Extracting, visualising and interpreting structure in geochemical data through compositional data analysis (CoDA):
Process Prediction and Predictive Mapping

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Evaluating Geochemical Data Using Multivariate Methods and Predictive Mapping

The Process of Predictive Mapping

Process Discovery

The use of empirical methods for identifying structure in data and forms the basis/justification to build or test models:

- Adjust data for censoring/missing values.
- Transform data to the logratio space (alr/clr/ilr).
- The use of different metrics (PCA, t-SNE, ICA, UMAP + others) to observe/discover patterns in the data.
- Discovery of processes through empirical analysis (principal component analysis, logratio analysis, multidimensional scaling, cluster analysis).
- Determine suitable classes for predictive mapping (e.g. lithologic units).
- Tag classes to sample sites where available using GIS.

The Process of Predictive Mapping

Process Validation

The use of modelled methods for process confirmation:

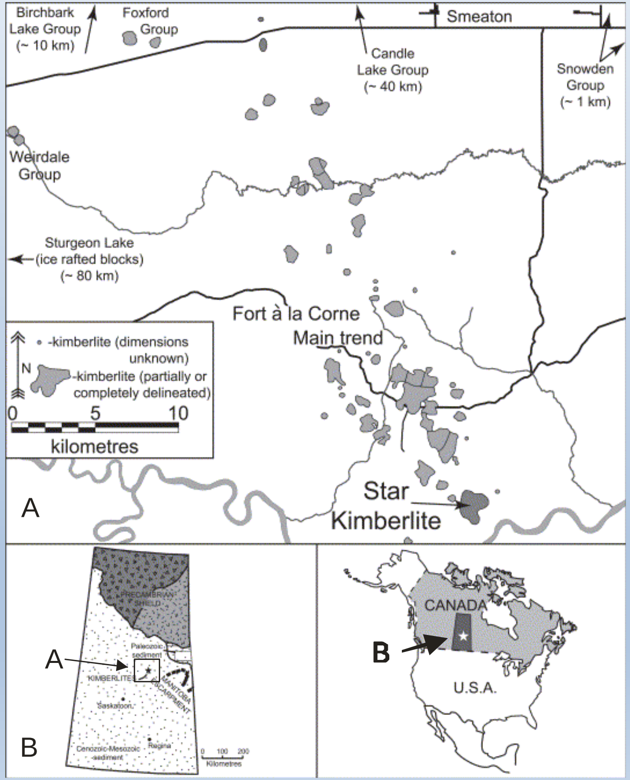
- Analysis of variance (AOV) to determine which elements or principal components give maximum separation of the classes.
- Methods of classification used for prediction (LDA, QDA, NN, LR, RF + others)
- Classification to determine measures of posterior probability or typicality from which a probability of class membership is assigned to each site. Other methods can be used (e.g. Random Forests).
- Spatial analysis to calculate semi-variograms and subsequent kriging (interpolation) to produce predictive maps for each class.

Calculate:

- **accuracy of prediction** for each class and overall accuracy.
- **precision** - the fraction of true positives/[true + false positives].
- **recall** - the fraction of true positives/false negatives.
- Estimates of accuracy are derived from Process Validation and based on the confusion matrix predicted classes vs. actual classes.

Kimberlite Classification using Lithogeochemistry

Local/Camp Scale < 1:50,000
Exploration scale studies and detailed geologic mapping.
Star Kimberlite – Fort a la Corne - Saskatchewan



- Lithogeochemical sampling program of drill core from a series of kimberlite eruptions.
- Kimberlite mineralogy varies from olivine bearing magmas to fractionated magmas contaminated by crust.
- Kimberlites analyzed the following oxides/elements converted to cation values :

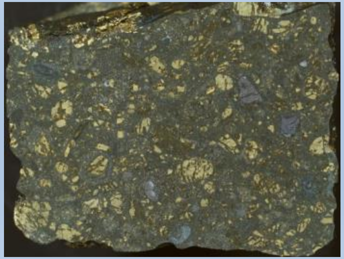
Si, Ti, Al, Fe, Mg, Ca, Na, K, P, Rb, Nb, Zr, Th, V, Cr, Co, Ni, La, Er, Yb, Y, Ga

Kimberlite Phases

Early Joli Fou

Mid Joli Fou

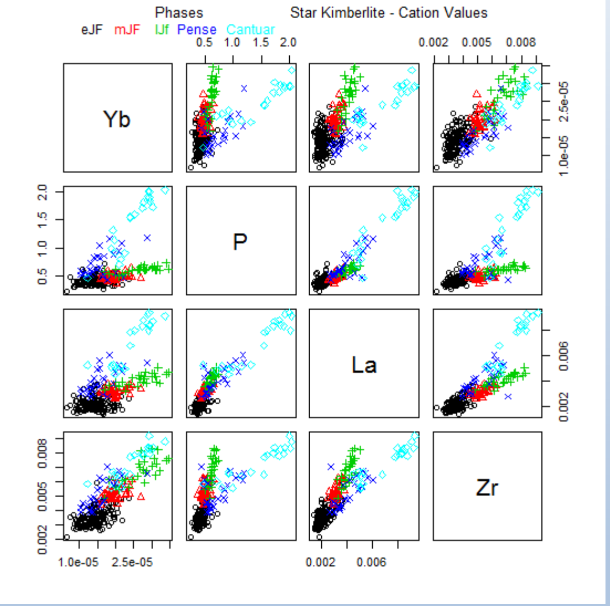
Late Joli Fou



Pense

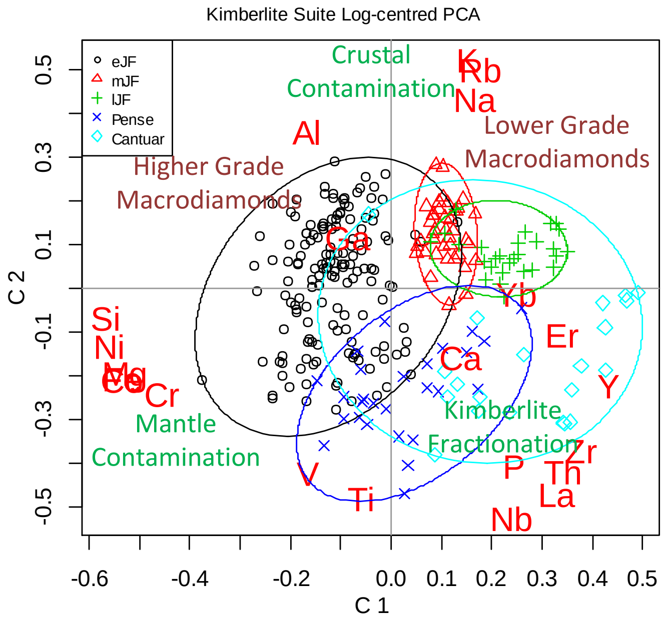
Cantuar

Process Discovery
Kimberlites – Logcentred PCA

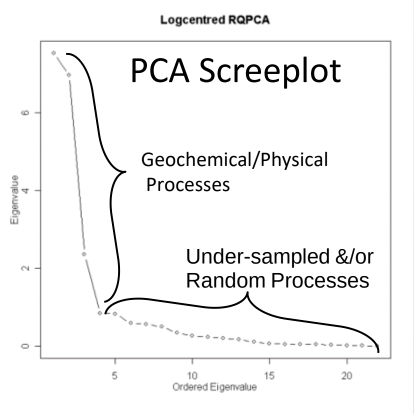


Kimberlite Fractionation Trends [stoichiometric control]

PCA Biplot



[Grunsky & Kjarsgaard, 2008]



ΣPC1-2 = 66%

ΣPC1-4 = 80%

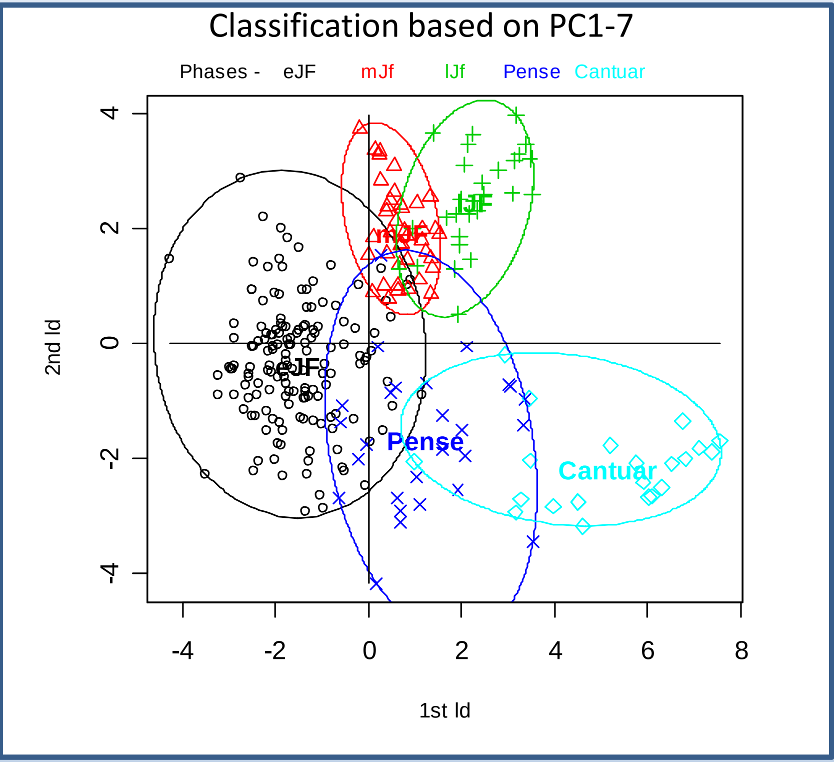
ΣPC1-7 = 90%

Overall variation

Signal PC 1-7

Noise PC 8-22

Kimberlite Suite
Linear Discriminant Analysis
Process Validation



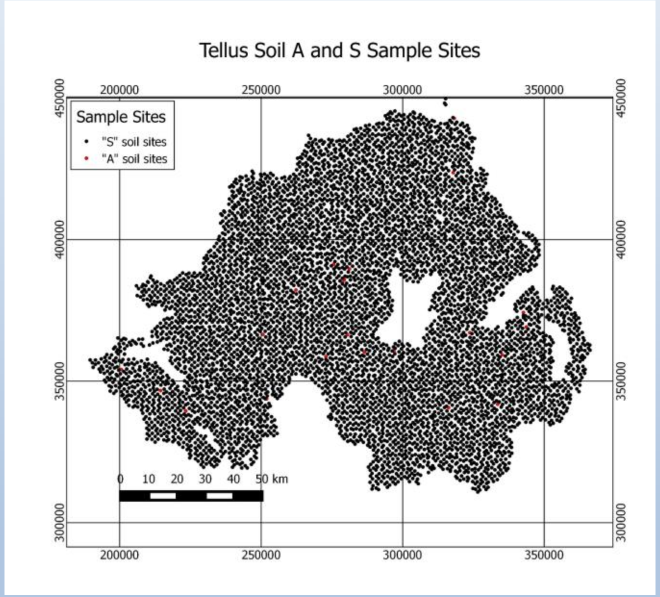
Accuracy/Confusion Matrix

	eJF	mJF	lJF	Pense	Cantuar
eJF	90.90	0.00	0.00	0.00	9.10
mJF	0.00	96.78	0.00	2.58	0.65
lJF	0.00	3.58	85.71	10.71	0.00
Pense	0.00	2.50	0.00	97.50	0.00
Cantuar	3.45	10.35	0.00	0.00	86.21

- The use of LDA enables the classification, and prediction of kimberlite phases that are relatively rich in diamonds.

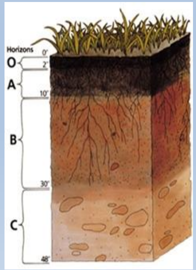
Predictive Lithologic Mapping from the Tellus data, Northern Ireland

Tellus Survey
"A" and "S" Sample Sites



Surface soil/ A sample (5-20 cm depth)
6862 sites
XRF analysis for major oxides and trace elements on pressed powder pellets (xrf) (6783 sites).
ICP (OES/MS) analysis by aqua regia (ar) digestion (6768 sites)
Fire assay for Au, Pd, Pt by ICP-MS

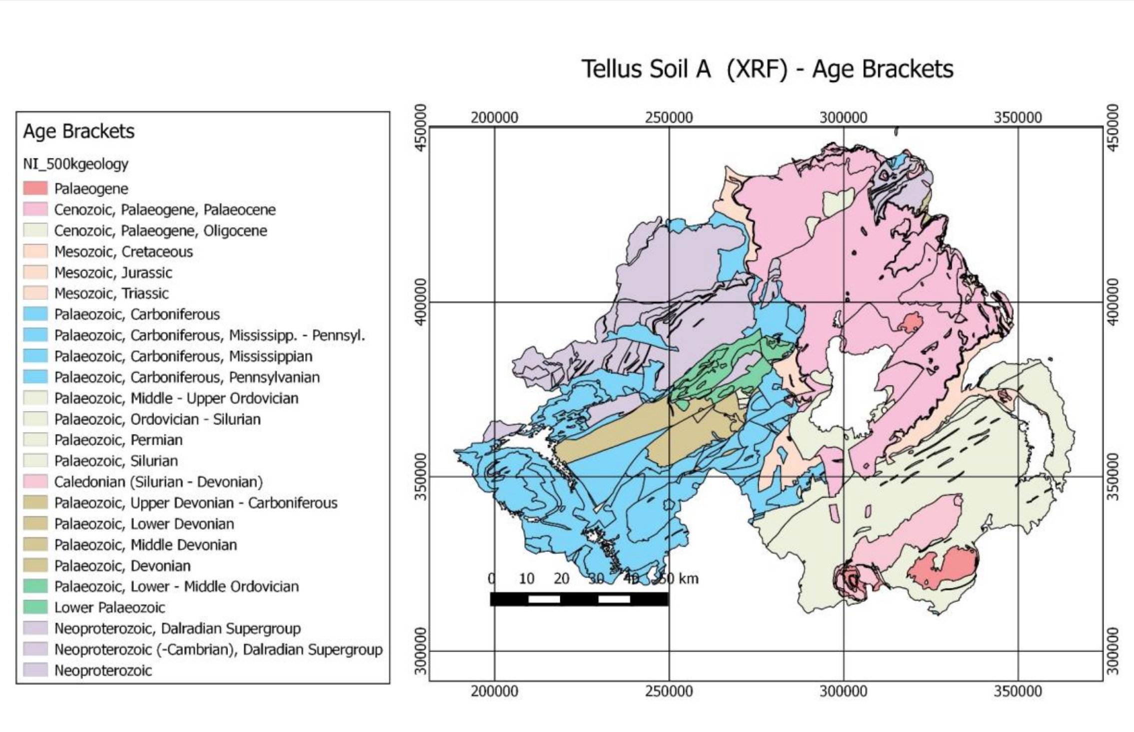
Deep soil/ S sample (35-50 cm depth)
6867 sites
ICP-OES/MS analysis by aqua regia (ar) digestion (6847 sites)
ICP-OES/MS analysis by 4 acid (4a) digestion (6859 sites)
Fire assay for Au, Pd, Pt by ICP-MS



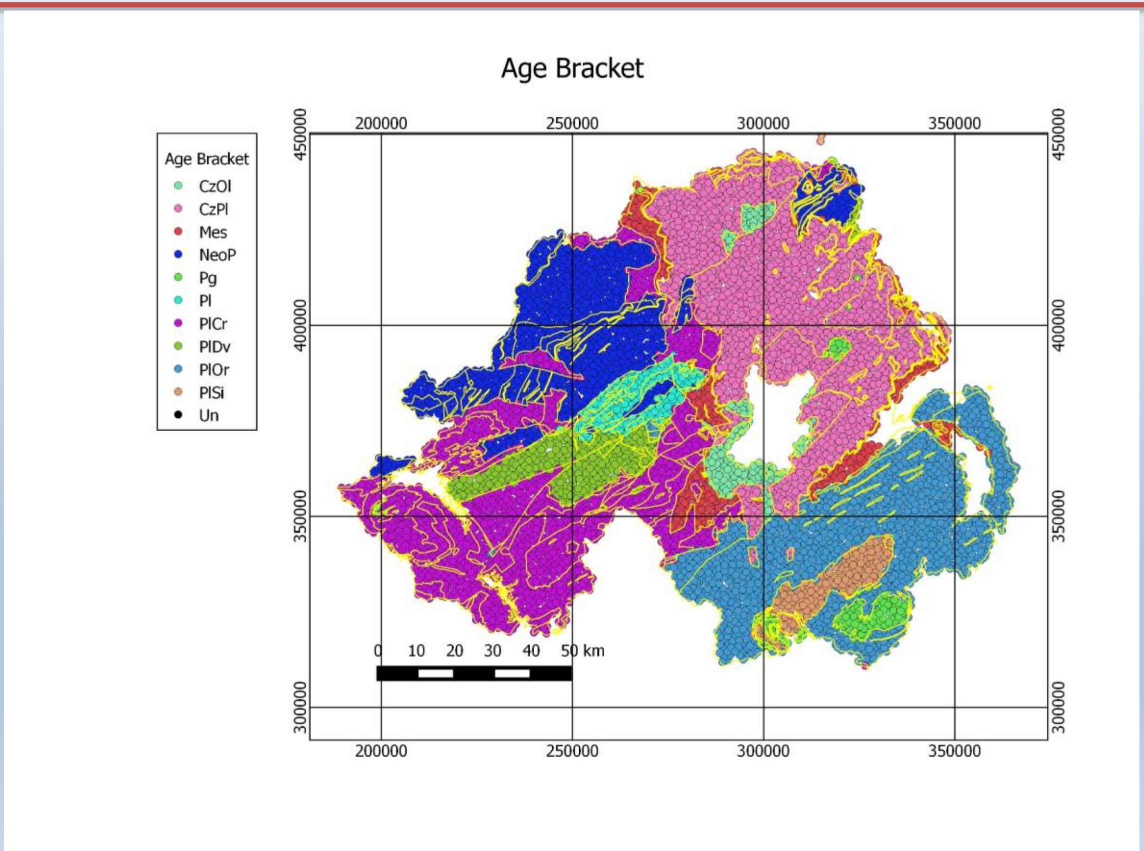
"A" zone – 5-20 cm depth

"S" zone – 35-50 cm depth

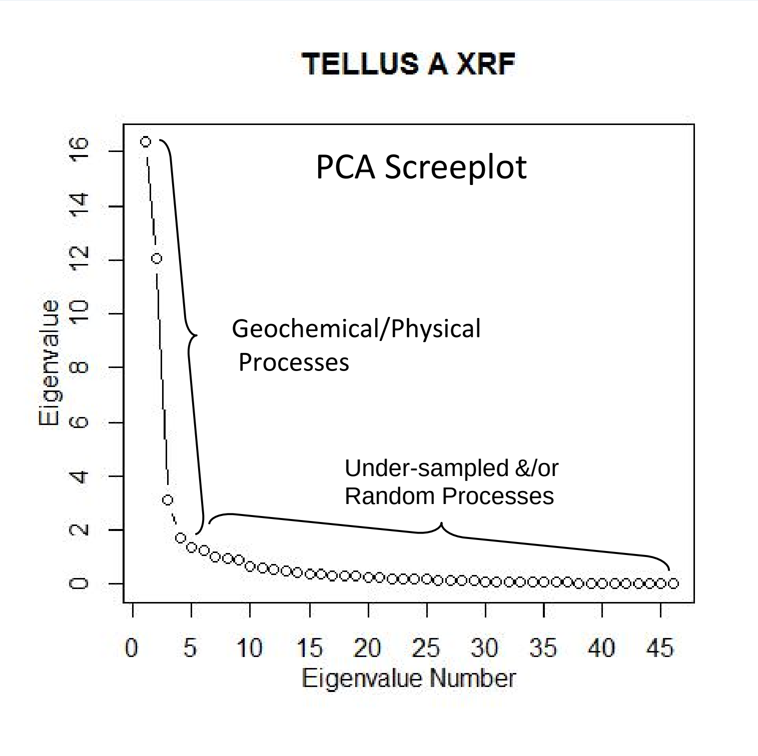
Predictive Mapping
Age Brackets



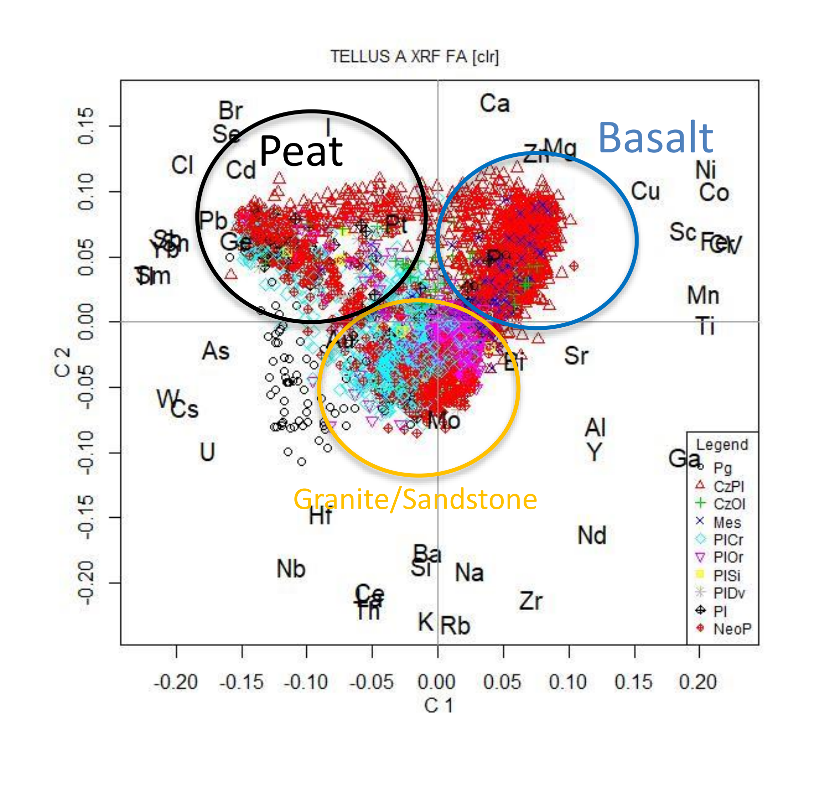
Age Brackets - Sample Sites



Principal Component Analysis



Colour/Symbol by Age Bracket



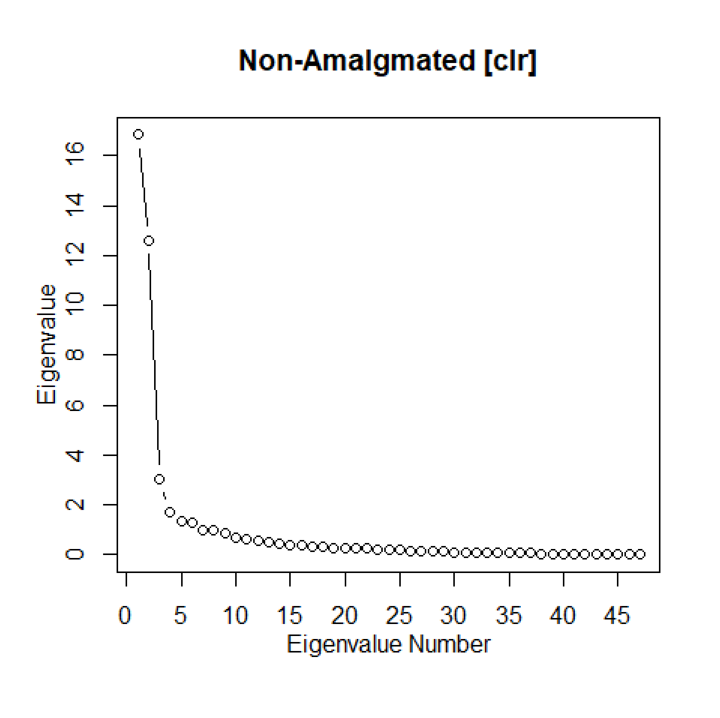
Amalgamation - Fit-for-purpose

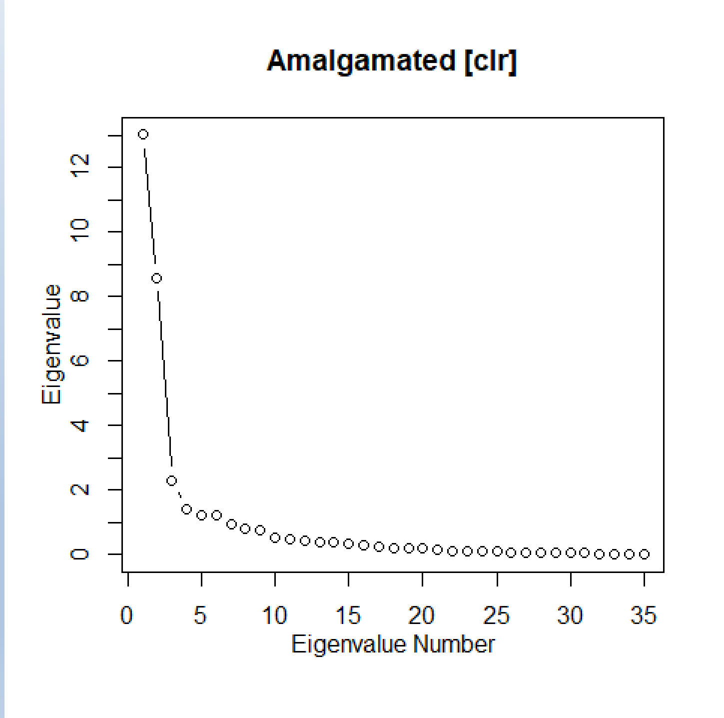
- There are cases where groups of elements are highly associated (correlated), such as rare earth elements (REE) where elements combine in specific lattice sites in minerals.
- These elements can create difficulty in linear algebraic methods where collinearity can result in non-unique solutions.
- Grouping these elements (amalgamating) reduces the risk of collinearity and simplifies the identification of processes.

Amalgamation

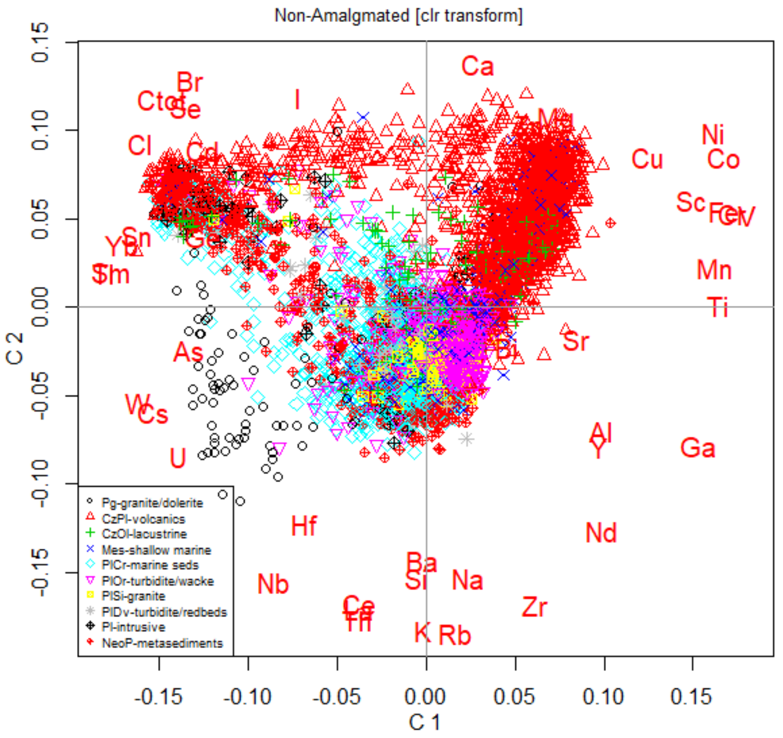
- Amalgamation of elements:
- LREE - La, Ce, Pr, Nd
- HREE - Lu, Yb, Er, Ho, Dy, Tb
- Mafic - Fe, Sc, V, Cr
- Feldspar (Cations)- Ba, Na, K,
- Feldspar (Anions) - Al, Ga

PCA Screeplots

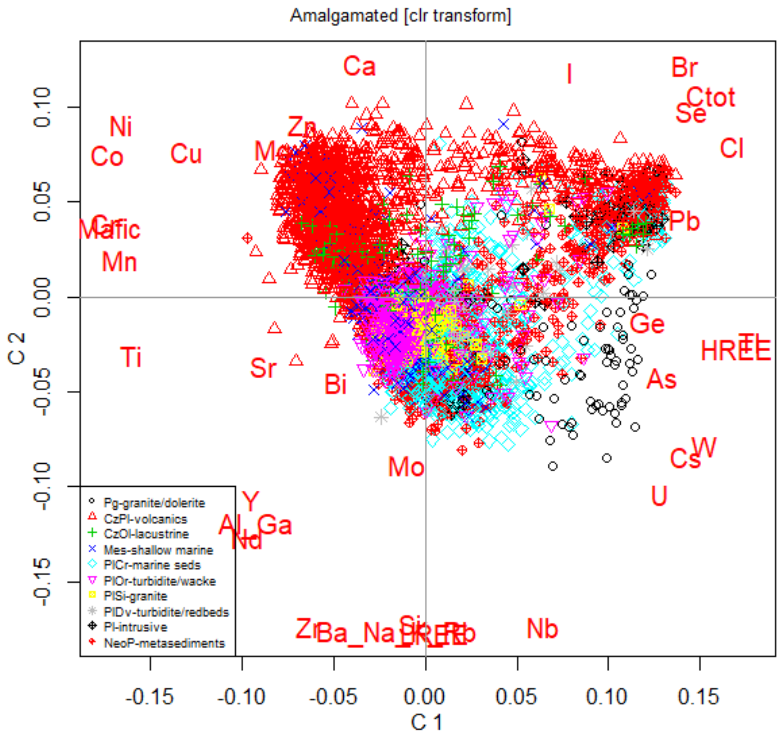




PCA Biplots



Non-Amalgmated [clr transform]
C 1
C 2
Pg-granite/dolerite
CzPl-volcanics
CzOl-lacustrine
Mes-shallow marine
PlCr-marine seds
PlOr-turbidite/wacke
PlSi-granite
PlDv-turbidite/redbeds
Pl-intrusive
NeoP-metasediments



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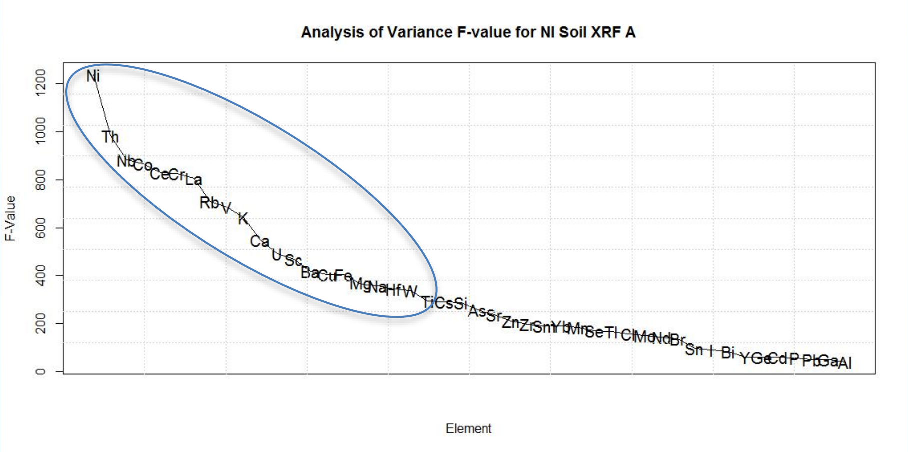
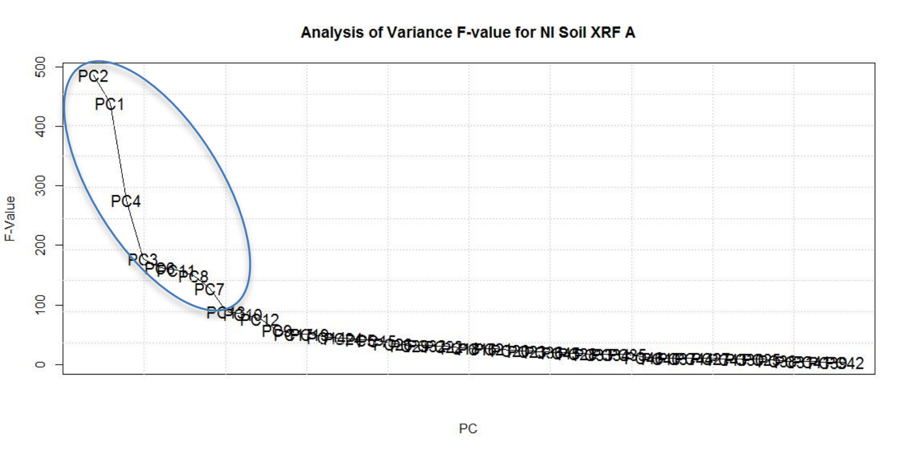
Analysis of Variance
Elements (clr) & Principal Components



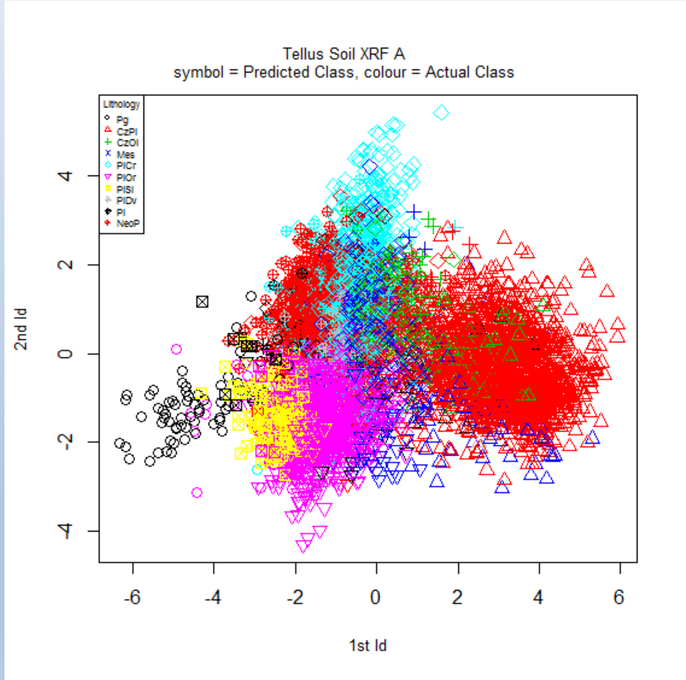
Many elements (>20) required for a useful discrimination between classes (Age Brackets)

Only 8 PCs required for a useful discrimination between classes (Age Brackets)

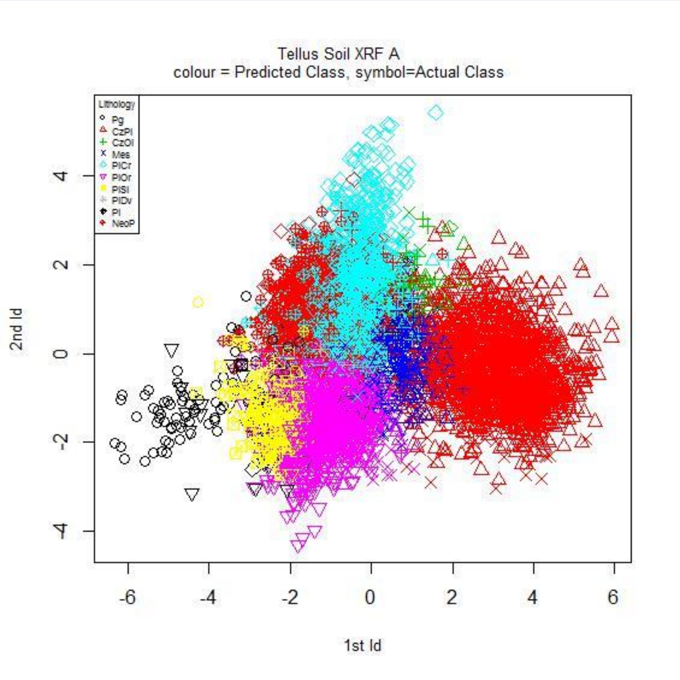


Linear Discriminant Analysis

Colour=Actual



Colour=Predicted



Not a significant difference

Classification Accuracy

Counts

predicted

true	CzOl	CzPl	Mes	NeoP	Pg	Pl	PlCr	PlDv	PlOr	PlSi
CzOl	11	42	37	6	0	0	56	0	2	0
CzPl	13	1448	74	54	0	9	71	0	21	1
Mes	4	69	57	10	0	0	132	0	58	0
NeoP	6	7	6	736	1	17	189	1	49	1
Pg	0	11	1	5	72	1	10	0	12	12
Pl	0	5	4	90	0	10	34	2	25	0
PlCr	8	8	32	216	1	15	1070	6	172	6
PlDv	1	2	1	95	0	0	35	27	142	1
PlOr	0	1	33	33	40	0	54	5	1117	28
PlSi	0	0	0	1	1	0	2	0	16	148

error rate = 30.93 %

%

predicted

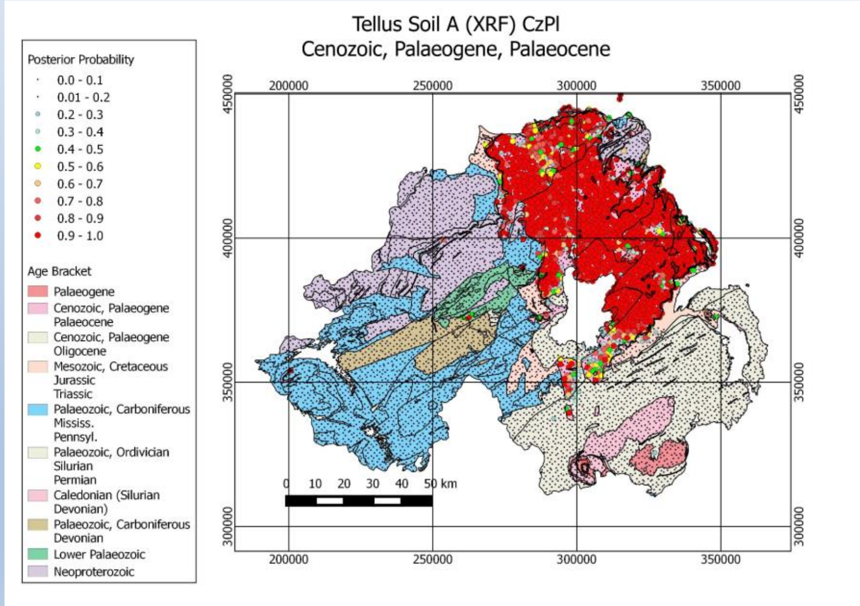
	CzOl	CzPl	Mes	NeoP	Pg	Pl	PlCr	PlDv	PlOr	PlSi
CzOl	**7.1**	27.3	24.0	3.9	0.0	0.0	36.4	0.0	1.3	0.0
CzPl	0.8	85.6	4.4	3.2	0.0	0.5	4.2	0.0	1.2	0.1
Mes	1.2	20.9	**17.3**	3.0	0.0	0.0	40.0	0.0	17.6	0.0
NeoP	0.6	0.7	0.6	**72.7**	0.1	1.7	18.7	0.1	4.8	0.1
Pg	0.0	8.9	0.8	4.0	**58.1**	0.8	8.1	0.0	9.7	9.7
Pl	0.0	2.9	2.4	52.9	0.0	**5.9**	20.0	1.2	14.7	0.0
PlCr	0.5	0.5	2.1	14.1	0.1	1.0	**69.8**	0.4	11.2	0.4
PlDv	0.3	0.7	0.3	31.2	0.0	0.0	11.5	**8.9**	46.7	0.3
PlOr	0.0	0.1	2.5	2.5	3.1	0.0	4.1	0.4	**85.2**	2.1
PlSi	0.0	0.0	0.0	0.6	0.6	0.0	1.2	0.0	9.5	**88.1**

Posterior Probability

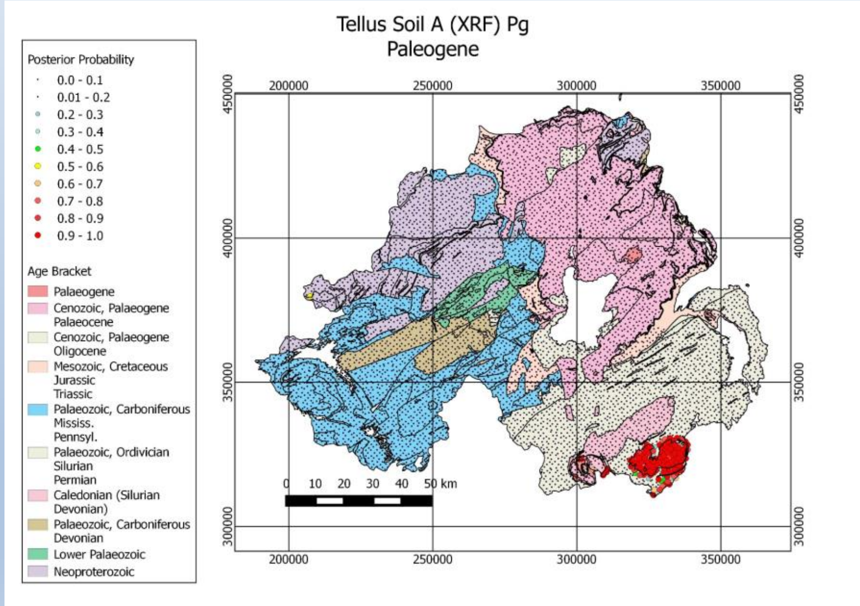
- A multivariate distance (Mahalanobis Distance - MD) is measure from a given observation (sample site) to the centroid of each Age Bracket class. Distances are based on the principal components used for the classification.
- The predicted class is assigned based on the shortest MD.
- Posterior probabilities are forced fits. An observation must belong to one class.

Posterior Probability

Paleogene – felsic granitoid rocks

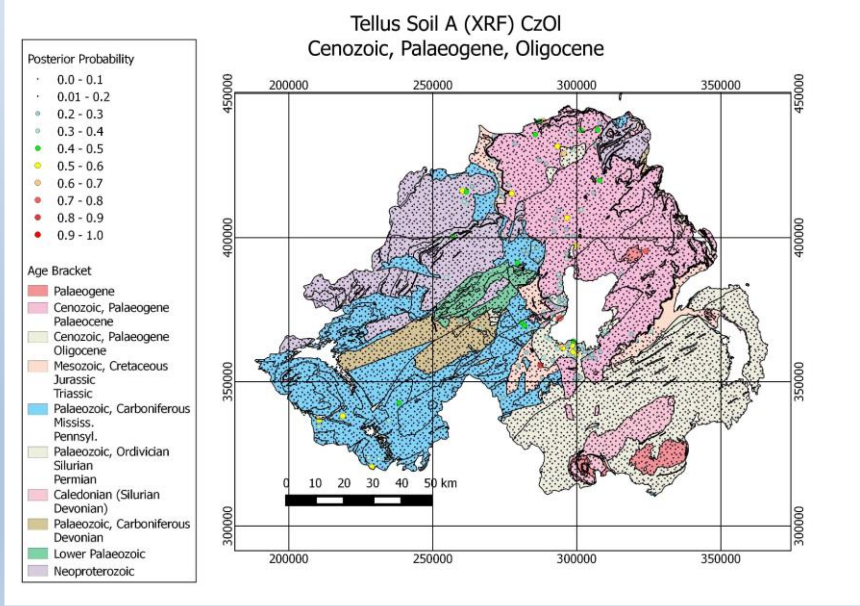


Cenozoic Basalts

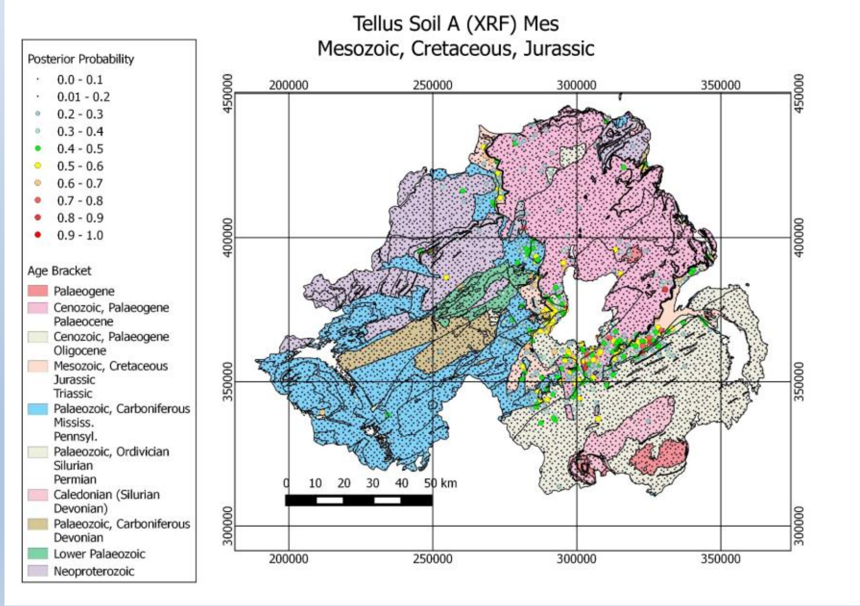


Posterior Probability

Lacustrine; Clay, sand & lignite

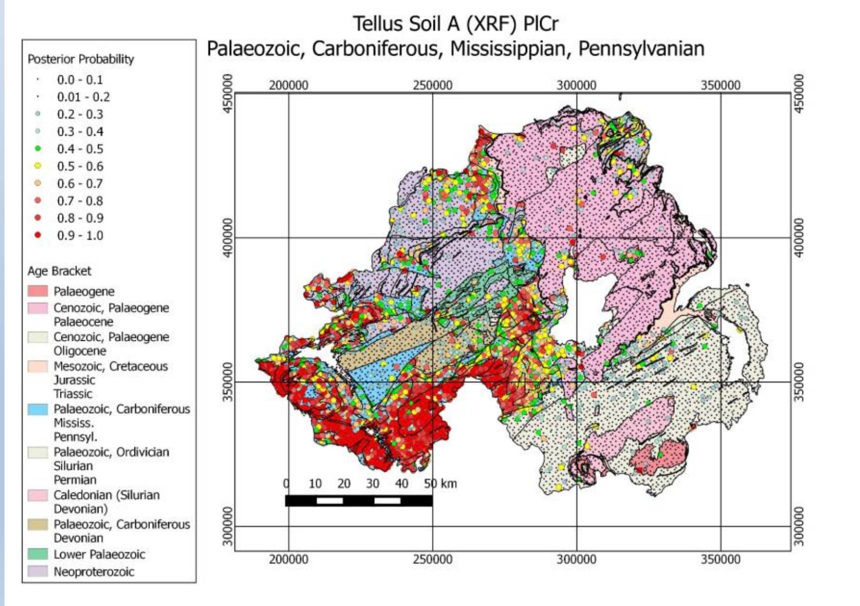


Continental redbed facies sandstone & mudstone

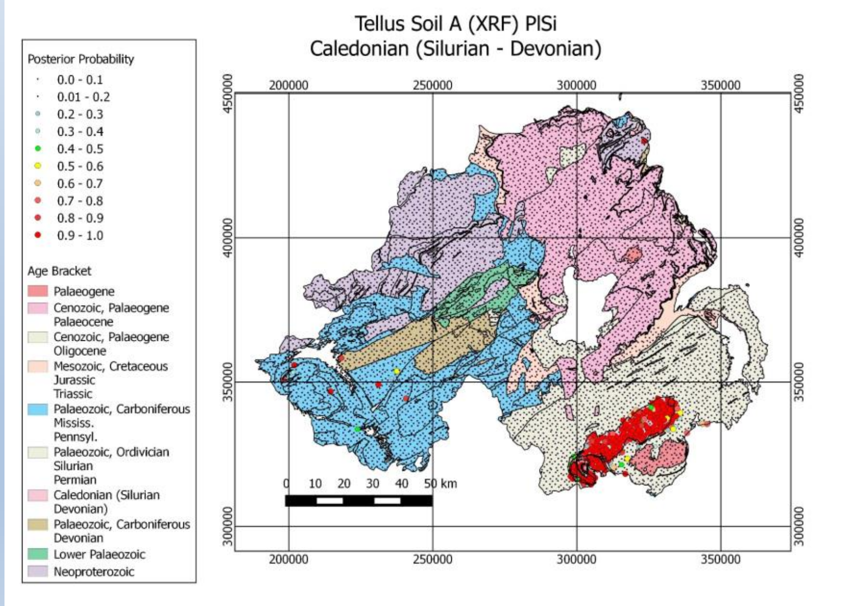


Posterior Probability

Basalt, trachyte, syenite & tuff + sediments

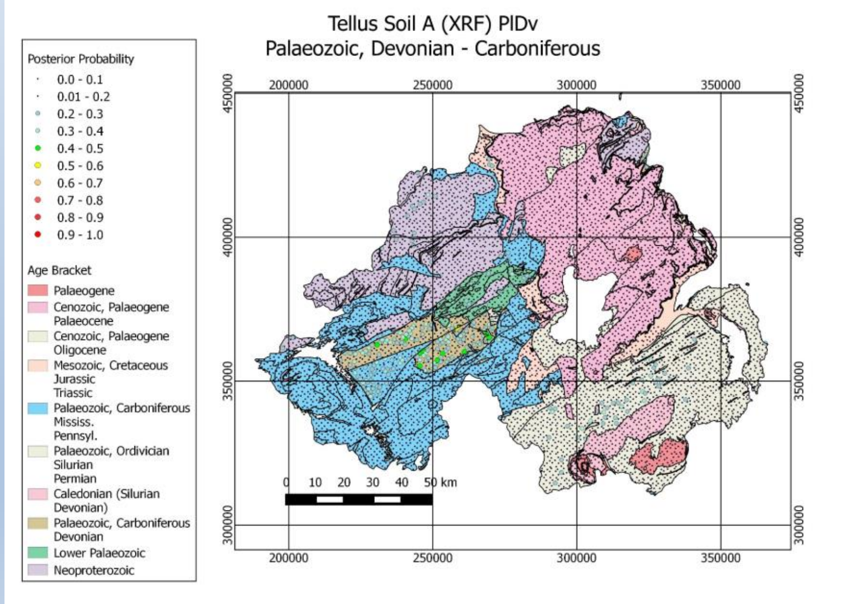


Appinite Suite, Granite, granodiorite

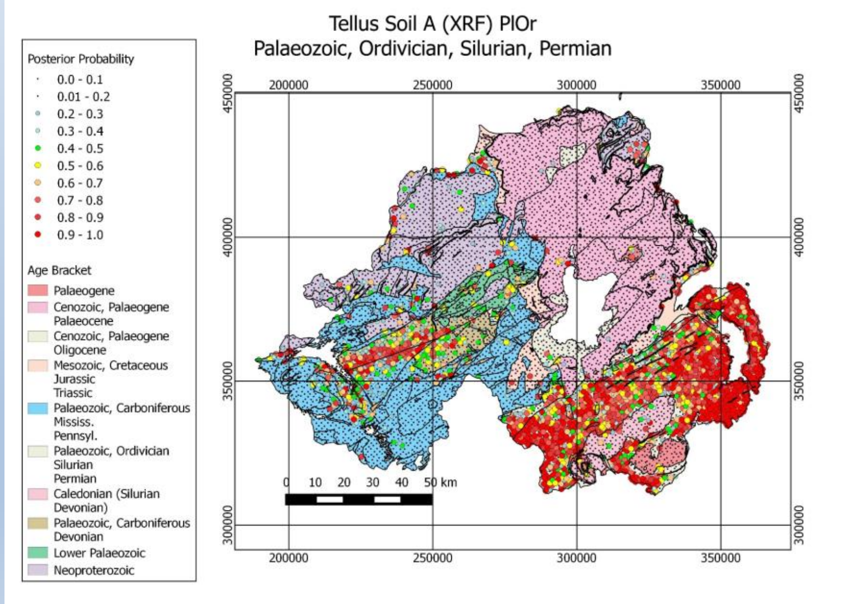


Posterior Probability

Basalt, andesite + sediments

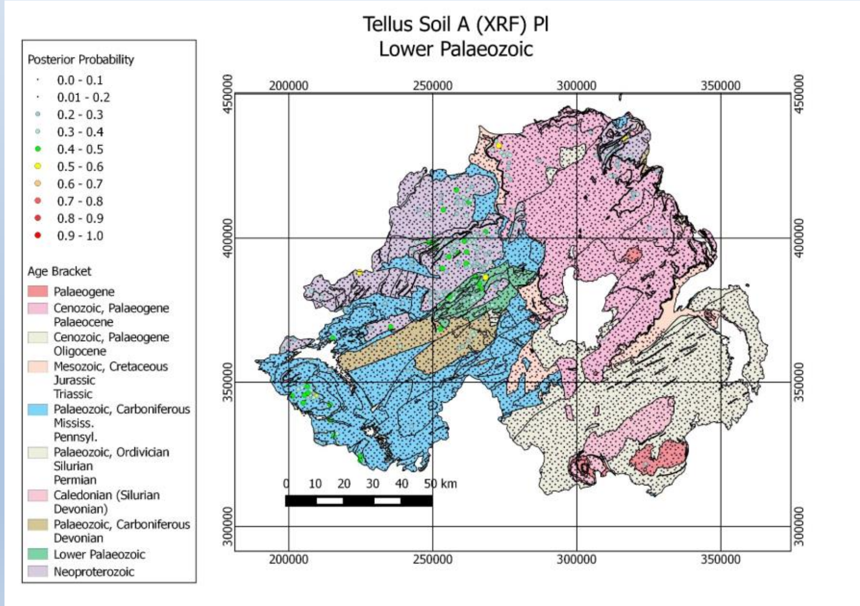


Paleozoic
Wackes/Conglomerate/Redbeds/Mudstone

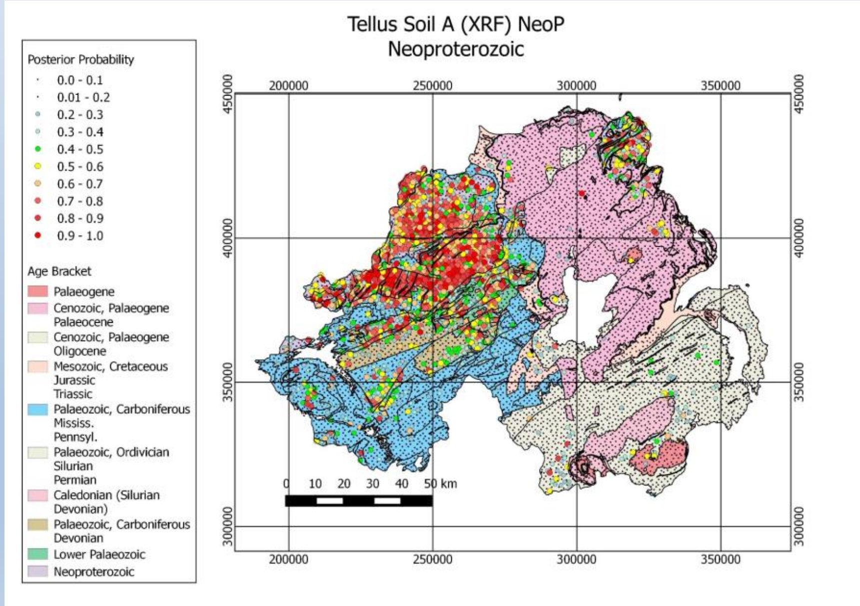


Posterior Probability

Paleozoic Granitoid/Gabbroic Rocks



Neoproterozoic Pelite/Semi-pelite/Psammite



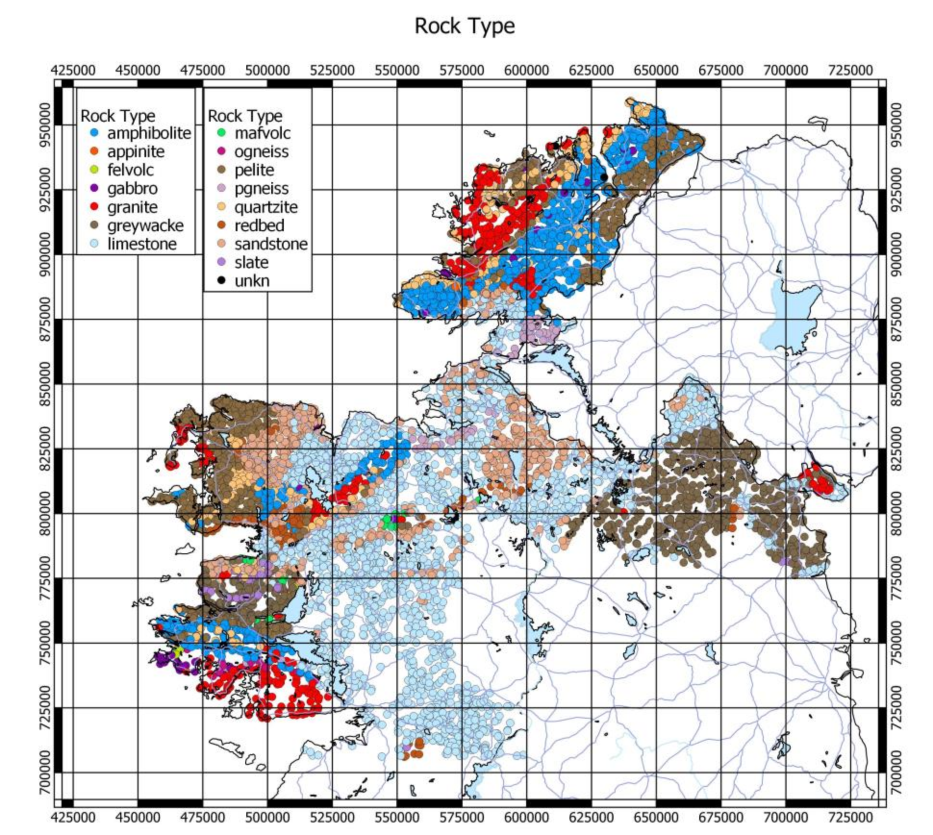
Predictive Lithologic Mapping from the Tellus data, Northwest Ireland

Gallagher, V., Grunsky, E., Fitzsimons, M., Browne, M., Lilburn, S. and Symons, J. (2021), Tellus Border and West Stream Water Data Analysis and Interpretation. Geological Survey Ireland report.

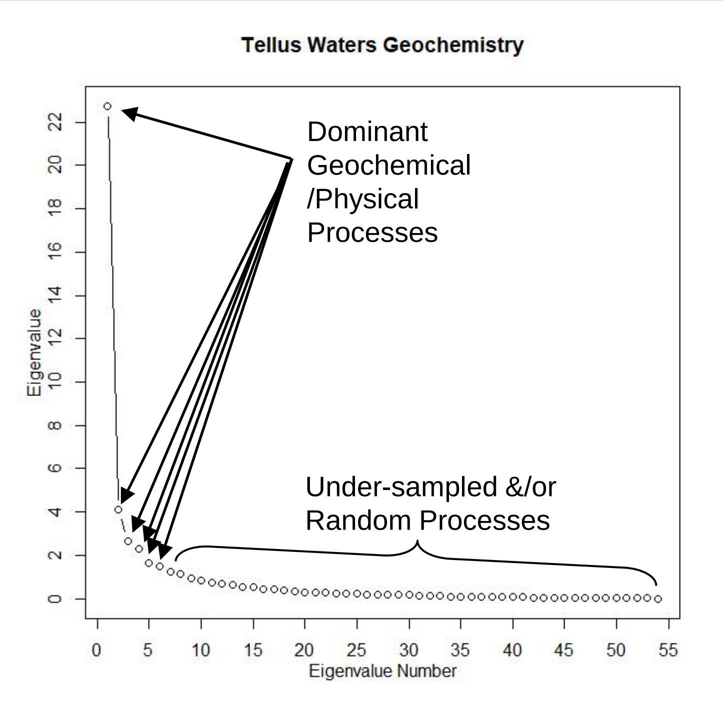
Evaluation of Tellus Waters Geochemistry Northwest Ireland

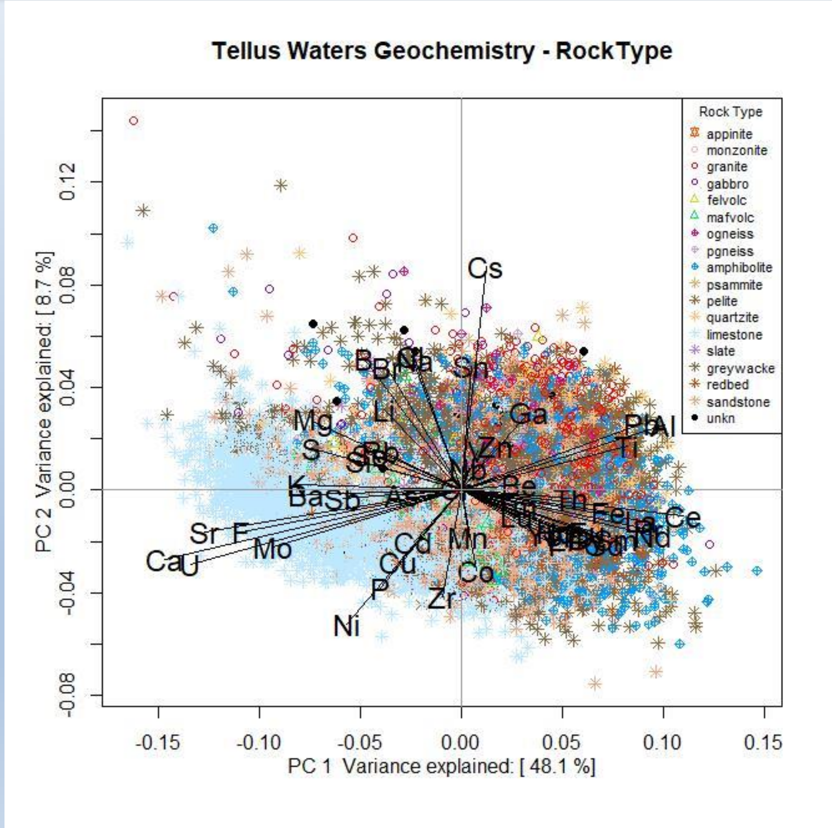
- Geological Survey of Ireland carried out a geochemical survey of surface waters.
- 6,739 stream water sites were sampled and studied.
- Intent to examine the usefulness of surface waters to reflect natural and anthropogenic influences.

Predicting Bedrock Lithologies from Tellus Waters Geochemistry

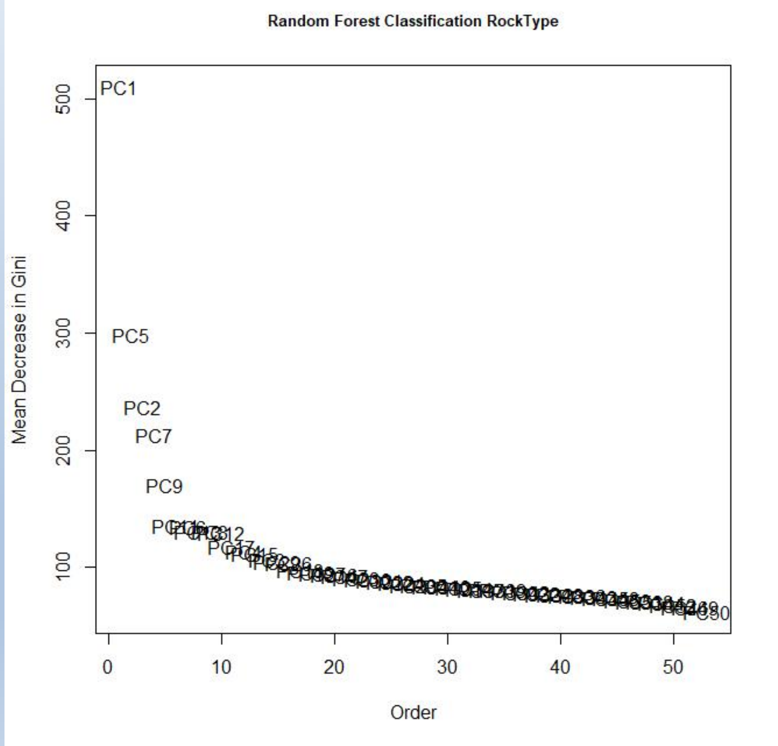


Principal Component Analysis





Random Forests Prediction of Rock Type



Waters RF Prediction - Rock Type - PCA

Counts

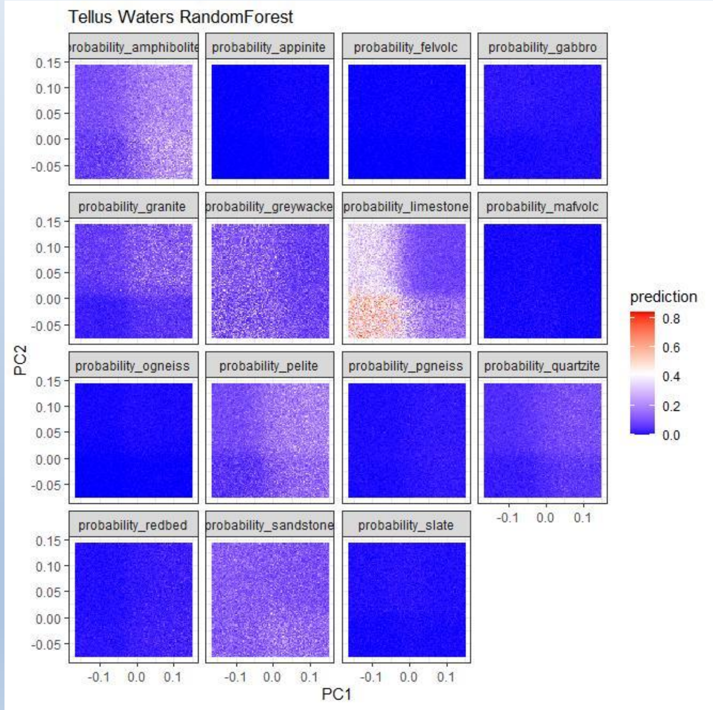
	amphibolite	appinite	felvolc	gabbro	granite	greywacke	limestone	mafvolc	ogneiss	pelite	pgneiss	quartzite	redbed	sandstone	slate
amphibolite	872	0	0	0	14	13	99	0	0	78	0	5	0	6	0
appinite	8	0	0	0	2	0	0	0	0	0	0	0	0	0	0
felvolc	2	0	0	0	1	4	0	0	0	1	0	0	0	0	0
gabbro	20	0	0	0	7	3	10	0	0	7	0	0	0	1	0
granite	60	0	0	0	318	13	41	0	0	35	0	2	0	7	0
greywacke	19	0	0	0	7	748	93	0	0	4	0	0	0	21	1
limestone	23	0	0	0	2	37	1735	0	0	2	0	0	1	63	0
mafvolc	3	0	0	0	0	10	18	0	0	0	0	0	0	5	0
ogneiss	4	0	0	0	5	1	1	0	0	5	0	0	0	0	0
pelite	242	0	0	0	16	29	61	0	0	489	0	3	0	14	0
pgneiss	35	0	0	0	0	1	20	0	0	7	6	0	0	2	0
quartzite	148	0	0	0	10	8	31	0	0	66	0	55	0	7	0
redbed	18	0	0	0	1	5	36	0	0	17	0	0	23	22	0
sandstone	69	0	0	0	0	22	338	0	0	22	0	0	0	501	0
slate	5	0	0	0	2	34	4	0	0	2	0	0	0	1	3

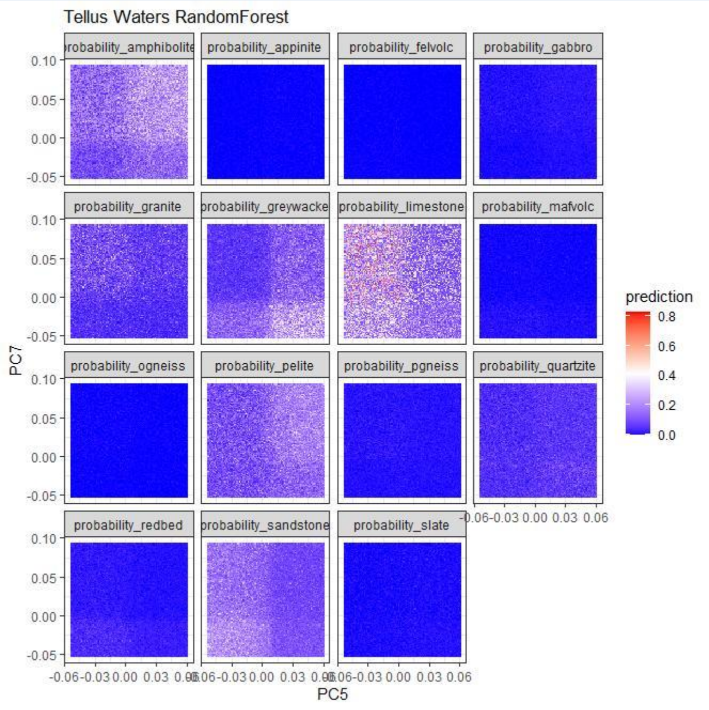
Accuracy %

	amphibolite	appinite	felvolc	gabbro	granite	greywacke	limestone	mafvolc	ogneiss	pelite	pgneiss	quartzite	redbed	sandstone	slate
amphibolite	**80.2**	0	0	0	1.3	1.2	9.1	0	0	7.2	0	0.5	0	0.6	0
appinite	80	**0**	0	0	20	0	0	0	0	0	0	0	0	0	0
felvolc	25	0	**0**	0	12.5	50	0	0	0	12.5	0	0	0	0	0
gabbro	41.7	0	0	**0**	14.6	6.2	20.8	0	0	14.6	0	0	0	2.1	0
granite	12.6	0	0	0	**66.8**	2.7	8.6	0	0	7.4	0	0.4	0	1.5	0
greywacke	2.1	0	0	0	0.8	**83.8**	10.4	0	0	0.4	0	0	0	2.4	0.1
limestone	1.2	0	0	0	0.1	2	**93.1**	0	0	0.1	0	0	0.1	3.4	0
mafvolc	8.3	0	0	0	0	27.8	50	**0**	0	0	0	0	0	13.9	0
ogneiss	25	0	0	0	31.2	6.2	6.2	0	**0**	31.2	0	0	0	0	0
pelite	28.3	0	0	0	1.9	3.4	7.1	0	0	**57.3**	0	0.4	0	1.6	0
pgneiss	49.3	0	0	0	0	1.4	28.2	0	0	9.9	**8.5**	0	0	2.8	0
quartzite	45.5	0	0	0	3.1	2.5	9.5	0	0	20.3	0	**16.9**	0	2.2	0
redbed	14.8	0	0	0	0.8	4.1	29.5	0	0	13.9	0	0	**18.9**	18	0
sandstone	7.2	0	0	0	0	2.3	35.5	0	0	2.3	0	0	0	**52.6**	0
slate	9.8	0	0	0	3.9	66.7	7.8	0	0	3.9	0	0	0	2	**5.9**

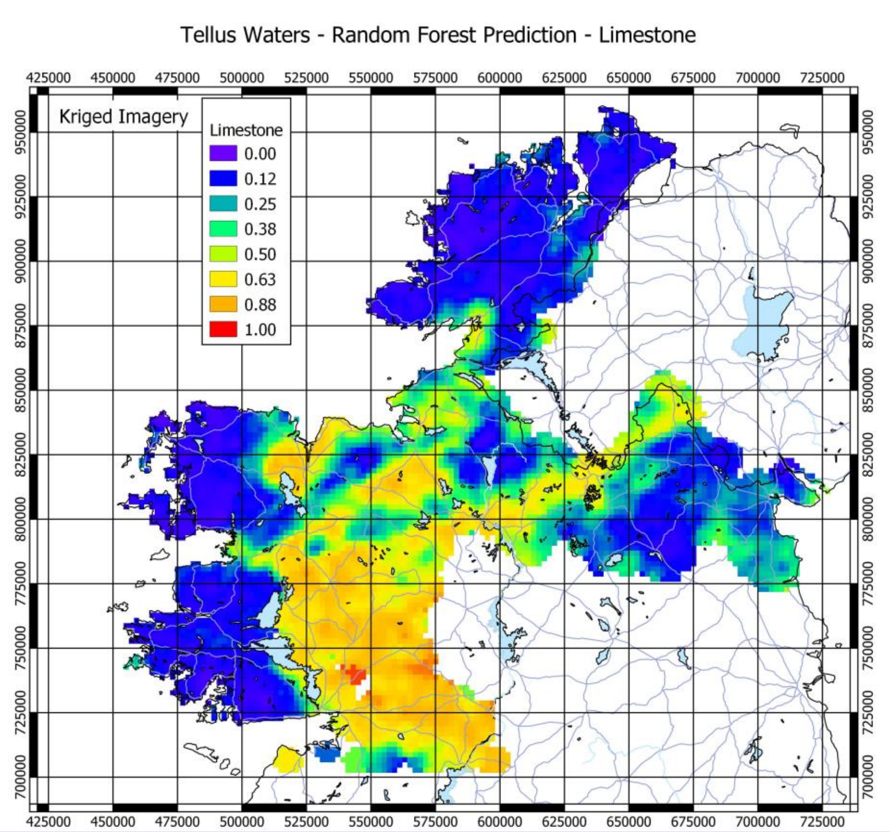
Overall Accuracy	69.73

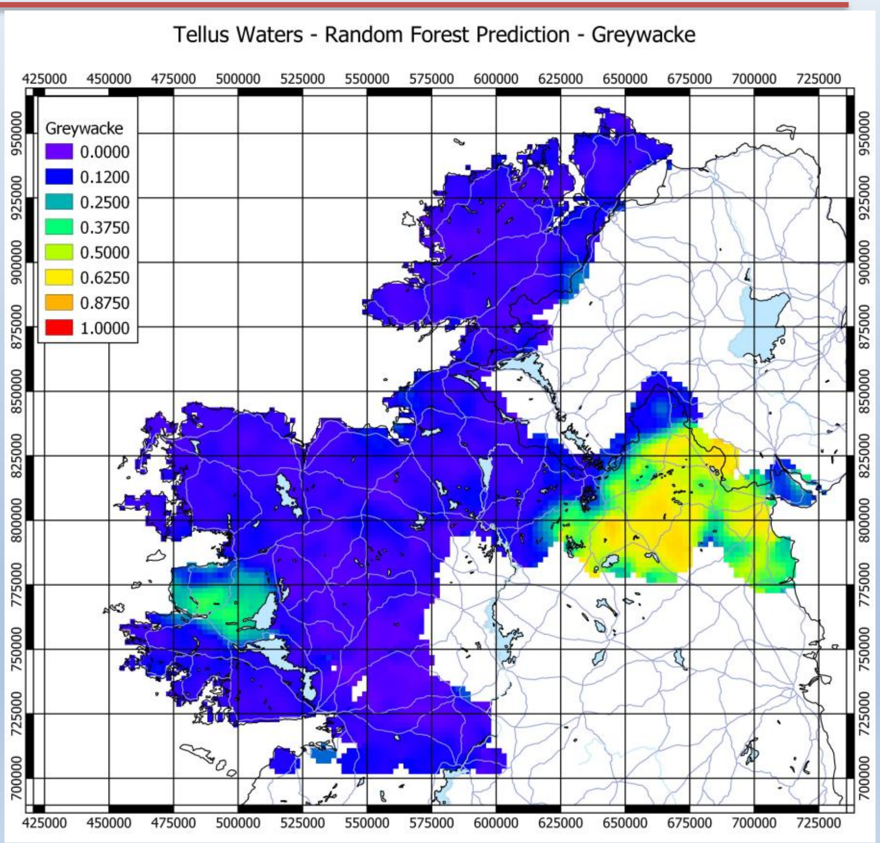
Random Forests - Prediction



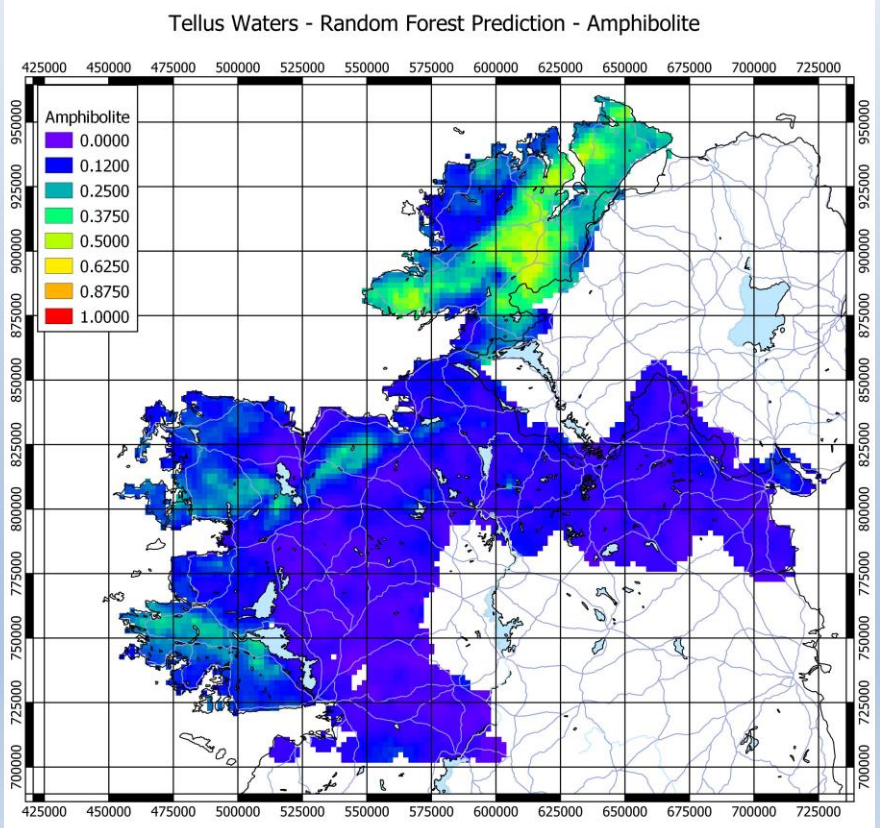


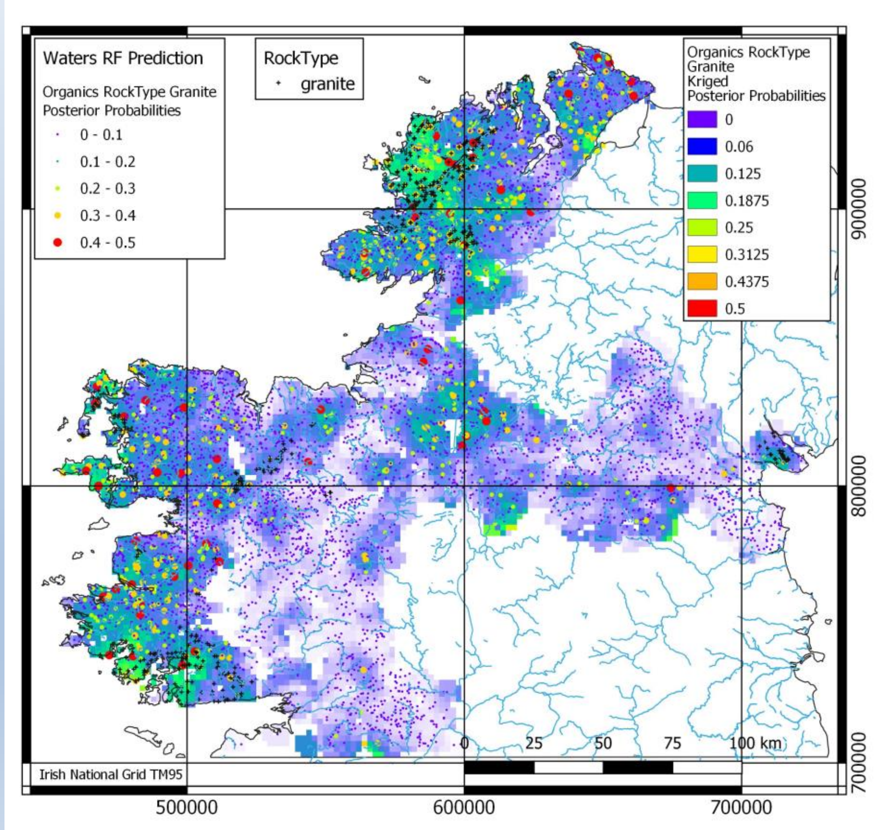
Random Forest Predictive Map





Random Forest Predictive Map





From surface sediment geochemical surveys to prediction of major crustal blocks

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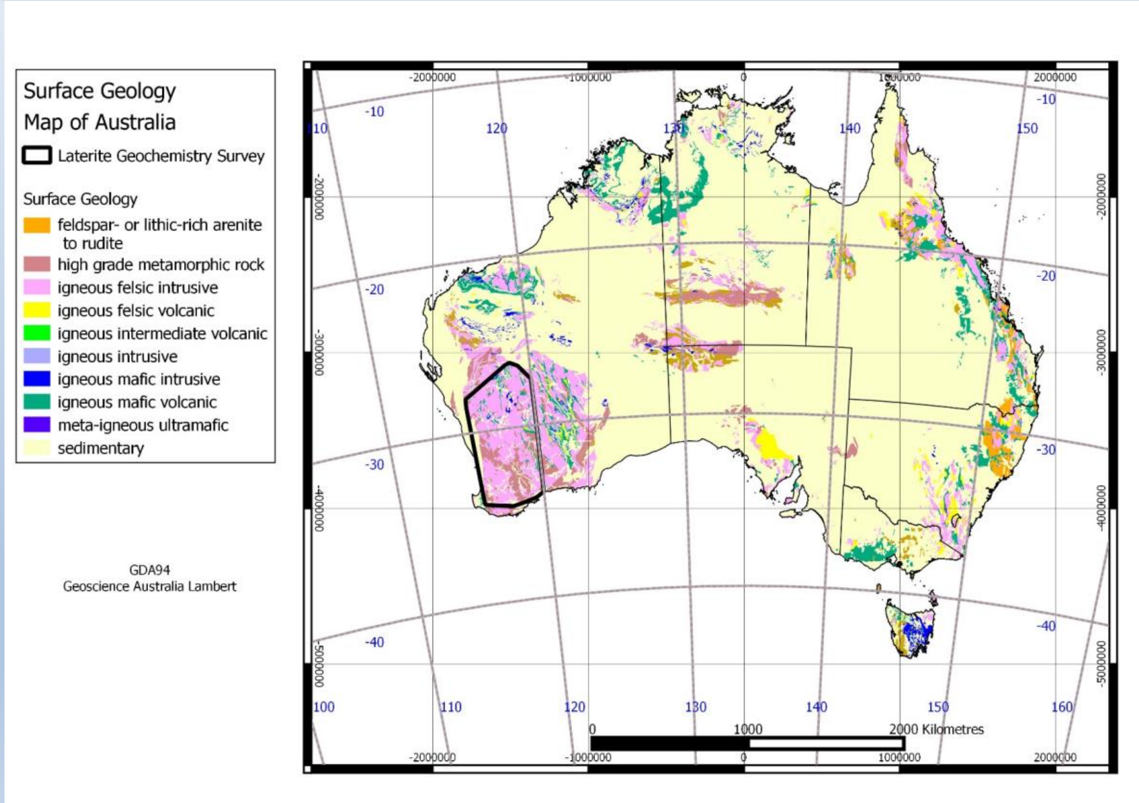
National Geochemical Survey Australia (with Patrice de Caritat, Geoscience Australia)

- National Geochemical Survey of Australia
- Geochemical composition (major, minor and trace elements) was determined on sediment samples collected as part of the National Geochemical Survey of Australia (NGSA) between 2006 and 2011 by Geoscience Australia and all States/NT geological surveys (www.ga.gov.au/ngsa).
- The NGSA collected catchment outlet (similar to floodplain/overbank) sediment samples from two depths (0-10 cm, and ~60-80 cm) in the sediment profile at 1186 sites across Australia.
- Collected samples were sieved to two grain-size fractions (<2 mm, and <75 µm) and analysed geochemically, resulting in four separate data sets (Caritat & Cooper, 2016).
- Whole-rock compositional data for 50 elements were used in this study.

Aim

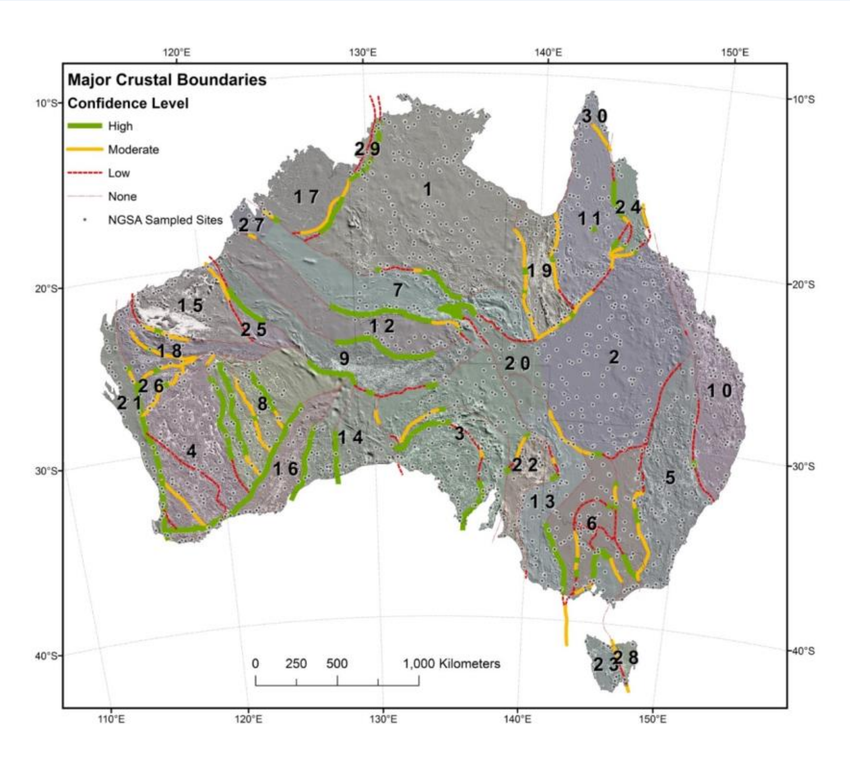
- Australia is composed of crustal blocks reflecting architecture of the continent
- National Geochemical Survey of Australia analysed surface regolith over continent
- The objective of this study is to use surface regolith compositional data for spatial prediction of membership to the major crustal blocks across the Australian continent
- Previous work has shown that the geochemistry of surficial materials (lake sediments, glacial till) can be used to define "type" compositions for the lithologies with which they represent based on statistical classification methods.

Surface Geology Map Australia



Major Crustal Blocks of Australia

- Classically interpreted from deep seismic reflection data and potential field geophysics.
- Fundamental geological units forming a continent,
- Boundaries often are crustal- or lithospheric-scale discontinuities that may act as melt and fluid conduits in a mineral system.

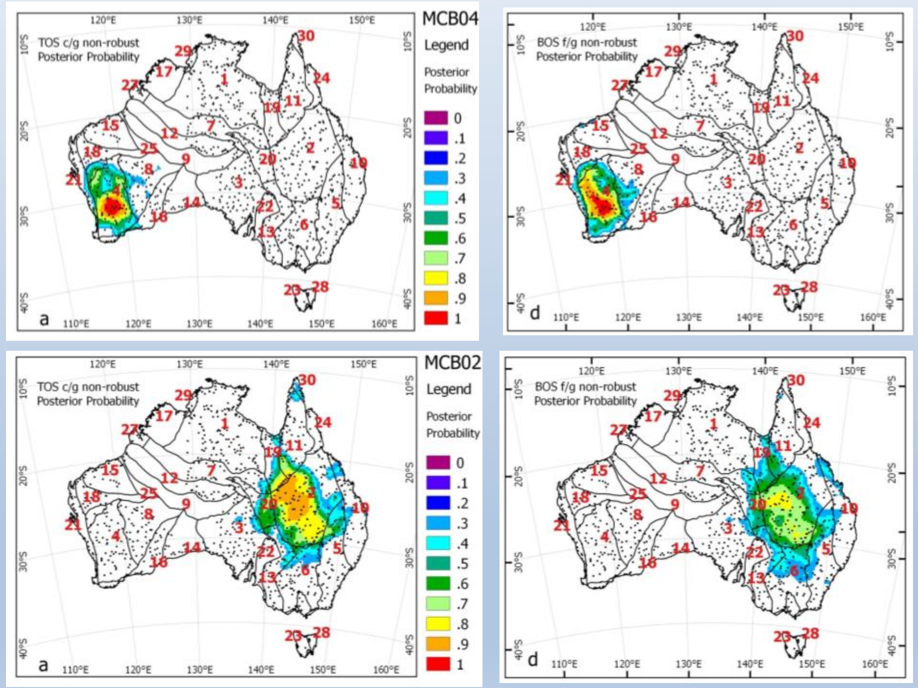


Methods

- Treat the geochemical data as compositions and apply logratio transforms.
- Compute Minimum/Maximum Autocorrelation Factors (Switzer and Green, 1984).
- Apply analysis of variance to MA factors based on MCB classification.
- Apply linear discriminant analysis to validate and provide a classification framework of the MCBs using non-   robust estimates of covariance.
- Soft indicator kriging to interpolate posterior probabilities derived from LDA.
- Derive most likely crustal block and measures of uncertainty.

Classification Accuracy

MCB	BOS c/g	BOS f/g	TOS c/g	TOS f/g
MCB01	0.81	0.85	0.87	0.82
MCB02	0.71	0.72	0.74	0.80
MCB03	0.67	0.69	0.67	0.74
MCB04	0.57	0.69	0.72	0.69
MCB05	0.41	0.24	0.42	0.44
MCB06	0.55	0.54	0.40	0.45
MCB07	0.42	0.53	0.53	0.56
MCB08	0.62	0.72	0.69	0.69
MCB10	0.42	0.44	0.46	0.63
MCB11	0.32	0.32	0.30	0.44
MCB12	0.48	0.48	0.39	0.30
MCB13	0.18	0.29	0.21	0.26
MCB14	0.83	0.89	0.94	0.89
MCB15	0.72	0.64	0.60	0.48
MCB16	0.19	0.26	0.23	0.19
MCB18	0.60	0.65	0.60	0.70
MCB19	0.16	0.12	0.04	0.16
MCB20	0.32	0.21	0.26	0.47
MCB21	0.56	0.44	0.49	0.62
MCB22	0.10	0.15	0.15	0.25
MCB23	0.33	0.43	0.29	0.24
MCB24	0.14	0.14	0.29	0.36

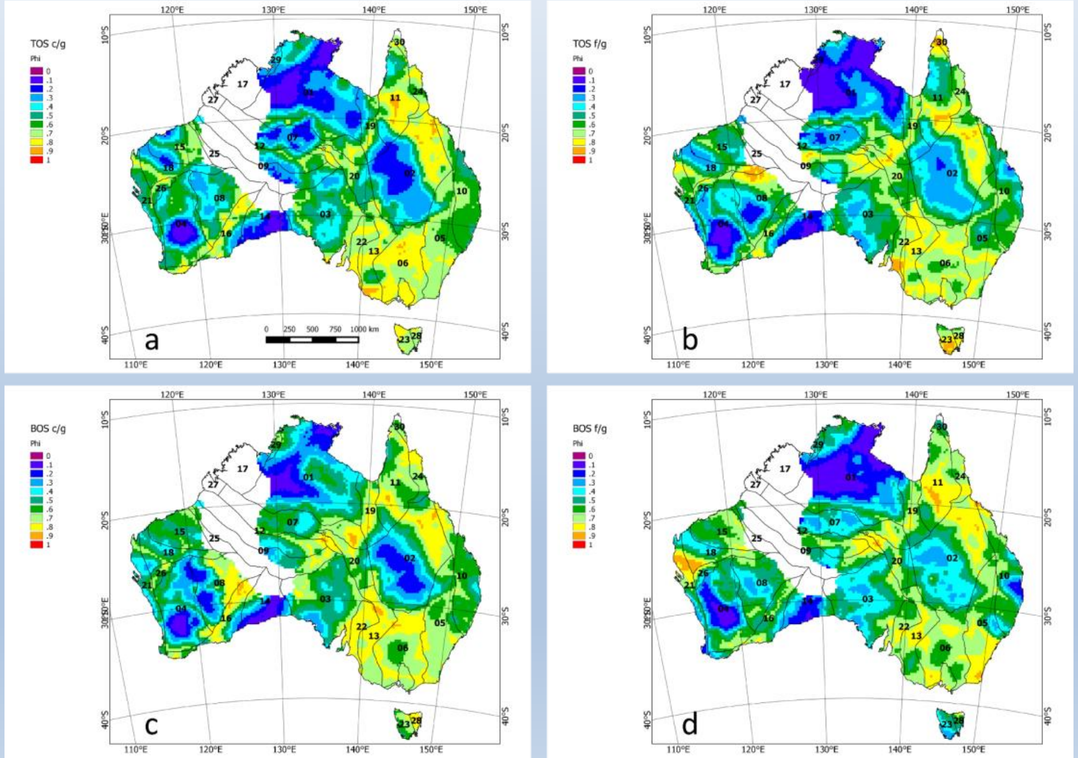


Posterior Probabilities, MCB04, MCB02, TOS c/g (left) and BOS f/g (right)

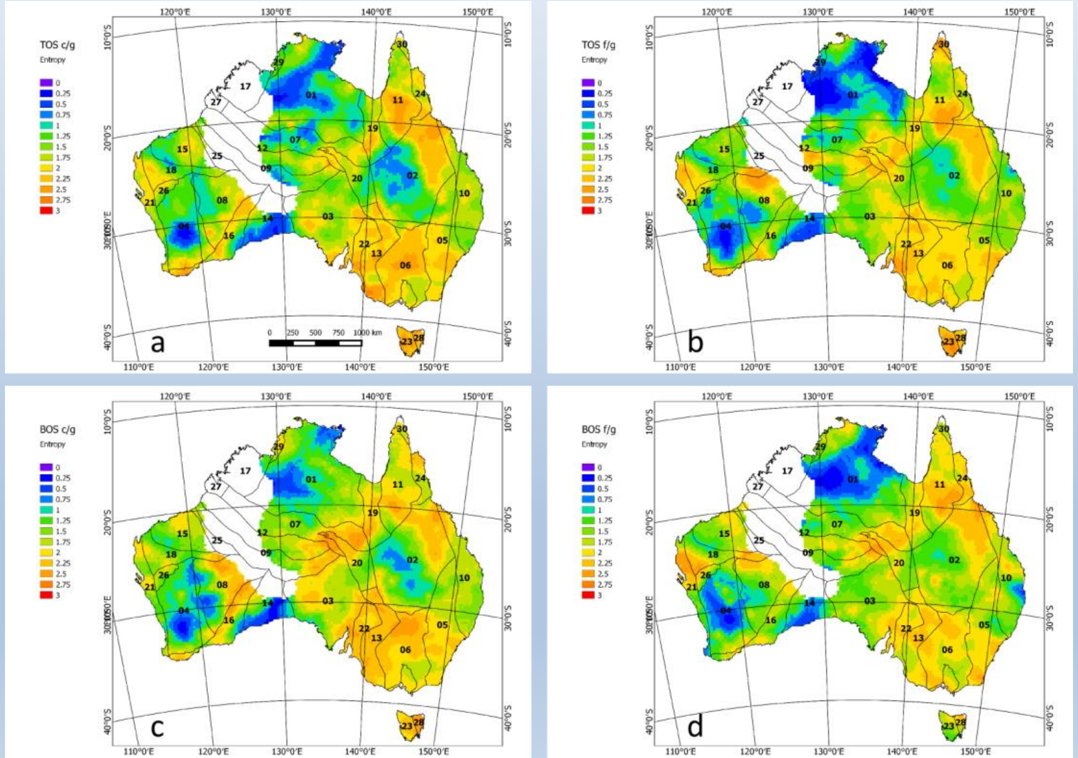
Measure of Uncertainty

- From the estimated posterior probabilities the following measures of spatial uncertainty about the allocation of a location to a specific MCB were computed:
- Local classification of uncertainty: $\varphi(x) = 1 - max_m(p_m(x))$
- Local entropy, given by $H(x) = -\sum_{i=1,p_i(x)\neq 0}^{K} p_i(x)\ln(p_i(x))$
- K denotes the number of classes
- The local classification uncertainty attains values from 0 to 1 and is close to 0 when class membership is reasonably certain. Similarly, the local entropy provides a measure of local randomness. The maximum value is given by $\ln K$, which is attained when all K MCBs are equiprobable, and its minimum value is 0, when the MCB is certain.

Measures of Uncertainty ($\boldsymbol{\varphi}$)



Measures of Uncertainty (Entropy)



In Conclusion …

- Geochemical survey data are well suited for identifying processes associated with mineralogy, weathering, transport.
- The use of multi-element geochemistry enables the recognition of processes through combinations of elements that reflect mineral stoichiometry. Soils, stream sediments, lithogeochemistry, laterite, etc. all have distinct mineral associations and are reflected in the inter-element associations.
- The geospatial association of geochemical survey sites with measures of underlying geology and surficial processes record the influence of igneous, sedimentary, mineralizing processes and the subsequent interaction with the biosphere (ecosystem) and climate.
- The use of advanced analytics and machine learning methods enhance the ability to "Discover" and "Validate/Predict" processes.
- The results demonstrated from predictive mapping confirm the capacity of geochemical data to test new hypotheses from which new geological/geochemical process maps can be created
- The establishment of training sets (specific lithologies, alteration, soils, ecosystems, landforms, climate) can assist in the study and prediction in areas where there is a lack of information.
- Overlap between classes (e.g. lithologies) is expected and the use of posterior probabilities can identify the degree of distinctiveness and overlap.
- The use of advanced analytics and machine learning methods provide an objective, repeatable and defensible framework from which processes can be identified, predicted and validated.

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Thanks for you attention.

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