (km)	Distance standard deviation (km)
Soybean	0.6119	0.0162	421.0144	17.5933
<i>Pinus</i>	0.4760	0.0142	388.1029	10.4444
<i>Betula</i>	0.4132	0.0354	504.3196	30.4044
<i>Quercus</i>	0.3844	0.0155	325.6389	8.2358
<i>Fagus</i>	0.3208	0.0237	179.3803	6.2309

A key limitation of the performance evaluation is that it does not explicitly account for spatial autocorrelation. The folds were geographically stratified so that each training set spanned the sampled domain, but the procedure did not enforce spatial separation between training and test observations. Nearby observations may therefore share environmental conditions, potentially producing optimistic performance estimates compared with stricter spatial-block or leave-region-out validation. Accordingly, the results should be interpreted as evidence that the models learned non-random geochemical structure rather than as final estimates of operational accuracy for regulatory deployment.

3.2 Soybean feature importance

The soybean feature-importance summary (Figure 3) shows a clear leading group of variables. Co, Ba, Mg, Se, Ni, Cu, Cs and Ca are consistently ranked near the top, although the exact order differs by model and by whether PI or CPI is used. A notable model-specific contrast is the reversal between Co and Cu: Co ranks more highly in Random Forest and XGBoost, whereas Cu ranks more highly in support-vector regression. The supplementary SHAP vector maps (Appendix Figure B4) suggest that this difference reflects how the architectures use spatial structure. Co separates the sampled domain into relatively distinct regions that can be represented efficiently by recursive tree splits, whereas Cu exhibits a smoother spatial gradient that is captured more strongly by the kernel-based support-vector model (Chen and Guestrin, 2016; Cortes and Vapnik, 1995). Disagreement among attribution results is therefore not necessarily statistical noise; it can reveal how different algorithms use the same geochemical information. The strongest variables have relatively compact intervals, indicating that their importance is not an artifact of a single model architecture or permutation definition. Lower-ranked variables have wider intervals and stronger disagreement, meaning that they contribute less uniquely and are more easily exchanged with correlated variables.

The leading soybean elements are environmentally plausible as provenance markers. The soil availability and plant uptake of trace metals such as Co, Ni and Cu are influenced by geological setting and soil properties, including pH and redox conditions (Galán et al., 2008; Alloway, 2013; Liu et al., 2021). Ca and Mg are major soil cations associated with mineralogy and agricultural management, while liming can alter nutrient availability in soybean production systems (Galán et al., 2008; Moreira et al., 2017). The distributions of Ba and Cs in soils and plants are likewise shaped by environmental and geochemical processes, making them plausible spatial markers (Sharma et al., 2025; Cook et al., 2007). Several of the elements here, including Ni,

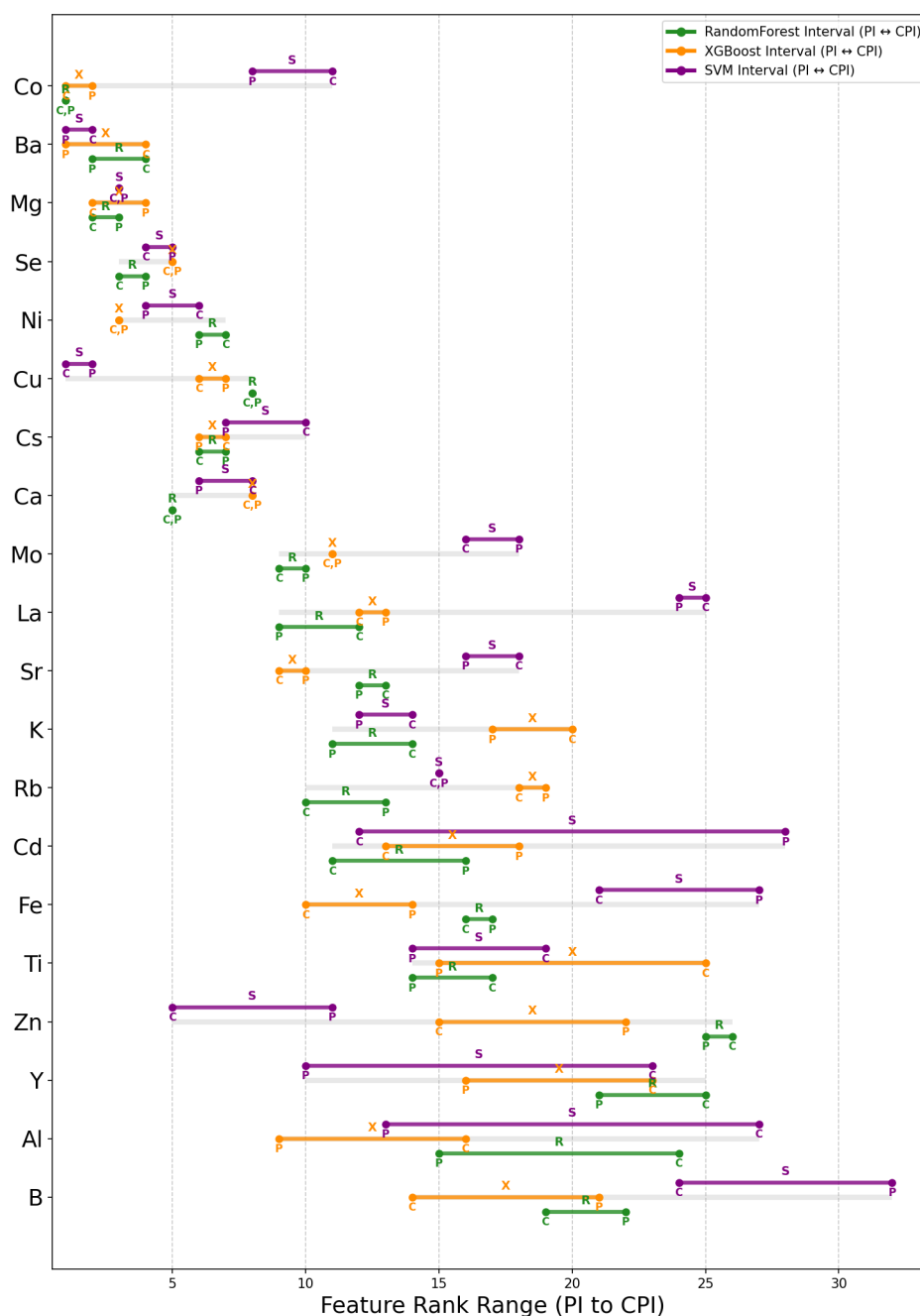


Figure 3. Summary of soybean feature-importance rankings across Random Forest, XGBoost and support-vector regression using classical permutation importance and conditional permutation importance. Each feature has three horizontal bars corresponding to the three models; bar endpoints indicate rankings under PI and CPI.

Ba, Co, Se and Ca, have also previously been reported as useful soybean-origin discriminators (Aparicio-Muriana et al., 2025; Maor et al., 2026; Soni et al., 2026; Zhou et al., 2023). The fact that CPI retains many of the same leading features strengthens confidence that the model is not only exploiting redundant correlations.

3.3 Timber feature importance is genus-specific

The combined rankings reveal both a shared elemental core and pronounced differences among timber genera. Table 2 provides a compact presence-absence comparison of the top-five sets: Fe is the only element shared by all four genera, Rb recurs in three, and the remaining markers are restricted to one or two genera. Figure 4 complements this overview by showing the within-genus ordering of the top elements and the extent to which their ranks vary across model architectures and permutation methods. *Betula*, *Fagus* and *Quercus* have a robust top 3, showing agreement between the models and PI metrics, whereas the *Pinus* figure shows there's no clear consensus across the three models.

Table 2. Presence of elements among the top five aggregated PI and CPI rankings for each timber genus across Random Forest, XGBoost and support-vector regression. A dot indicates that an element occurs in the genus-specific top-five set.

Genus	Fe	Rb	Br	Cl	Sr	Zn	Bi	Cu	Mn	Ni	Pb	S
<i>Betula</i>	•	•			•				•		•	
<i>Fagus</i>	•		•	•			•					•
<i>Pinus</i>	•	•	•	•		•						
<i>Quercus</i>	•	•			•			•		•		

Several conclusions follow from Figure 4. First, genus-specific modelling is justified, as each genus has its own unique fingerprint panel. The dominant markers for *Pinus* differ from those for the hardwood genera, suggesting that gymnosperm and angiosperm timber do not translate environmental chemistry into wood chemistry in the same way. Second, some elements recur across genera. Fe and Rb form a broad baseline of useful timber markers, consistent with previous timber-tracing work in which elements such as Fe, Rb, Cl, Ca, Pb, Si, Sr and Zn contributed to spatial prediction in similar genera (Mortier et al., 2024). Third, most key timber markers have either anthropogenic or geogenic origins. Sr is widely interpretable as a marker of bedrock and soil mineralogy (Dubchak, 2018), while Fe availability is controlled by soil pH and redox processes and can therefore encode local edaphic conditions (Morrissey and Guerinot, 2009). Pb, important especially in hardwoods and a top marker of *Betula*, may capture historical pollution or industrial deposition, consistent with known spatial variability of heavy metals in agricultural and forest environments (Tóth et al., 2016).

3.4 SHAP analysis

The permutation-based rankings were complemented by SHAP beeswarm plots, which show both the relative importance of each feature and the direction in which high or low feature values shift model predictions. Figure 5 was constructed to contrast

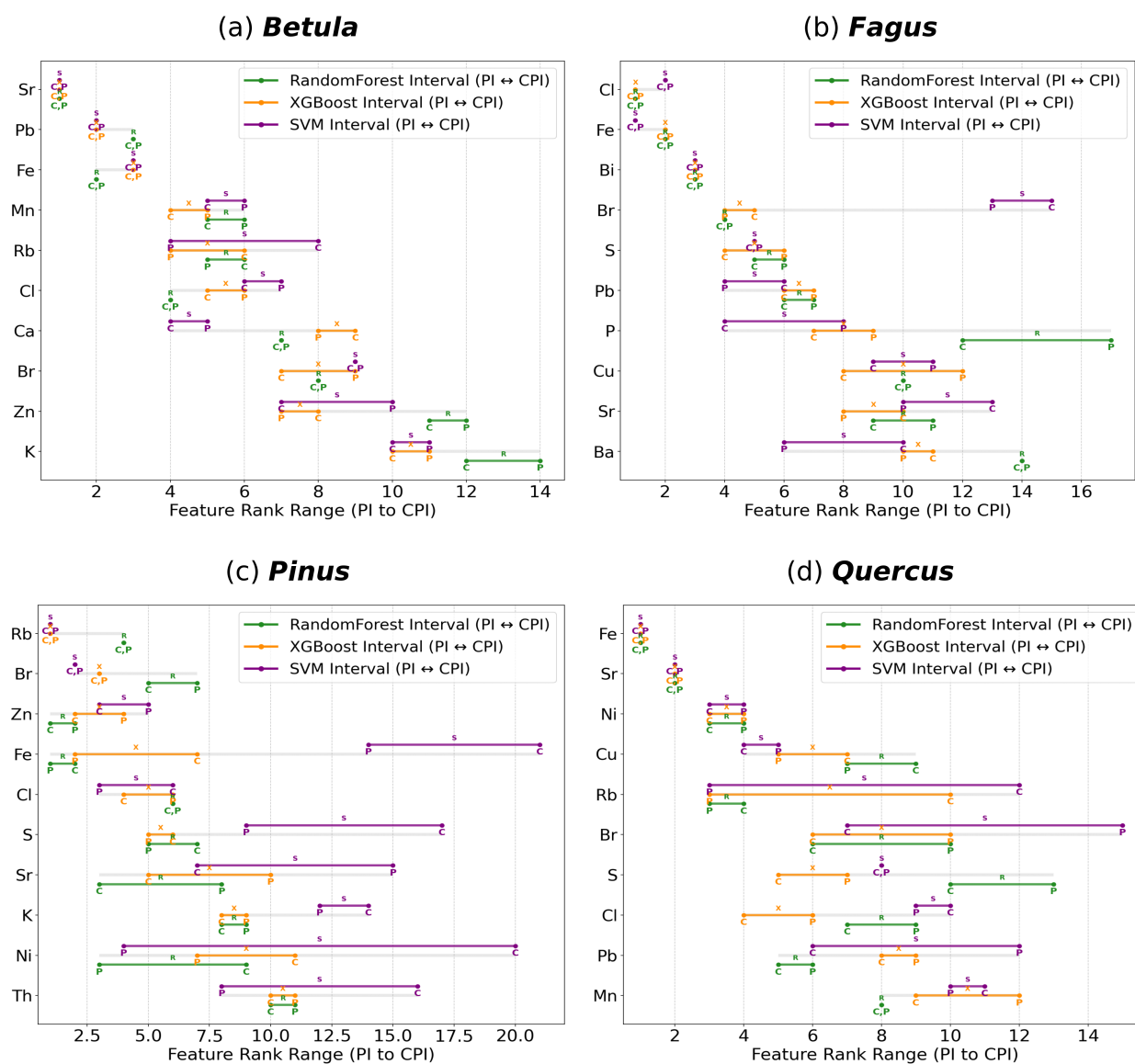


Figure 4. Top-ten timber feature-importance rankings across Random Forest, XGBoost and support-vector regression using classical and conditional permutation importance.



a tree ensemble with a kernel-based model, using XGBoost and support-vector regression, respectively. Soybean and *Pinus* were shown because they had the strongest predictive performance within the agricultural and timber datasets, while latitude provides the widest spatial axis for the soybean domain and a common north–south axis for comparing feature effects. For soybean, Ba, Mg and Se appear among the most influential variables in both models, supporting the conclusion that these elements encode robust north–south geographic information. For *Pinus*, Rb, Br and Zn recur across both models, although their ordering and the other leading variables differ. The plots also show that model architecture affects how the same chemical signal is used. XGBoost produces more clustered SHAP patterns, consistent with tree-based splitting into discrete regions of feature space, whereas the support-vector model produces smoother and more continuous SHAP spreads. The corresponding latitude beeswarm plots for *Betula*, *Fagus* and *Quercus* under these two models are available in the supplementary figures (Appendix Figure B2).

Figure 6 gives a spatially explicit example of how a single feature can affect individual coordinate predictions. In the Random Forest soybean model, high Se values in the northern part of the sampling domain support northward predictions, whereas low-Se samples in central Brazil are pulled southward, illustrating that an important feature can improve model structure overall while still contributing locally misleading spatial pushes for some samples.

The supplementary soybean SHAP vector maps provide further insight into agreement and disagreement among models (Appendix Figure B4). Ba produces substantial spatial contributions in all three architectures, consistent with its high global importance. By contrast, the Co concentration pattern is divided into relatively distinct geographic regions and is used more strongly by Random Forest and XGBoost, whereas the smoother spatial variation in Cu is used more strongly by support-vector regression. Ni illustrates a different form of model dependence: XGBoost assigns it a pronounced, predominantly east–west contribution, while its spatial effect is weaker in Random Forest and support-vector regression. Together, these examples show that an element’s importance depends not only on the strength of its spatial pattern but also on whether that pattern can be represented effectively by a particular model architecture. An additional *Pinus* support-vector regression map for Bi is provided in Appendix Figure B5 and is discussed further in the following section.

3.5 Feature-set reduction and operational relevance

The cumulative feature-addition analyses showed that near-optimal performance can often be achieved with a limited core of top-ranked variables. Across most dataset–model combinations, performance approached the full-panel threshold rapidly and then remained broadly stable. However, some support-vector regression trajectories instead overshot the full-panel performance before declining as lower-ranked variables were added. This pattern suggests that these models can be sensitive to noisy, redundant or weakly informative predictors.

Figure 7 illustrates these behaviours using ordinary permutation-importance rankings. The soybean Random Forest reaches approximately full-model performance with its first seven elements and remains stable thereafter. The *Betula* support-vector regression model continues improving to a peak near nine elements before declining as lower-ranked variables are introduced, showing that a reduced panel can outperform the complete feature set. The *Pinus* support-vector regression trajectory based on CPI shows related fluctuations (Appendix Figure B3). In that trajectory, the early decrease when Bi is added is consistent with

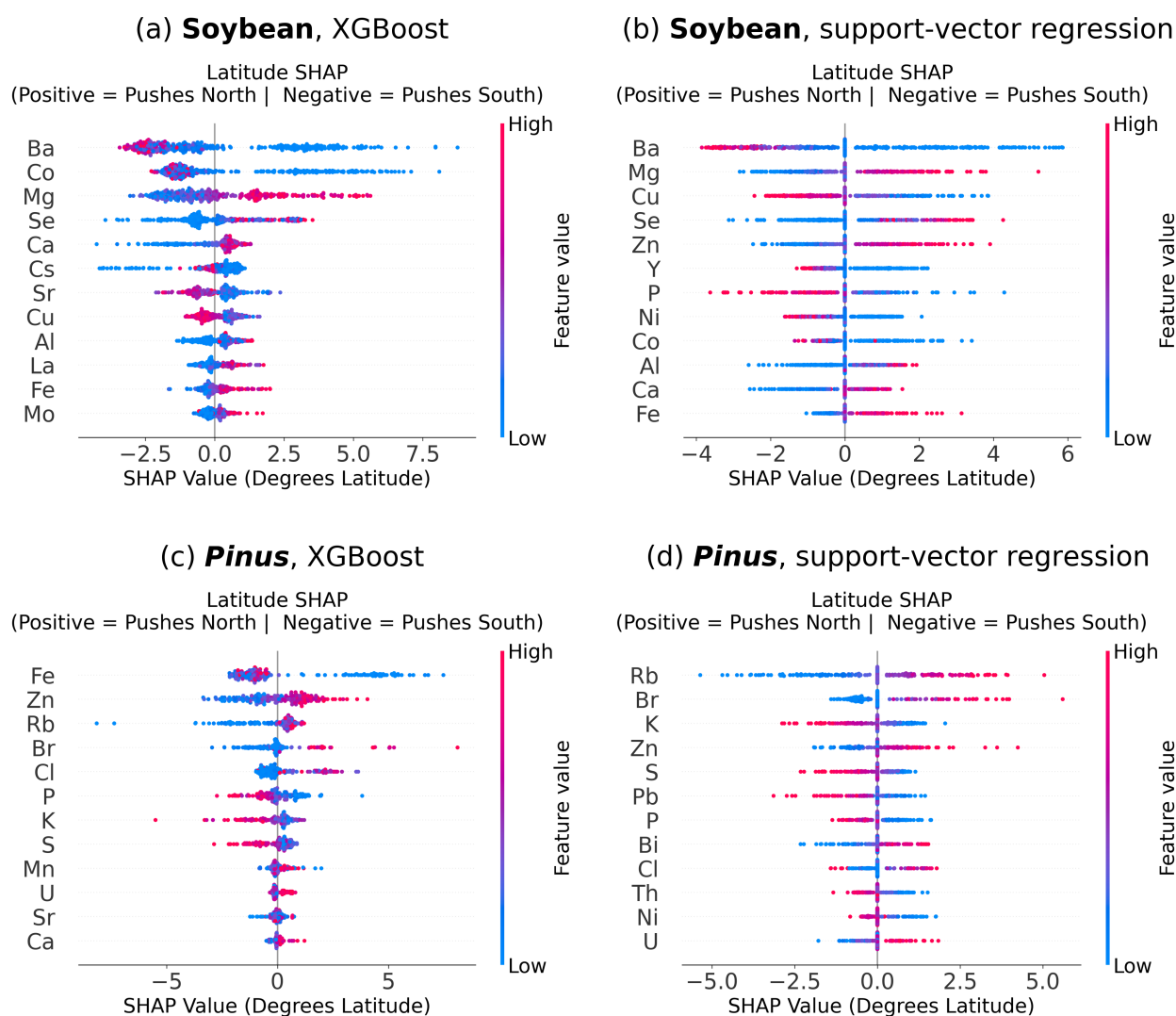


Figure 5. SHAP beeswarm plots comparing feature impacts on latitude predictions for soybean (a, b) and *Pinus* (c, d) using XGBoost (a, c) and support-vector regression (b, d). Elements are ranked by mean absolute SHAP importance within each model. The x-axis represents SHAP values in degrees latitude, where positive values push predictions northward and negative values push predictions southward. Marker colour indicates the relative concentration of each element, from low (blue) to high (red).

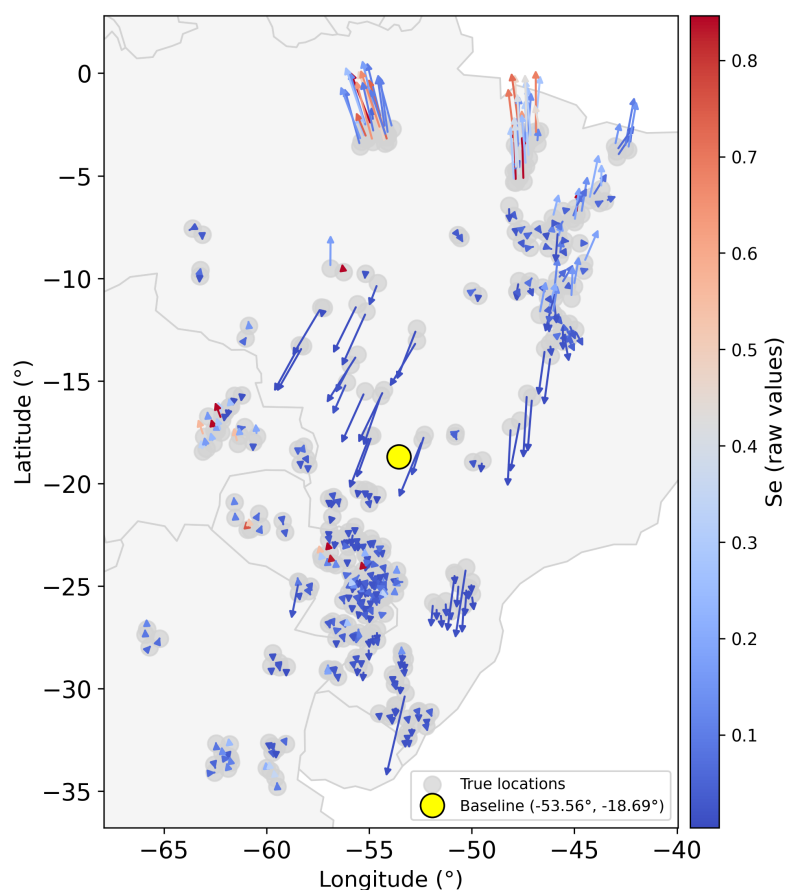


Figure 6. SHAP vector map for the Se-RF interaction in the soy dataset. The gray circles indicate the true (jittered) locations of the soy samples, while the yellow dot marks the global baseline prediction (mean predicted longitude and latitude) for each model. Arrows originate at the true locations and indicate the direction of the SHAP spatial push with respect to the baseline. Northern samples exhibit high Se values (red arrows), causing low-Se samples (dark blue) situated in central-Brazil to be incorrectly pulled southward.



295 its SHAP vector map, which shows heterogeneous and sometimes opposing local spatial pushes (Appendix Figure B5). This provides a model-based explanation for why adding a globally ranked feature need not improve cross-validated performance in every subset.

These findings have practical consequences. Smaller panels can reduce laboratory costs (and as such make chemical testing for harvest location more affordable), simplify quality control and make traceability models easier to communicate, while
300 excluding unstable variables may also improve robustness. However, feature-set reduction should be applied cautiously. An element panel that works for South American soybean cannot be assumed to work for European timber, and a *Betula* panel cannot be assumed to work for *Pinus*. Feature reduction should therefore be treated as a validated, commodity-specific design decision rather than a universal optimisation.

4 Conclusions

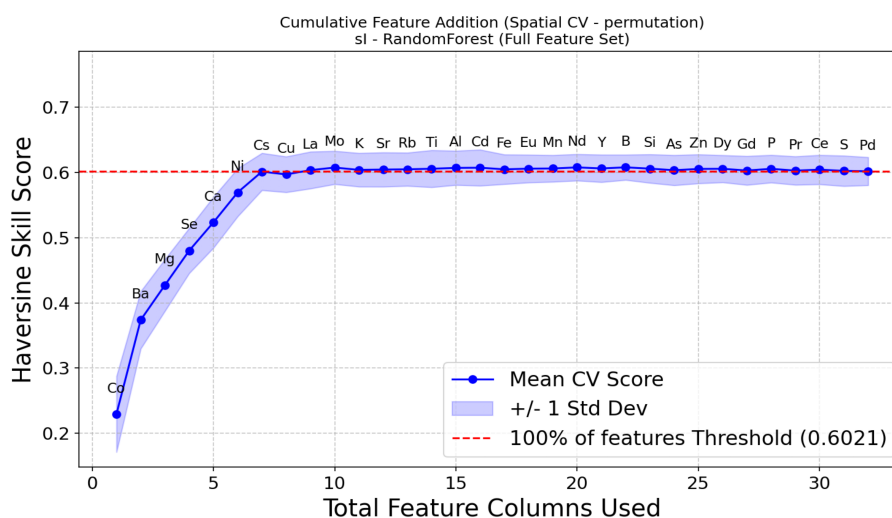
305 Multi-element fingerprints contained meaningful geographic information for both soybean and timber, although predictive strength and the elements carrying that information differed between commodities and among timber genera. The combined use of PI, CPI, SHAP and cumulative feature-addition analysis showed that much of this information can be associated with smaller element sets, while also revealing where importance depends on the model architecture or on correlations among predictors. The most defensible provenance markers are therefore not simply those with the highest importance score, but those
310 that contribute to prediction, remain influential across complementary attribution methods and have plausible environmental or biological interpretations.

The present HSS results should not yet be interpreted as estimates of operational accuracy in unknown supply chains. The validation design did not enforce spatial separation between training and test observations, the geographic reference domains remain incomplete and the feature-addition analyses used fixed rankings rather than recalculating conditional relevance for
315 each subset. Future work should combine stricter spatial-block and region-withholding validation with independent external datasets, uncertainty estimates for predicted coordinates and adaptive or nested feature selection. Log-ratio transformations should also be evaluated to account more explicitly for the compositional structure of elemental profiles.

Despite these limitations, the study demonstrates how chemical origin prediction can move from black-box modelling toward transparent evidentiary analysis. Reporting predictive skill together with stable feature sets, correlation-aware importance and
320 local SHAP explanations makes the basis of individual predictions more visible and auditable. Explainable machine learning can therefore strengthen elemental fingerprinting as an independent line of evidence for environmental commodity tracing, provided that models and reduced element panels are validated for their specific commodity, taxonomic group and geographic reference domain.



(a) **Soybean**, Random Forest



(b) **Betula**, support-vector regression

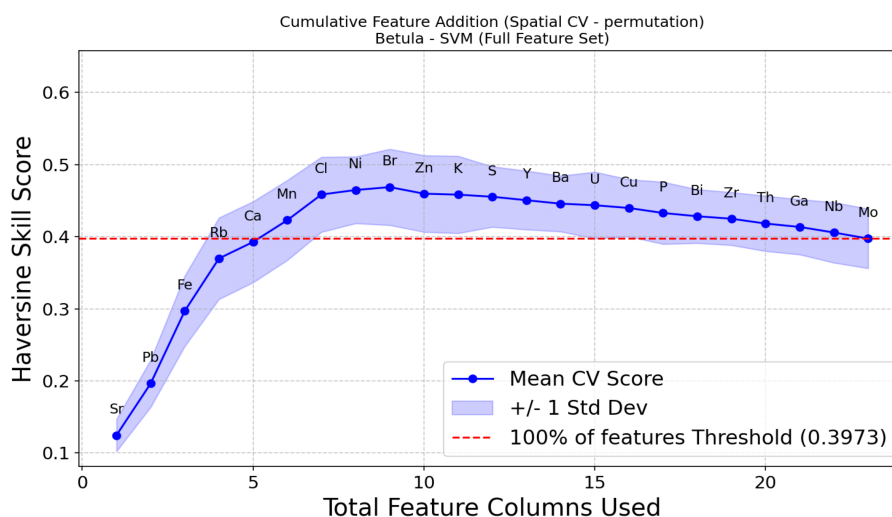


Figure 7. Cumulative feature-addition analyses using ordinary permutation-importance rankings for (a) the soybean Random Forest and (b) the *Betula* support-vector regression model. The blue line shows mean Haversine skill score across spatial cross-validation folds, shading indicates ± 1 standard deviation and the dashed red line marks performance with the full feature set. Element labels identify the variable added at each step.



Appendix A: Model Performance Tables

325 Tables A1–A5 provide the full model-performance summaries across the five folds of the separate performance-evaluation cross-validation. Each table reports both Haversine skill score (HSS) and Haversine distance error in kilometres.

Table A1. Performance metrics across the five evaluation folds for the soybean dataset. Standard deviation, minimum and maximum are calculated across folds.

Metric	Model	Mean	Standard deviation	Minimum	Maximum
HSS	XGBoost	0.6281	0.0393	0.5725	0.6904
HSS	Support-vector regression	0.6118	0.0237	0.5795	0.6419
HSS	Random Forest	0.5957	0.0303	0.5551	0.6493
Haversine distance (km)	XGBoost	403.6395	46.9411	334.5690	480.4459
Haversine distance (km)	Support-vector regression	420.5854	21.0205	386.9926	443.9024
Haversine distance (km)	Random Forest	438.8183	39.0774	378.9234	500.0740

Table A2. Performance metrics across the five evaluation folds for the *Betula* dataset. Standard deviation, minimum and maximum are calculated across folds.

Metric	Model	Mean	Standard deviation	Minimum	Maximum
HSS	XGBoost	0.4538	0.0318	0.3915	0.4796
HSS	Random Forest	0.3963	0.0291	0.3532	0.4437
HSS	Support-vector regression	0.3894	0.0540	0.3235	0.4484
Haversine distance (km)	XGBoost	469.3952	29.3856	431.6704	521.7315
Haversine distance (km)	Random Forest	518.6766	25.3516	488.1504	554.5575
Haversine distance (km)	Support-vector regression	524.8870	49.9925	469.5267	596.0436

Table A3. Performance metrics across the five evaluation folds for the *Fagus* dataset. Standard deviation, minimum and maximum are calculated across folds.

Metric	Model	Mean	Standard deviation	Minimum	Maximum
HSS	Random Forest	0.3434	0.0355	0.2923	0.4003
HSS	XGBoost	0.3230	0.0527	0.2386	0.3855
HSS	Support-vector regression	0.2961	0.0395	0.2283	0.3467
Haversine distance (km)	Random Forest	173.5215	9.1438	164.4720	190.5287
Haversine distance (km)	XGBoost	178.6931	10.2408	168.4554	191.6938
Haversine distance (km)	Support-vector regression	185.9263	7.6330	176.5011	192.7255



Table A4. Performance metrics across the five evaluation folds for the *Pinus* dataset. Standard deviation, minimum and maximum are calculated across folds.

Metric	Model	Mean	Standard deviation	Minimum	Maximum
HSS	Support-vector regression	0.4899	0.0525	0.4026	0.5613
HSS	XGBoost	0.4765	0.0629	0.4188	0.5894
HSS	Random Forest	0.4616	0.0555	0.3751	0.5242
Haversine distance (km)	Support-vector regression	377.9423	47.1845	320.1553	460.0416
Haversine distance (km)	XGBoost	387.5568	51.4016	299.6502	444.1617
Haversine distance (km)	Random Forest	398.8096	48.9215	348.0124	481.2383

Table A5. Performance metrics across the five evaluation folds for the *Quercus* dataset. Standard deviation, minimum and maximum are calculated across folds.

Metric	Model	Mean	Standard deviation	Minimum	Maximum
HSS	Support-vector regression	0.3969	0.0434	0.3441	0.4740
HSS	XGBoost	0.3893	0.0524	0.3435	0.4909
HSS	Random Forest	0.3671	0.0383	0.3329	0.4351
Haversine distance (km)	Support-vector regression	318.9836	24.5793	274.1741	344.1713
Haversine distance (km)	XGBoost	323.0837	29.7825	265.4025	349.8079
Haversine distance (km)	Random Forest	334.8495	23.4174	294.4811	365.1480

Appendix B: Supplementary Figures

Figure B1 visualises the spatial behaviour of the soybean coordinate predictions discussed in the main text. Figure B2 provides the additional timber latitude beeswarm plots referenced in the SHAP interpretation, and Figure B3 provides the supplementary cumulative feature-addition result. The subsequent SHAP vector maps show how selected elemental concentrations push individual coordinate predictions away from each model's baseline prediction. They complement the main-text Se example (Figure 6) by showing additional soybean and timber feature–model interactions, including the *Pinus* support-vector regression interaction with Bi.

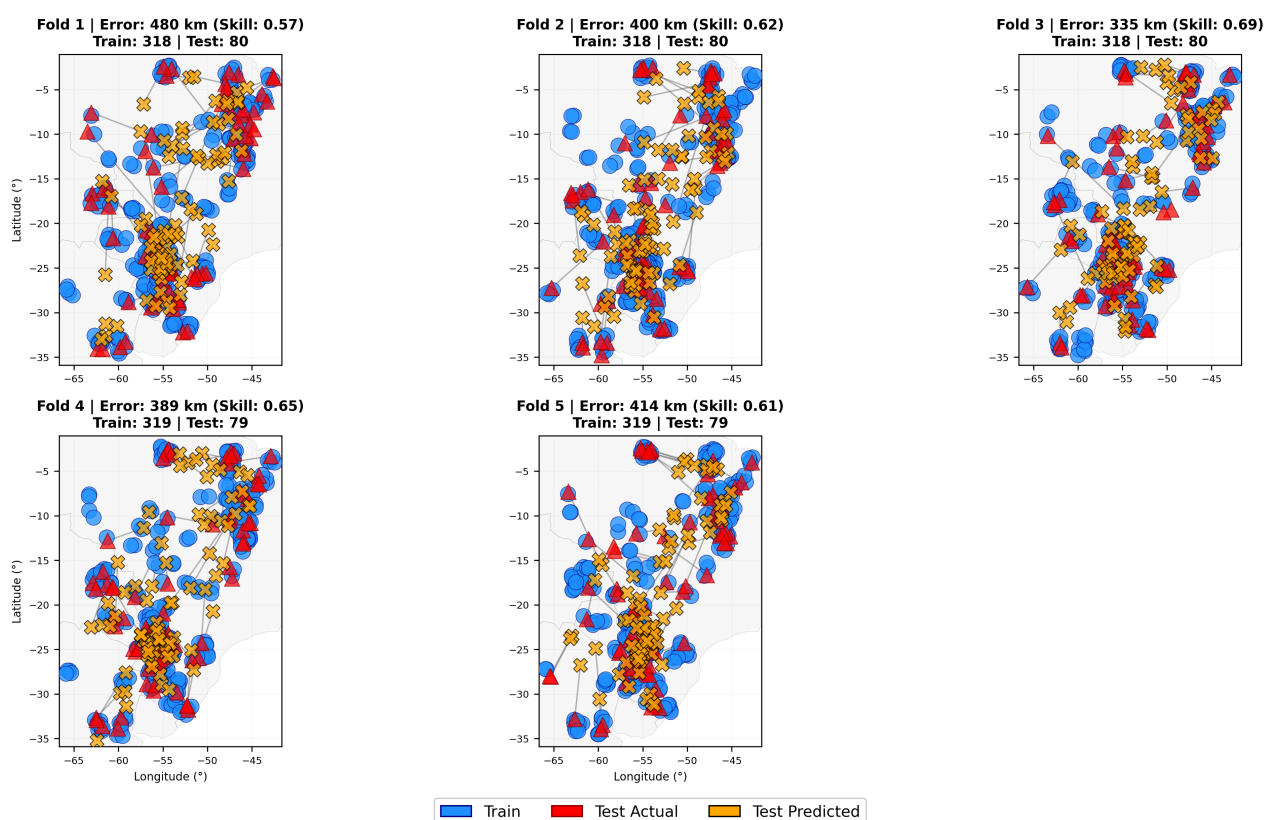


Figure B1. Visualisation of five-fold spatial cross-validation results for the XGBoost soybean model. The dataset was partitioned using spatial clustering to produce geographically stratified folds. Each panel shows training samples, true test locations, predicted coordinates and error vectors connecting true and predicted locations.

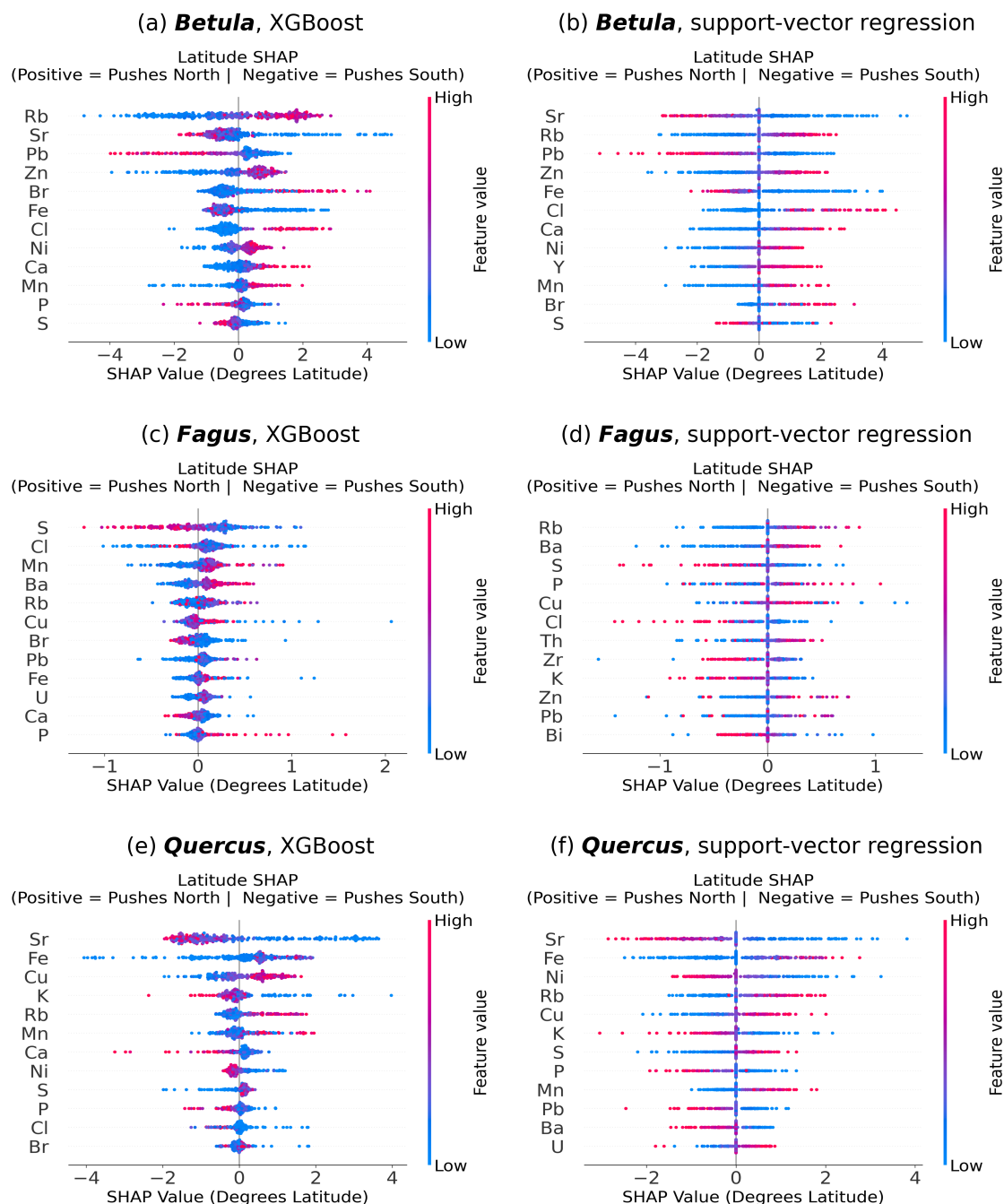


Figure B2. Supplementary SHAP beeswarm plots comparing feature impacts on latitude predictions for *Betula* (a, b), *Fagus* (c, d) and *Quercus* (e, f) using XGBoost (a, c, e) and support-vector regression (b, d, f). Elements are ranked by mean absolute SHAP importance within each model. Positive SHAP values push predictions northward and negative values push predictions southward, while marker colour indicates relative elemental concentration from low (blue) to high (red).

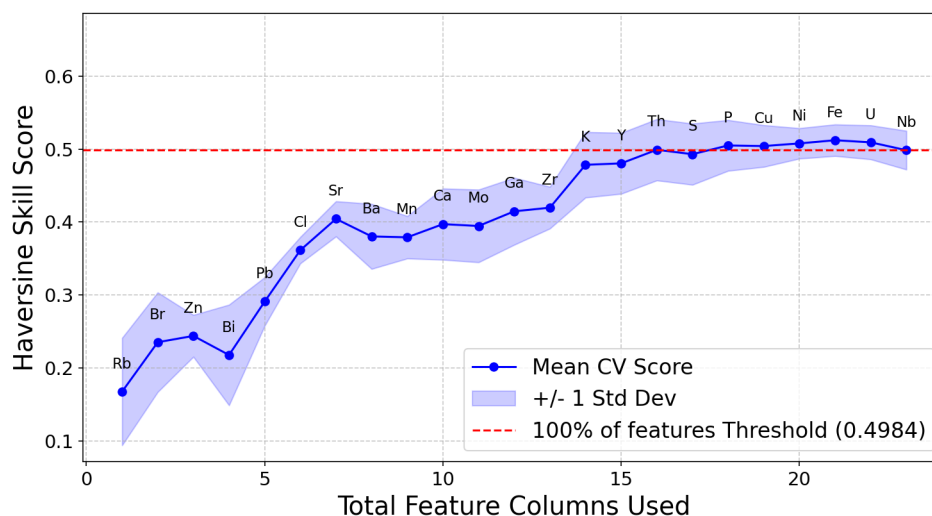


Figure B3. Supplementary cumulative feature-addition analysis for the *Pinus* support-vector regression model using conditional-permutation-importance rankings. The blue line shows mean Haversine skill score across spatial cross-validation folds, shading indicates ± 1 standard deviation and the dashed red line marks performance with the full feature set. Element labels identify the variable added at each step.

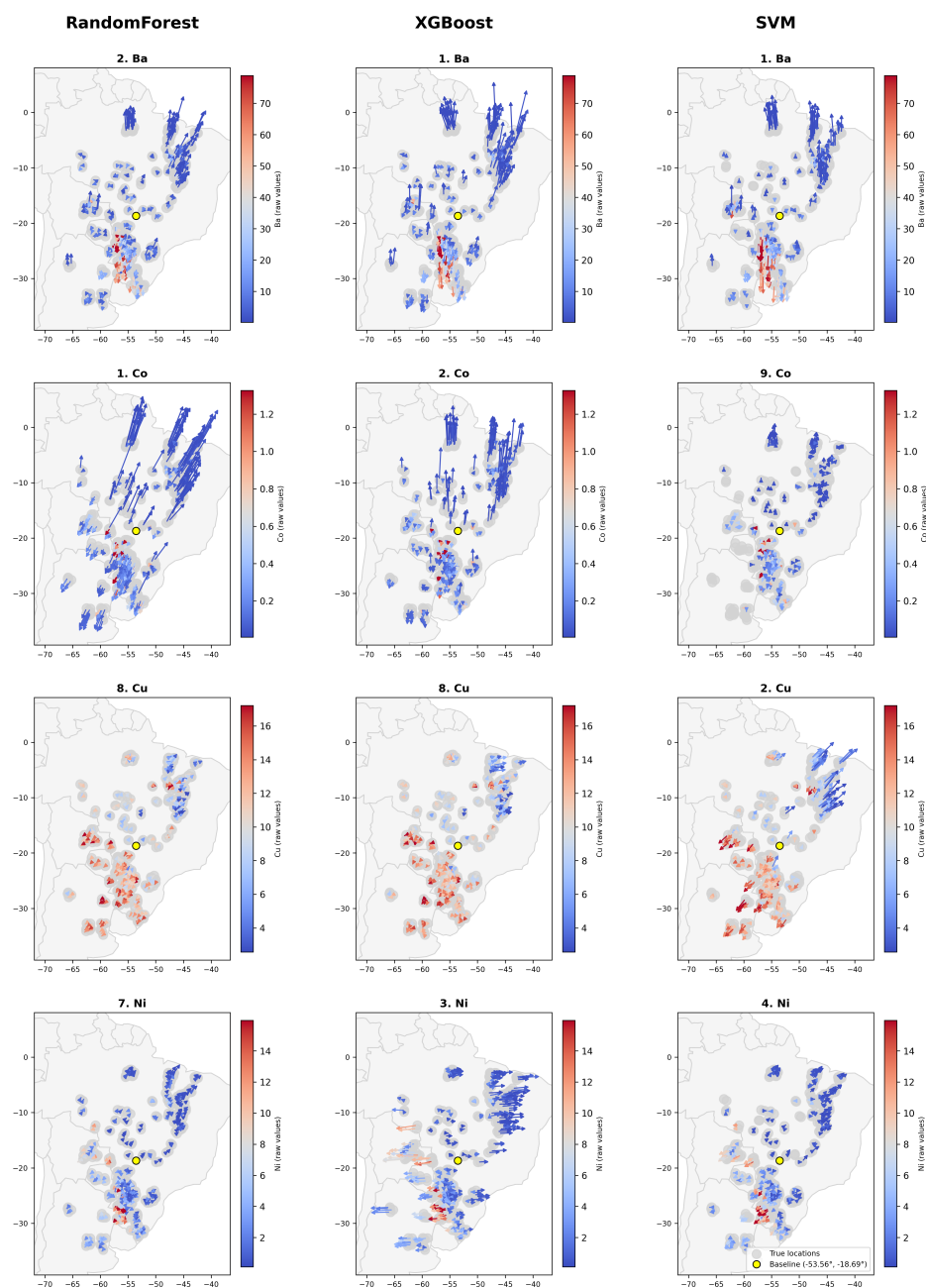


Figure B4. Supplementary soybean SHAP vector maps comparing Ba, Co, Cu and Ni across Random Forest, XGBoost and support-vector regression. Columns correspond to model architectures and rows correspond to elements. Arrows originate at the true sample locations and show the direction and magnitude of each element's contribution to predicted longitude and latitude relative to the model baseline. Colours indicate raw elemental values from low (blue) to high (red).

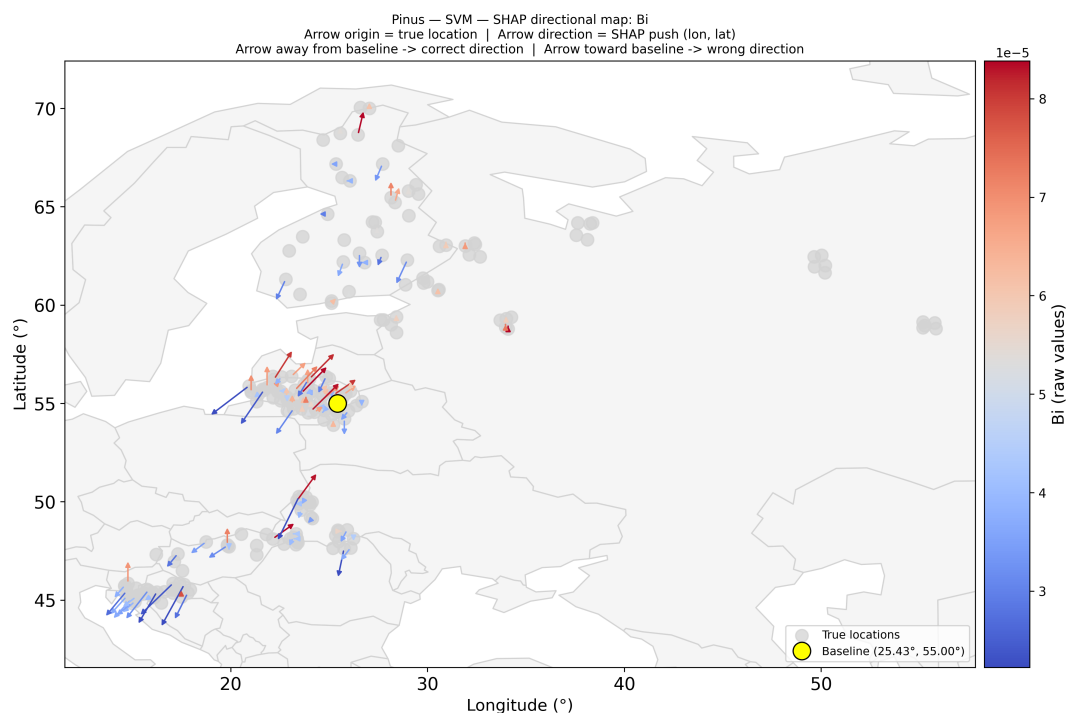


Figure B5. Supplementary SHAP vector map for the Bi interaction in the *Pinus* support-vector regression model. Arrows originate at the true sample locations and show the direction and magnitude of the Bi contribution to predicted longitude and latitude relative to the model baseline. Colours indicate raw Bi values from low (blue) to high (red).



335 *Code and data availability.* The data are available upon reasonable request from victor.deklerck@worldforestid.org. Analysis code, including hyperparameter-search settings and random seeds, is available at <https://github.com/WanderLabaere/commodity-tracing-interpretability>.

Author contributions. Conceptualization: SJ, WW and VD; Data curation: WL, SJ, BB, CC, LAM, Formal Analysis: WW, and SJ; Methodology: SJ, WW and VD; Writing (original, review and editing): all.

Competing interests. The authors declare that they have no conflict of interest.

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