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REPORT

Report no.: 2000.84 | ISSN 0800-3416 | Grading: Open

Title:
Prediction of the spatial structure of censored data by robust statistical methods

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Client:
Ministry of the environment/NGU

County:
Finnmark (N-Finland, NW-Russia)

Commune:

Map-sheet name (M=1:250.000)
None

Map-sheet no. and -name (M=1:50.000)

Deposit name and grid-reference:

Number of pages: 43 Price (NOK): 215,-
Map enclosures:

Fieldwork carried out:	Date of report:	Project no.:	Person responsible:
1995	07.08.2000	2590.02	

Summary:

Censored data are a well-known problem when dealing with regional geochemical data. Often many analytical results for some of the most interesting variables, for example gold (Au), are reported as below detection limits. With a high proportion of censored data, distribution estimators and many statistical tests will not perform. The regional structure of the data as displayed in a geochemical map may also get lost or be a poor approximation of reality. However, very many other variables are often available from the same sample sites. A method to recover censored data, based on robust principal component analysis (PCA) and robust multiple regression is introduced. All other available information from each sample site is used to predict the censored data. It is first used to recover the regional data structure for a test data set where the regional distribution is known. Subsequently it is used to predict the regional data structure for a number of elements in topsoil and C-horizon samples from the Kola Project where a large proportion of the reported analytical results was below detection. Although the method tends to an overestimation of the predicted values, the regional structure of the data can be recovered, thus permitting more effective use of the geochemical maps in mineral exploration campaigns.

Keywords: Kola Peninsula	Censored data	Multiple regression
Geochemical mapping	Detection limit	Prediction
Robust statistics	C-Horizon	Topsoil

CONTENTS

1. INTRODUCTION

When analysing geological samples, censored data, i.e., caused by a high proportion of samples returning values below detection, are a difficulty commonly encountered for a number of elements. In a first attempt to deal with the problem, geochemists often tend to replace all results below the detection limit with the value of the actual detection limit or ½ of that value. Doing this, at least the information that a low concentration can be expected at this sample site is preserved and geochemical maps covering all sample locations can be drawn. Statistically, however, this approach is not acceptable. A high proportion of censored data results in many problems in conventional statistical analysis (e.g., Cohen, 1959; El-Shaarawi, 1989; El-Shaarawi and Esterby, 1992; Helsel and Hirsch, 1992). For example, all estimators of location and spread will be seriously biased. A number of techniques have been suggested to predict censored data (e.g., Miller, 1976; Dempster et al., 1977; Buckley and James, 1979; Schmee and Hahn, 1979; Aitkin, 1981; Stein, 1992; Militino and Ugarte, 1999). As long as information about the censored part of the data population is only needed for a more reliable estimate of location or for statistical tests, the problem is relatively easy to overcome. For example the cumulative distribution function can be used to predict median and percentiles for censored data.

In geochemical mapping, however, the problem is different. When strongly censored data are used for geochemical mapping, noisy maps, showing little or no regional structure, will be the result, even when smoothing methods like kriging are used to produce a smoothed surface map (see Reimann et al., 1998). The problem cannot be overcome by estimating the population because for geochemical mapping, a concentration at each individual sample site is needed. Strongly left-censored data were encountered for a number of interesting elements (e.g., As, Au, Cs, Hg, Mo, Sb, Ta, U) in a large environmental geochemical mapping project in the European Arctic. From 1992-1998 the Geological Surveys of Finland (GTK) and Norway (NGU) and the Central Kola Expedition (CKE) in Russia carried out a major geochemical mapping project (see World Wide Web site http://www.ngu.no/Kola) across a 188,000 km^2 area north of the Arctic Circle (Figure 1). In the summer and autumn of 1995, terrestrial moss, topsoil (0-5 cm), organic topsoil (humus 0-3 cm or less if the organic layer was thinner than 3 cm) and complete podzol profiles (5 horizons) were sampled throughout the survey area. The average sampling density was one station per 300 km^2. The whole data set describing the regional

distribution patterns of up to 50 elements in 5 different sample media is available in the form of a geochemical atlas (Reimann et al., 1998). Table 1 summarises the complete analytical program for topsoil and C-horizon samples and gives an indication for which elements severely censored data were encountered due to insufficient detection limits.

When more than about 30-40% of all values were below detection, the resulting geochemical maps were generally noisy and had so little information value that many were not shown in the geochemical atlas (Reimann et al., 1998). The alternative was to show black and white point source maps marking the location of the high outliers. These maps are collected in Reimann (1998). However, the regional data structure, as revealed in a complete geochemical map, can give important hints about element sources and enrichment processes. Thus the question arises whether or not it is possible to predict the "lower", censored end of a data distribution with high enough reliability to recover at least this regional structure. For this purpose it is not necessary to get an exact estimate of concentration at each site.

For estimating censored data, regression methods based on ordinary least squares (OLS) have been used (Miller, 1976; Buckley and James, 1979; Koul et al., 1981). A method called tobit regression (Judge et al., 1985; Cohn, 1988) is similar to OLS, with the exception that the coefficients are fitted by maximum-likelihood estimation. However, these methods, including the sometimes suggested logistic regression (Helsel and Hirsch, 1992), are still sensitive with respect to data outliers and do not perform well if more than 25-50% of the data are censored. Extreme data outliers and a very high proportion of censored data are, however, very typical when dealing with, for example, gold analyses. Even one single data outlier (which is sufficiently large) can cause complete breakdown of classical estimators. An easy way for still obtaining stable results is to remove this outlier. However, there are not many situations where outliers are obvious at first glance. In general it is extremely difficult to identify “multivariate” outliers, and usually computationally intensive robust methods must be used for this task (Rousseeuw and Van Zomeren, 1990).

Another approach, functioning with higher portions of censored data, uses the Expectation-Maximisation (EM) algorithm (Dempster et al., 1977). By assuming an idealised data distribution (e.g. log-normality), an alternating scheme is applied for estimating the censored data. Militino and Ugarte (1999) generalised this algorithm to spatial data. The resulting estimations are, however, based on the least squares criterion, and thus also quite sensitive

with respect to outliers. In addition regional geochemical data show almost never a normal or a log-normal distribution (Reimann and Filzmoser, 2000).

Thus a different approach, able to handle a high proportion of censored data, imprecise measurements and extreme data outliers is needed. This situation calls for the use of robust statistical techniques that are not sensitive with respect to data outliers. These methods will, of course, also work for "clean" data although the statistical efficiency is in general lower than for classical methods. The basic principle of robust methods is to fit the majority of the data. Robust statistics allows for deviations from strict parametric models and can thus be seen as a compromise between parametric and nonparametric statistics (e.g., Hampel et al., 1986).

One possibility for robustly estimating censored data is to treat the data as a contingency table. By assuming that each entry in the table consists of a general mean, a row effect, a column effect, and an error term, the cells with censored data can be estimated. Croux and Filzmoser (1999) developed a method for robustly estimating such cells based on robust alternating regression. However, if one column (or row) includes more than 25% censored data, this method will not give reliable results.

An alternative is to use robust regression for the prediction. Nowadays a variety of robust regression techniques exist which are also fast to compute (Rousseeuw and Leroy, 1987). As a general rule, these techniques require more observations than variables. In practise the number of observations should be at least twice as large as the number of variables or more, depending on the method. When dealing with a large amount of censored data and a large number of available predictor variables, as it is the case for the Kola data, this prerequisite is not fulfilled. The use of only some selected predictor variables may cause loss of information. In such a case the most important information of the complete data set can be extracted by first performing a robust principal component analysis (PCA) on the predictors. Like all other robust methods a robust PCA has the advantage of not being influenced by data outliers. The robust PCA method used here is based on the idea of projection pursuit and was introduced by Li and Chen (1985). Filzmoser (1999) successfully used a slightly modified method (Croux and Ruiz-Gazen, 1996) for the Kola data set. This method has several further advantages. For example the number of observations can be smaller than the number of variables; it is not necessary to compute all principal components, i.e., one can stop at a desired number of components, and a fast algorithm exists already (Croux and Ruiz-Gazen, 1996).

In this report a statistical method is used based on a combination of robust PCA and robust regression, using all other available information to predict one censored variable in order to:
- Test the method by using a variable where all data are known but the lower 50, 60, 70 and 80% of the distribution were deleted and then predicted. Regional smoothed surface geochemical maps are constructed using the original and the predicted values (80% deleted).
- Predict the missing results for the exploration-relevant elements As, Au, Cs, Hg, Mo, Sb, Ta, U and Zn in Topsoil and/or C-horizon samples from the Kola project, and to construct regional maps based on these results. Note that the regional structure cannot be recovered for elements where more than about 80% of all analytical results are below detection.

2. THE KOLA PROJECT DATA

Sampling

A detailed description of the sample-site selection criteria and the sampling method is given in Äyräs and Reimann (1995) and in Reimann et al. (1998). Complete podzol profiles were dug at carefully selected sites and about 2 kg of the C-horizon material was sampled. The samples were air dried and subsequently sieved to <2 mm using nylon screening. Topsoil samples were taken from the uppermost 5 cm of the soil layer, independent of soil horizons. A large composite sample from at least 10 sites within a 100 m x 100 m area was taken. The samples were air dried and sieved to <2 mm using nylon screening.

Chemical analyses

Analytical procedures and all analytical results are detailed in Reimann et al. (1998). In short, a 2 g subsample of the <2 mm fraction of the C-horizon samples was digested in aqua regia (3:1 HNO_3:HCl) at 90^o C at the GTK laboratory. The solutions were analysed by ICP-AES for 32 elements (Niskavaara, 1995), and by graphite furnace atomic absorption spectrometry (GFAAS) for Ag, As, Cd and Pb. A second aliquot was analysed after pre-concentration using reductive co-precipitation (Niskavaara and Kontas, 1990) for Bi, Sb, Se and Te by GFAAS. Aqua regia extraction will not result in total element concentrations. The analysed values will strongly depend on the differences in mineralogy between samples, and will generally reflect secondary geochemical processes such as weathering, scavenging of elements by Fe-oxides/hydroxides and/or the amount of sulphides and clay minerals in the individual sample.

Furthermore the C-horizon samples were analysed for major elements (Al, Ca, Fe, K, Mg, Mn, Na, P, Si, Ti) by XRF in NGU laboratory. Both topsoil and C-horizon samples were analysed for more than 30 other elements using instrumental neutron activation analyses (INAA) by Activation Laboratories Ltd. in Canada. These two techniques result in total element concentrations that will largely be governed by geological processes. Table 1 summarises the complete analytical program for topsoil and C-horizon samples, showing the detection limits and the percentage of samples below detection as well as indicating which elements have been included as explanatory variables in this study.

Data Analysis

For robust PCA and robust multiple regression analysis the S-PLUS software package (Mathsoft – http://www.splus.mathsoft.com/, Venables and Ripley, 1997) was used. For variables with a low percentage of values below detection, results for these samples were set to ½ of the detection limit. All geochemical maps were produced using the DAS®-software package (Dutter et al., 1992). Kriging was performed using the software package GEOSAN (Dutter, 1996). For the maps using the original Au data another approach to mapping was used. These values are mapped with just one symbol, an expanding dot, whose size grows in relation to concentration as suggested by Björklund and Gustavsson (1987).

3. ROBUST PCA AND ROBUST REGRESSION TO PREDICT CENSORED DATA

In the following, a brief description of the methods used to predict the censored data is given. As a first step the raw data are log-transformed and standardised to at least approach normality and avoid problems with heteroscedasticity. Let $X = \{x_1, x_2, \mathrm{K}, x_n\}$ be a data matrix with the observations $x_i \in \Re^p$ $(i = 1, \mathrm{K}, n)$. Assume that the first (k-1) projection directions (i.e. robust estimations of the eigenvectors) $\hat{\gamma}_1, \mathrm{K}, \hat{\gamma}_{k-1}$ are already known. Then a projection matrix is defined by

$$P_1 = I_p, \qquad P_k = I_p - \sum_{j=1}^{k-1} \hat{\gamma}_j \hat{\gamma}_j^{\mathrm{T}} .$$

P_k stands for projection on the orthogonal complement of the space spanned by the first (k-1) projection directions. The *k*-th projection direction is then defined as the maximum of the function

$$a \rightarrow S_n(x_i^{\mathrm{T}} a; 1 \le i \le n)$$

under the conditions $a^{\mathrm{T}} a = 1$ and $P_k a = a$. The latter condition ensures orthogonality to previously found projection directions. S_n is a robust measure of spread, e.g., the median absolute deviation (MAD). For a sample $\{y_1, \mathrm{K}, y_n\} \subset \Re$ the median absolute deviation is defined as

$$\mathrm{MAD}_n(y_1, \mathrm{K}, y_n) = 1.486 \operatorname*{med}_i | y_i - \operatorname*{med}_j y_j |$$

where the constant 1.486 is a consistency factor for normal distribution. Taking the classical sample standard deviation for S_n would result in classical PCA.

Croux and Ruiz-Gazen (1996) also give an algorithm for the above maximisation problem since in general no exact solution exists. Instead of scanning the whole space of possible solutions, it is proposed to check for directions *a* belonging to the set

$$A_{n,k}(X) = \left\{ \frac{P_k(x_i - \hat{\mu}_n(X))}{\left\| P_k(x_i - \hat{\mu}_n(X)) \right\|}; 1 \le i \le n \right\}.$$

$\hat{\mu}_n$ is a robust location estimator like the L_1-median which is defined by

$$\hat{\mu}_n(X) = \operatorname*{minimize}_{\mu \in \Re^p} \sum_{i=1}^{n} \left\| x_i - \mu \right\|.$$

It is very robust (breakdown value 50%) and orthogonally equivariant (Hössjer and Croux, 1995). As a simple but crude approximation one could also take the median of each component.

Robust PCA reduces the number of variables to a number $k < p$ of components $\{(z_{i1}, \mathrm{K}, z_{ik}); 1 \le i \le n\}$ including the main variation of the data set. For choosing *k* the same rules as used in classical PCA can be applied (e.g., the scree-plot; Jackson, 1991). These principal components (PCs) can now be used as predictors for the censored variable (response). Note that the problem of co-linearity can never occur because the PCs are orthogonal to each other. Since the prediction should not be influenced by outlying observations, robust regression is advisable. Very robust regression techniques with good statistical properties are LMS (least median of squares) and LTS (least trimmed squares) regression (Rousseeuw, 1984). For the latter a fast algorithm was developed recently (Rousseeuw and Van Driessen, 1998).

Suppose that *n-m* out of *n* observations of the response variable are below the detection limit. Without loss of generality, these *n-m* observations can be arranged as the last observations in the original data set (and hence the same arrangement for the PCs). For regression only the first m values can be used. The residual r_i of observation i $(1 \le i \le m)$ is defined as the difference between the observed response value y_i and the corresponding fitted value, hence

$$r_i(\hat{\beta}_0, \mathrm{K}\,, \hat{\beta}_k) = y_i - (\hat{\beta}_0 + \hat{\beta}_1 z_{i1} + \hat{\beta}_k z_{ik})\,.$$

The regression coefficients $\beta_0, \beta_1, \mathrm{K}\,, \beta_k$ are estimated according to the LTS criterion which is given by

$$\underset{(\hat{\beta}_0, \mathrm{K}\,, \hat{\beta}_k)}{\text{minimize}} \sum_{i=1}^{h} (r_i^2)_{i:m}$$

where $(r^2)_{1:m} \le (r^2)_{2:m} \le \Lambda \le (r^2)_{m:m}$ are the ordered squared residuals. The LTS criterion resembles that of least squares but does not count the largest squared residuals, thereby allowing the LTS to steer clear of outliers. A choice of $h \approx 0.75 \cdot m$ is a good compromise between robustness and statistical efficiency. Although the parameter estimations are not consistent because the observations are spatially dependent this robust regression method will still give quite reliable results.

At the basis of the estimated regression coefficients $\hat{\beta}_0, \mathrm{K}\,, \hat{\beta}_k$ and because the complete matrix of principal component scores is available, the values of the response variable below the detection limit can be predicted by

$$y_i = \hat{\beta}_0 + \hat{\beta}_1 z_{i1} + \hat{\beta}_k z_{ik}$$

for $i = m+1, \mathrm{K}\,, n$. The result is a set of predicted data for the censored part of the distribution. This is combined with the upper existing data and then used for geochemical mapping. This approach guarantees that the original real information is not lost but used in the maps.

The quality of the fit can be determined by the coefficient of determination also called R^2. For the LTS this is a robust measure which is defined by:

$$R^2 = 1 - \frac{\sum_{i=1}^{h} (r_i^2)_{i:m}}{\sum_{i=1}^{h} \left((y_i - \tilde{y})^2 \right)_{i:m}}$$

where the denominator has to be minimised over $\tilde{y}$ (Rousseeuw and Leroy, 1987).

4. TEST

To test the prediction quality of the suggested method, several elements (Ag, As, Bi, Cr, Pb) without any censored data were used. As an example, Fig. 2 (upper left) shows the CDF-diagram for Cr, analysed by INAA. To simulate a detection limit problem, first the lower 50% and then the lower 60%, 70% and 80% of all values were deleted (Fig. 2 – upper right: Cr with 80% of the data deleted), and then predicted using the remaining values and all other available variables. For the example Cr with 80% censoring the robust coefficient of determination was 0.7. This indicates that the fit for the existing data is quite good. A detailed analysis of the residuals is shown in Fig. 3. The structure of the plot is influenced by the fact that the laboratory delivered Cr-concentrations rounded to 10 mg/kg steps above 100 mg/kg (see CDF-diagram for Cr, Fig. 2). The plot shows clearly the existence of outliers which are plotting outside the critical values ±2.5. Fortunately such outliers do not influence robust regression.

Because the regression model used for the prediction is fitted to the upper 20% of the data only, an increasing tendency to overestimated concentrations at the lower end of the distribution was observed. One of the reasons can be visualised in the CDF-diagram for Cr (Fig. 2) where several breaks occur in the curve. This problem could not be overcome and requires further research. It means that the actual concentration at each site cannot be reliably predicted. However, most of the data structure as visible in the maps could be recovered. Figure 4 shows as an example two maps for Cr. One is based on the original data the second one on the predicted concentrations, combined with the original values from the upper 20% of the distribution. The map based on the predicted concentrations demonstrates that the original regional structure is still visible. The actual concentrations, however, have changed significantly at the lower end of the distribution. All other elements tested (Ag, As, Bi, and Pb) showed comparable results. The upper limit for a "successful" prediction of the regional data structure was between 70% and 80% of censored data. As this value depends on the

predicted element and may also depend on the number of available variables for the prediction it may be special for the Kola data set and should not be taken as a generalisation.

5. APPLICATION FOR GOLD

Following the successful test, the regional structure for Au was predicted for the C-horizon and the Topsoil samples. The original data distributions of the Au analyses in C-horizon and Topsoil samples as received from the laboratory are given in Fig. 2 (lower two CDF-diagrams). Figure 5 shows a combination of Au maps. The upper maps show the original Au values as point source map, based on the "growing dot technique" (Bjørklund and Gustavsson, 1987). In the middle, kriging (Journel and Huijbregts, 1978) is used to produce smoothed colour surface maps. Both maps show the extremely "noisy" nature of the gold data. They can hardly be used to detect any regional structure in the data. Only some "hot spots" can be defined. Figure 6 shows the variograms obtained when using these data. These variograms indicate that the regional distribution is governed by the well-known nugget effect. The nugget effect is an artefact of insufficient precision in sampling and analysis (Harris, 1982) and not a necessary characteristic of the regional gold distribution. No regional structure exists in these data. The lower two variograms (Fig. 6) show the situation after the real data were combined with the predicted concentrations for the censored part of the distribution. A regional dependency is now visible. The lower two smoothed surface maps (Fig. 5) are based on the predicted concentrations, combined with the existing data and were kriged using these variograms. Both maps show a very clear regional structure, which could, for example, be used for developing gold exploration concepts for this area. For Au the robust coefficient of determination was 0.4 for the C-horizon and 0.45 for the Topsoil.

6. APPLICATION FOR OTHER ELEMENTS

Given the good results obtained so far, the technique was subsequently used routinely to recover the regional structure for a number of other elements that showed severe detection limit problems (see Table 1), but that are of great interest for mineral exploration. Table 2 summarises for which elements the prediction was carried out and gives the coefficients of determination. In figures 7 to21 the resulting colour surface maps are presented in the same format as used for the colour maps given in the Kola Atlas (Reimann et al., 1998).

7. CONCLUSIONS

A combination of robust PCA and robust multiple regression analysis can be used to recover information on the inherent regional data structure even for strongly left-censored variables. Although the actual concentrations will be overestimated because the model is build on the upper end of the data distribution, the geochemical map will still show the regional distribution for the predicted element. Results get better when many explanatory variables are available. For the Kola data set, even with up to 80% of censored data, the regional structure could be successfully recovered. The recovery of the regional data structure will allow much more effective use of the resulting geochemical maps from censored data in regional mineral exploration campaigns.

8. ACKNOWLEDGEMENTS

The authors wish to thank the Kola Ecogeochemistry team for their assistance both in the field and in the laboratory, and for many interesting discussions. R. Dutter's assistance with variograms and kriging and his many helpful comments were highly appreciated. N. Cook improved the English presentation of this manuscript and provided us at the same time with a very useful review. The Norwegian participation in the Kola Project was financed by the Norwegian Ministry of the Environment and with special project funds from the Norwegian Ministry of Foreign Affairs. Support by the Vienna University of Technology for C.R.'s stay in Vienna was highly appreciated.

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10. TABLES

Table 1: Analytical program for the C-horizon and the Topsoil samples, Kola Project. DL: detection limit, % < DL: percentage of samples that reported below the detection limit.

Table 2: Predicted variables for topsoil and C-horizon and coefficient of determination.

11. FIGURES

Figure 1: General location map of the Kola Project area.

Figure 2: Cumulative distribution function (CDF-) diagrams for: upper left: Cr, original data; upper right: Cr after removal of 80% of the data at the lower end (artifical censoring), lower left: Au in the C-horizon (original data); lower right: Au in Topsoil (original data).

Figure 3: Residual plot of LTS regression for Cr with 80% of censored data.

Figure 4: Maps showing the original regional distribution of Cr in the C-horizon samples and the regional map based on predicted values; 80% of all values at the lower end of the distribution were removed and then predicted.

Figure 5: Maps showing the regional distribution of Au in the C-horizon and Topsoil from the Kola Project area. Upper maps: original data mapped using the growing dot technique (Björklund and Gustavsson, 1987); middle: kriged smoothed surface maps using the original data, lower maps: kriged smoothed surface maps using the original and predicted values.

Figure 6: Variograms as obtained when using the original data and the predicted values.

Figure 7: As in topsoil, 62.9% of all results were below detection.

Figure 8: As in C-horizon, 71.9% of all results were below detection.

Figure 9: Au in topsoil, 74.4% of all results were below detection.

Figure 10: Au in C-horizon, 72.4% of all results were below detection.

Figure 11: Cs in C-horizon, 61.4% of all results were below detection.

Figure 12: Hg in C-horizon, 56% of all results were below detection.

Figure 13: Mo in C-horizon, 76.5% of all results were below detection.

Figure 14: Sb in topsoil, 50.6% of all results were below detection.

Figure 15: Sb in C-horizon, 75.1% of all results were below detection.

Figure 16: Ta in topsoil, 78.1% of all results were below detection.

Figure 17: Ta in C-horizon, 78.4% of all results were below detection.

Figure 18: U in topsoil, 64.1% of all results were below detection.

Figure 19: U in C-horizon, 48.8% of all results were below detection.

Figure 20: Zn in topsoil, 68.5% of all results were below detection.

Figure 21: Zn in C-horizon, 39.1% of all results were below detection.

ELEMENT	NAME	UNIT	METHOD	DL	% < DL C-horizon	USED	% < DL Topsoil	USED
Ag	Silver	mg/kg	aqua regia, GF-AAS	0.001	0.2	YES	na	
Ag_NAA	Silver	mg/kg	INAA	5	100	NO	100	N0
228Ac	Actinium228	Bq/kg	Gamma-ray spectroscopy	0.8	na	NO	0	YES
Al	Aluminium	mg/kg	aqua regia, ICP-AES	10	0	YES	na	NO
Al_XRF	Aluminium	mg/kg	XRF	300	0	YES	na	NO
241Am	Americium241	Bq/kg	Gamma-ray spectroscopy	0.3	na	NO	75.1	NO
As	Arsenic	mg/kg	aqua regia, GF-AAS	0.1	1.7	YES	na	NO
As_NAA	Arsenic	mg/kg	INAA	0.5	71.9	NO	62.9	NO
Au	Gold	mg/kg	INAA	0.002	72.4	NO	74.4	NO
B	Boron	mg/kg	aqua regia, ICP-AES	3	89.4	NO	na	NO
Ba	Barium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Ba_NAA	Barium	mg/kg	INAA	50	0	YES	5.1	YES
Be	Beryllium	mg/kg	aqua regia, ICP-AES	0.05	0	YES	na	NO
Bi	Bismuth	mg/kg	aqua regia, GF-AAS	0.005	2.5	YES	na	NO
214Bi	Bismuth214	Bq/kg	Gamma-ray spectroscopy	0.2	na	NO	7.7	YES
Br_NAA	Bromine	mg/kg	INAA	0.5	25.4	NO	5.1	YES
Ca	Calcium	mg/kg	aqua regia, ICP-AES	3	0	YES	na	NO
Ca_NAA	Calcium	mg/kg	INAA	10000	22.8	NO	55.5	NO
Ca_XRF	Calcium	mg/kg	XRF	50	0	YES	na	NO
Cd	Cadmium	mg/kg	aqua regia, GF-AAS	0.001	0	YES	na	NO
Ce	Cerium	mg/kg	INAA	3	0	YES	1.8	YES
Co	Cobalt	mg/kg	aqua regia, ICP-AES	0.2	0	YES	na	NO
Co_NAA	Cobalt	mg/kg	INAA	1	0.2	YES	1.8	YES
Cr	Chromium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Cr_NAA	Chromium	mg/kg	INAA	5	0	YES	4.6	YES
Cs	Cesium	mg/kg	INAA	1	61.4	NO	88.1	NO
134Cs	Cesium134	Bq/kg	Gamma-ray spectroscopy	0.1	na	NO	86	NO
137Cs	Cesium137	Bq/kg	Gamma-ray spectroscopy	0.1	na	NO	0	YES
Cu	Copper	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Eu_NAA	Europium	mg/kg	INAA	0.2	0	YES	11.2	YES
Fe	Iron	mg/kg	aqua regia, ICP-AES	10	0	YES	na	NO
Fe_NAA	Iron	mg/kg	INAA	100	0	NO	0	YES
Fe_XRF	Iron	mg/kg	XRF	200	0	YES	na	NO
Hf_NAA	Hafnium	mg/kg	INAA	1	0	YES	4.8	YES
Hg	Mercury	mg/kg	aqua regia, CV-AAS	0.06	56	NO	na	NO
Hg_NAA	Mercury	mg/kg	INAA	1	99.2	NO	99.5	NO
Ir_NAA	Iridium	mg/kg	INAA	0.005	100	NO	100	NO
K	Potassium	mg/kg	aqua regia, ICP-AES	200	0.5	YES	na	NO
K_XRF	Potassium	mg/kg	XRF	40	0	YES	na	NO
40K	Potassium40	Bq/kg	Gamma-ray spectroscopy	10	na	NO	1.2	YES
La	Lanthanum	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
La_NAA	Lanthanum	mg/kg	INAA	0.5	0	YES	0	YES
Li	Lithium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Lu_NAA	Lutetium	mg/kg	INAA	0.05	0	YES	7.1	YES
Mg	Magnesium	mg/kg	aqua regia, ICP-AES	5	0	YES	na	NO
Mg_XRF	Magnesium	mg/kg	XRF	200	0	YES	na	NO
Mn	Manganese	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Mn_XRF	Manganese	mg/kg	XRF	80	0	YES	na	NO
Mo	Molybdenum	mg/kg	aqua regia, ICP-AES	0.2	76.5	NO	na	NO
Mo_NAA	Molybdenum	mg/kg	INAA	1	84	NO	88.1	NO
Na	Sodium	mg/kg	aqua regia, ICP-AES	15	0	YES	na	NO
Na_NAA	Sodium	mg/kg	INAA	100	0	NO	0	YES
Na_XRF	Sodium	mg/kg	XRF	200	0	YES	na	NO
Nd	Neodymium	mg/kg	INAA	5	1.3	YES	38.9	NO
Ni	Nickel	mg/kg	aqua regia, ICP-AES	1	0	YES	na	NO
Ni_NAA	Nickel	mg/kg	INAA	20	86.3	NO	92.8	NO
P	Phosphorus	mg/kg	aqua regia, ICP-AES	7	0	YES	na	NO
P_XRF	Phosphorus	mg/kg	XRF	40	0	YES	na	NO
Pb	Lead	mg/kg	aqua regia, GF-AAS	0.2	0	YES	na	NO
Rb_NAA	Rubidium	mg/kg	INAA	15	6.3	YES	31.5	NO
S	Sulphur	mg/kg	aqua regia, ICP-AES	5	0.5	NO	na	NO
Sb	Antimony	mg/kg	aqua regia, GF-AAS	0.01	53.9	NO	na	NO
Sb_NAA	Antimony	mg/kg	INAA	0.1	75.1	NO	50.6	NO

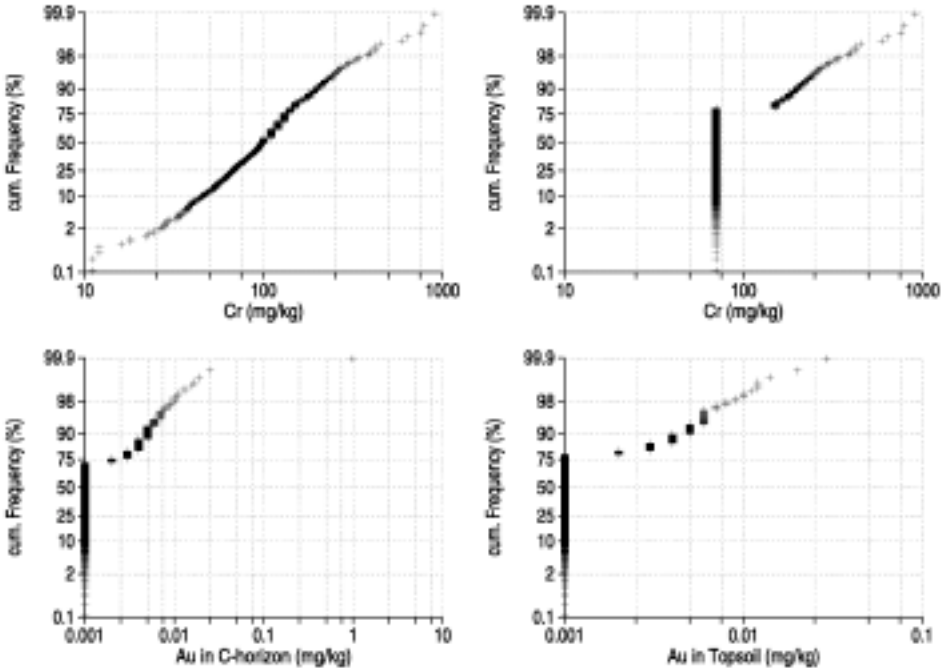
ELEMENT	NAME	UNIT	METHOD	DL	% < DL C-horizon	USED	% < DL Topsoil	USED
Sc	Scandium	mg/kg	aqua regia, ICP-AES	0.1	0.2	YES	na	NO
Sc_NAA	Scandium	mg/kg	INAA	0.1	0	YES	0	YES
Se	Selenium	mg/kg	aqua regia, GF-AAS	0.01	4.1	YES	na	NO
Se_NAA	Selenium	mg/kg	INAA	3	99	NO	99.2	NO
Si	Silicon	mg/kg	aqua regia, ICP-AES	10	0	YES	na	NO
Si_XRF	Silicon	mg/kg	XRF	2300	0	YES	na	NO
Sm_NAA	Samarium	mg/kg	INAA	0.1	0	YES	0.3	YES
Sr	Strontium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Sr_NAA	Strontium	mg/kg	INAA	500	86.5	NO	92.8	NO
Ta_NAA	Tantalum	mg/kg	INAA	0.5	78.4	NO	78.1	NO
Tb_NAA	Terbium	mg/kg	INAA	0.5	72.4	NO	91.6	NO
Te	Tellurium	mg/kg	aqua regia, GF-AAS	0.003	22.6	NO	na	NO
Th	Thorium	mg/kg	aqua regia, ICP-AES	3	0.5	YES	na	NO
Th_NAA	Thorium	mg/kg	INAA	0.2	0	YES	4.6	YES
Ti	Titanium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Ti_XRF	Titanium	mg/kg	XRF	30	O	YES	na	NO
U_NAA	Uranium	mg/kg	INAA	0.5	48.8	NO	64.1	NO
V	Vanadium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
W_NAA	Tungsten	mg/kg	INAA	1	97.9	NO	94.4	NO
Y	Yttrium	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Yb_NAA	Ytterbium	mg/kg	INAA	0.2	0	YES	3.8	YES
Zn	Zinc	mg/kg	aqua regia, ICP-AES	0.5	0	YES	na	NO
Zn_NAA	Zinc	mg/kg	INAA	50	39.1	NO	68.5	NO
LOI	Loss on Ignition	wt.-%	GRAVIMETRIC	0.1	0	NO	0	YES
pH	pH		water extraction, pH-electrode	0.1	O	NO	0	YES
EC	Electrical Conductivity	mS/m	water extraction, potentiometric	1	0	NO	0	YES

Variable	Topsoil R^2	C-horizon R^2	Techn.
As	0.34	0.85	INAA
Au	0.45	0.40	INAA
Ca	0.48	0.57	INAA
Cs	-	0.81	INAA
Hg	-	0.53	CV-AAS
Mo	-	0.20	ICP-AES
Sb	0.31	0.70	INAA
Ta	0.49	0.65	INAA
U	0.35	0.58	INAA
Zn	0.37	0.73	INAA

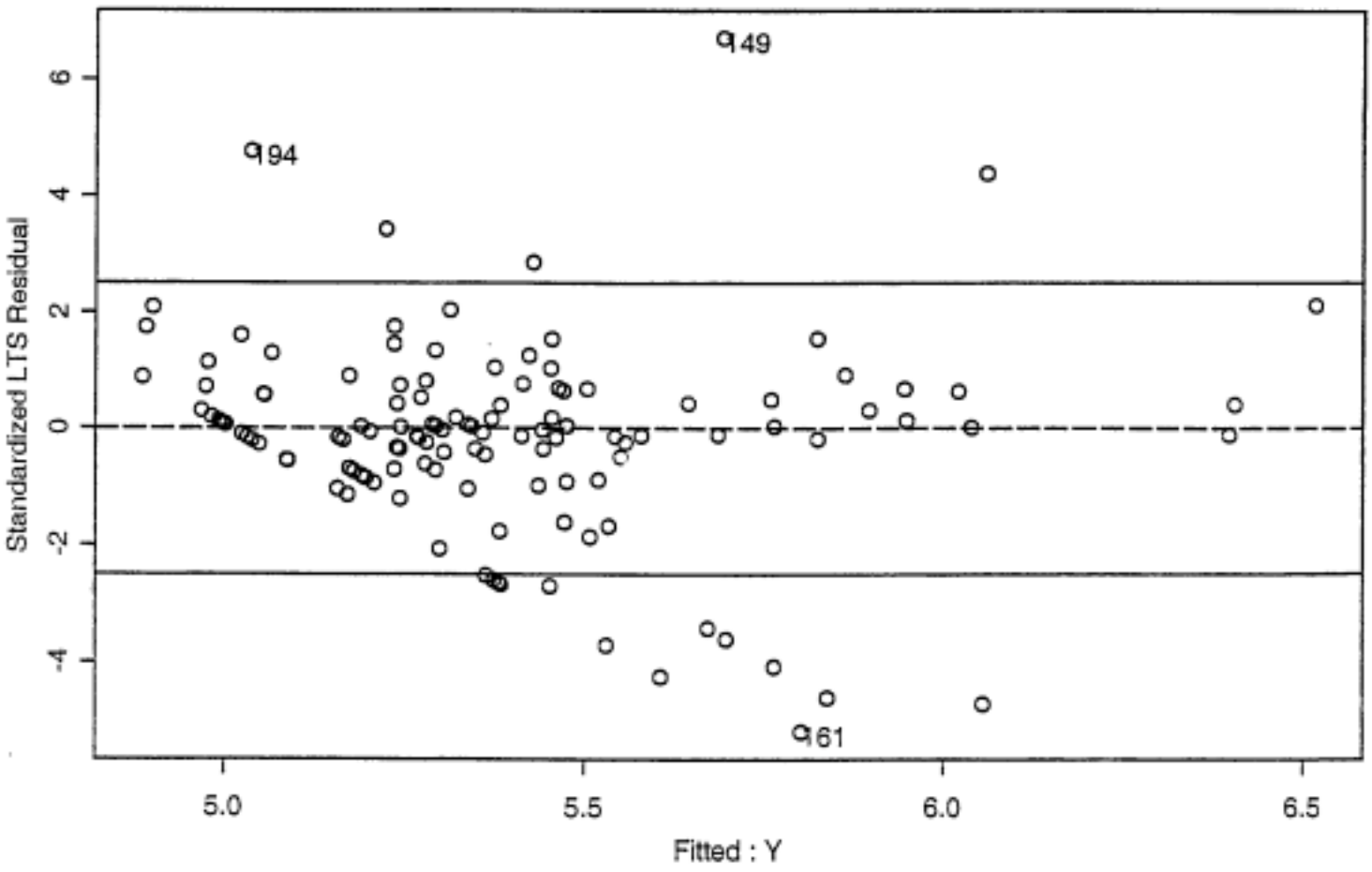
Table 2: Coefficient of determination for the predicted variables


N
0 50 100 km
Barents Sea
NORWAY
Lakselv
KIRKENES
NIKEL
ZAPOLJARNIJ
24 degrees E
Murmansk
Ivalo
OLENEGORSK
MONCHEGORSK
APATITY
FINLAND
KIROVSK
KOVDOR
KANDALAKSHA
35.5 degrees E
RUSSIA
Polar Circle
Rovaniemi

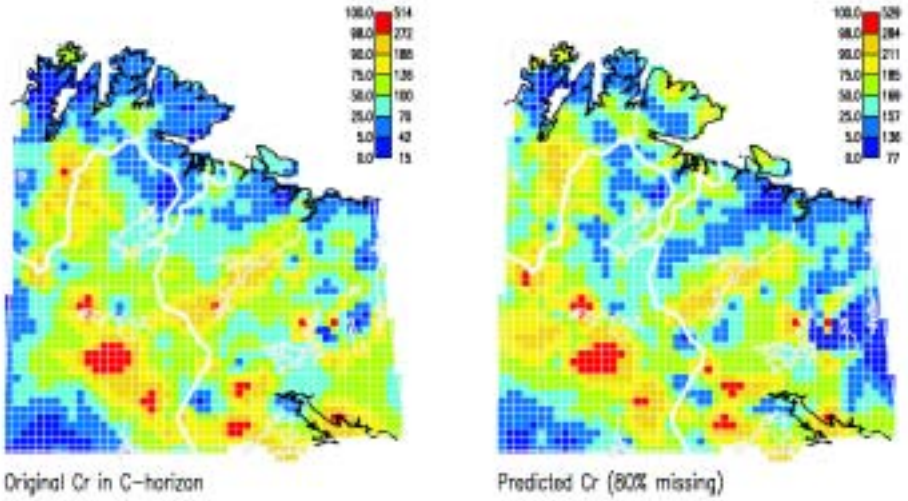
Figur 1


cum. Frequency (%)
99.9
98
90
75
50
25
10
2
0.1
10
100
1000
Cr (mg/kg)
cum. Frequency (%)
99.9
98
90
75
50
25
10
2
0.1
10
100
1000
Cr (mg/kg)
cum. Frequency (%)
99.9
98
90
75
50
25
10
2
0.1
0.001
0.01
0.1
1
10
Au in C-horizon (mg/kg)
cum. Frequency (%)
99.9
98
90
75
50
25
10
2
0.1
0.001
0.01
0.1
Au in Topsoil (mg/kg)

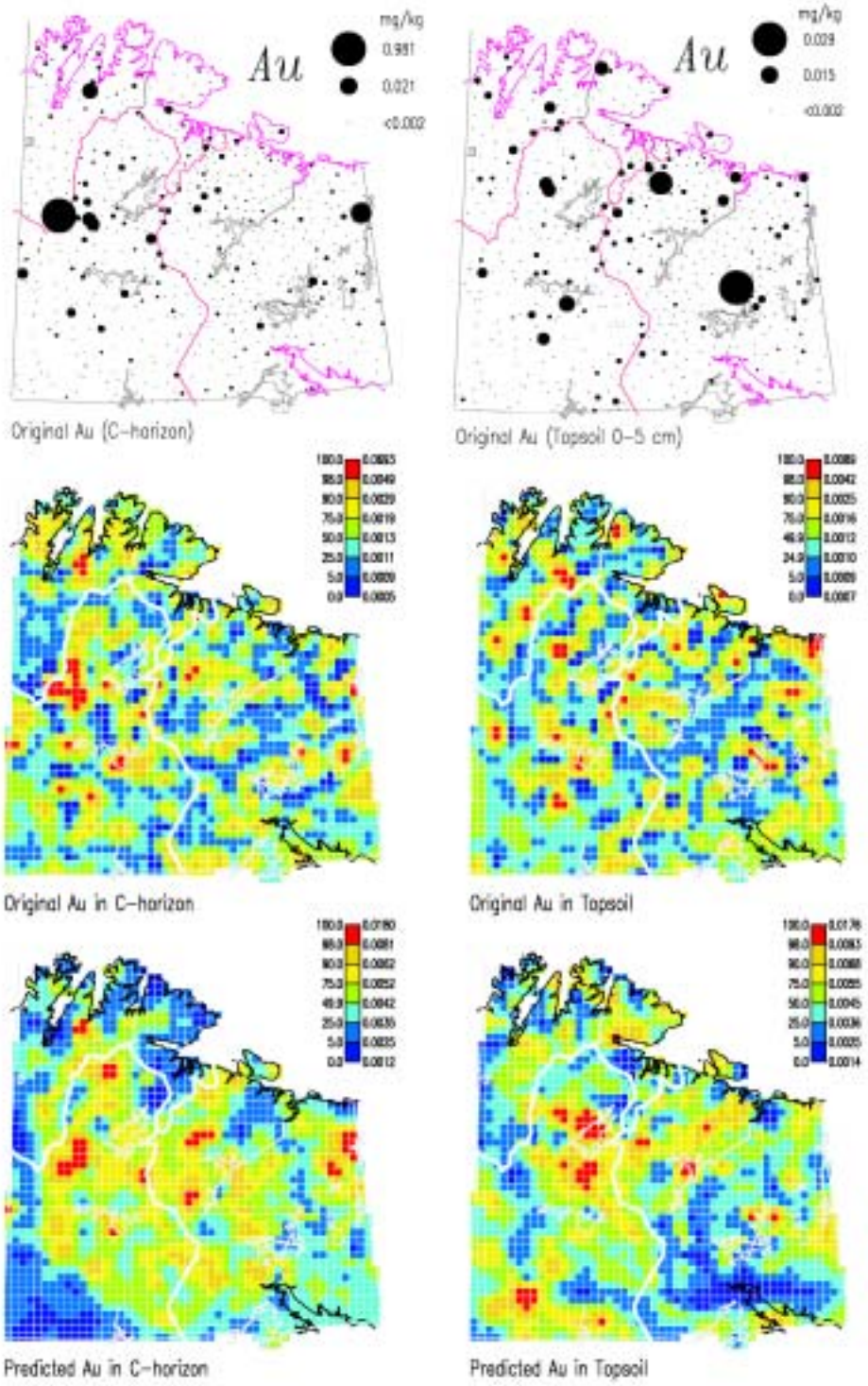
Figur 2


Standardized LTS Residual
Fitted : Y
49
94
61
6
4
2
0
-2
-4
5.0
5.5
6.0
6.5

Figur 3



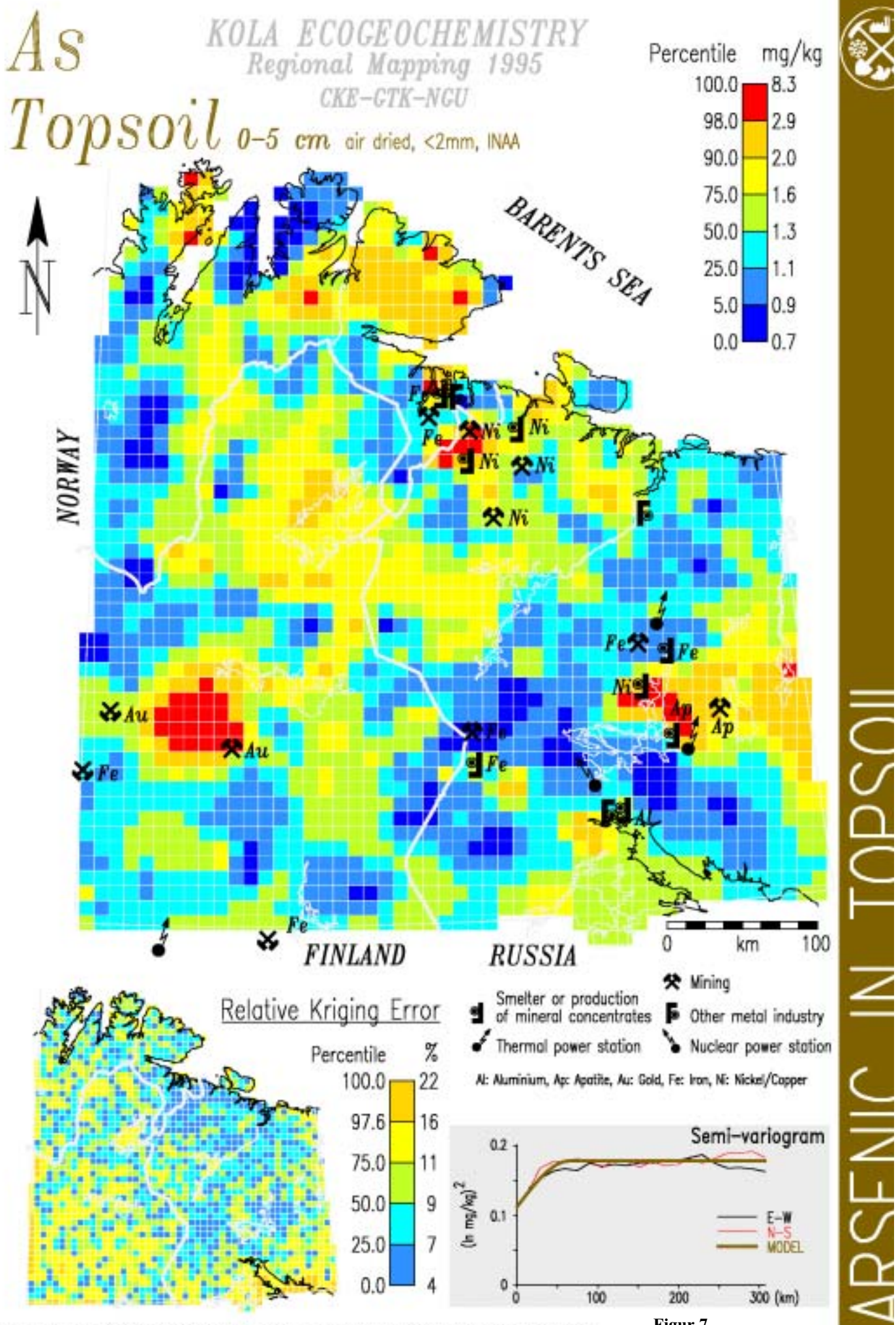
Figur 4


Au
mg/kg
0.981
0.021
<0.002
Original Au (C-horizon)
Au
mg/kg
0.029
0.015
<0.002
Original Au (Topsoil 0-5 cm)
Original Au in C-horizon
Original Au in Topsoil
Predicted Au in C-horizon
Predicted Au in Topsoil

Figur 5

Au
C-horizon, original data
Au
C-horizon, predicted data
Au
Topsoil, original data
Au
Topsoil, predicted data
E-W
N-S
MODEL
(ln mg/kg)²
0
100
200
300 km
0.2
0.4
0.6
0.1

Figur 6

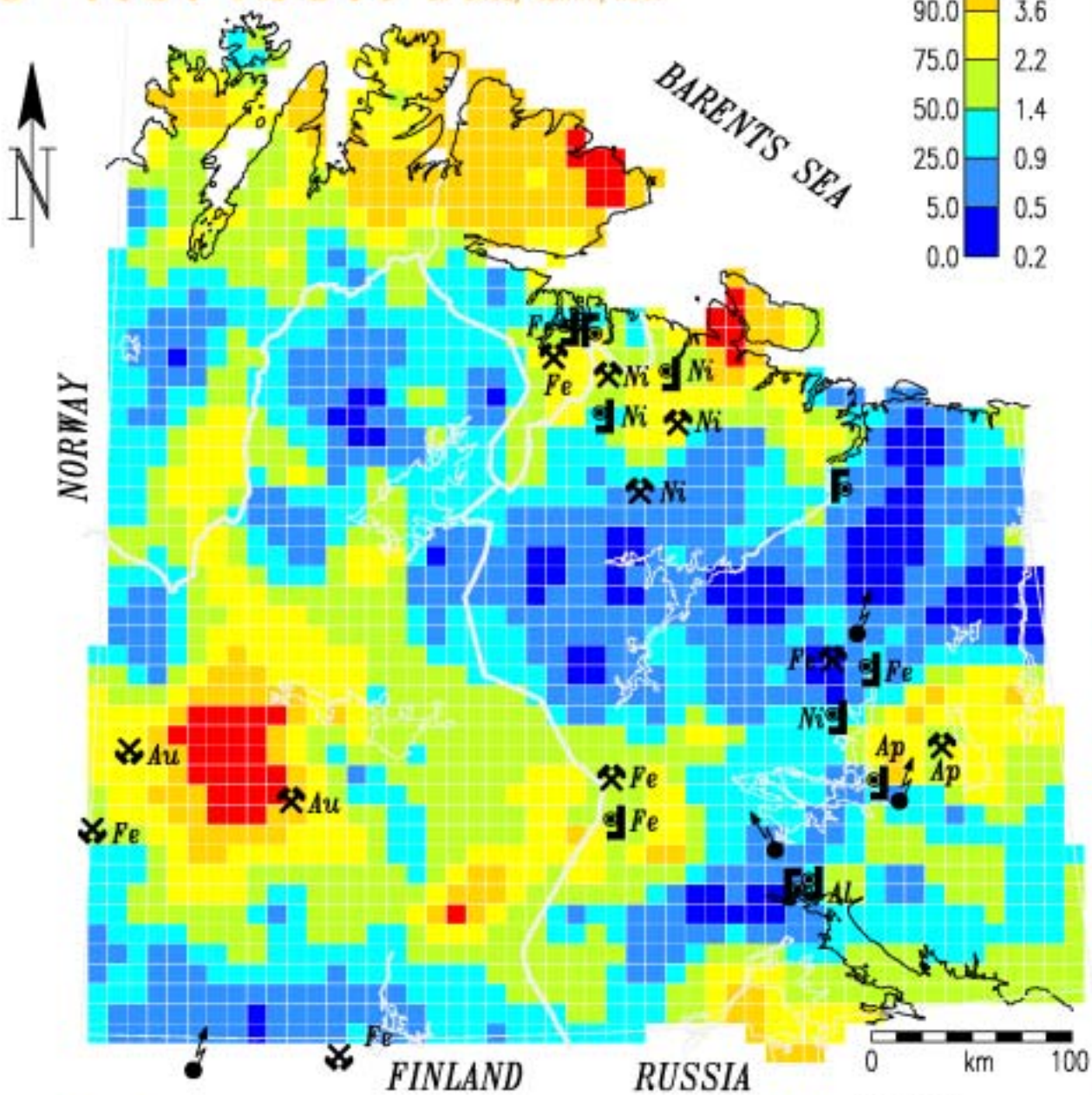

As
Topsoil 0–5 cm air dried, <2mm, INAA
KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU
Percentile mg/kg
100.0 8.3
98.0 2.9
90.0 2.0
75.0 1.6
50.0 1.3
25.0 1.1
5.0 0.9
0.0 0.7
BARENTS SEA
NORWAY
FINLAND
RUSSIA
0 km 100
Relative Kriging Error
Percentile %
100.0 22
97.6 16
75.0 11
50.0 9
25.0 7
0.0 4
Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station
Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper
Semi-variogram
E–W
N–S
MODEL
(ln mg/kg)²
0 100 200 300 (km)
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)
ARSENIC IN TOPSOIL

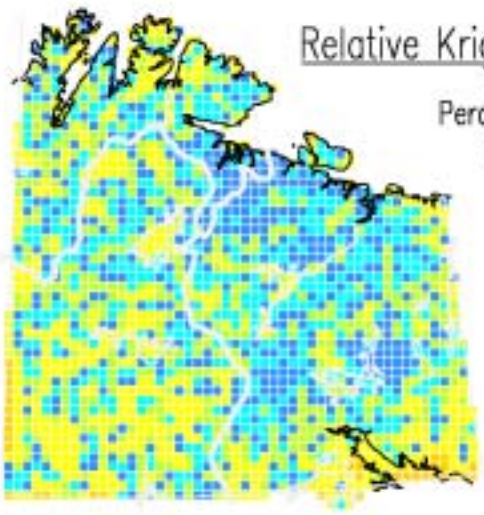
Figur 7

As C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

air dried, <2mm, INAA



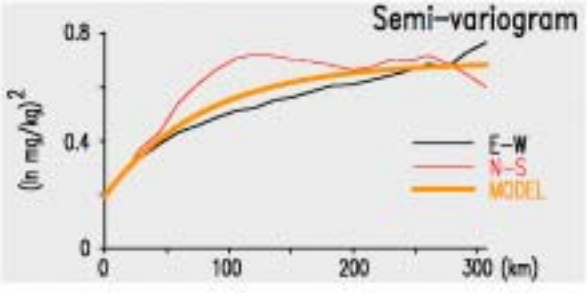


Relative Kriging Error

Percentile	%
100.0	44
98.0	32
75.0	22
50.0	18
25.0	15
0.0	9

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper

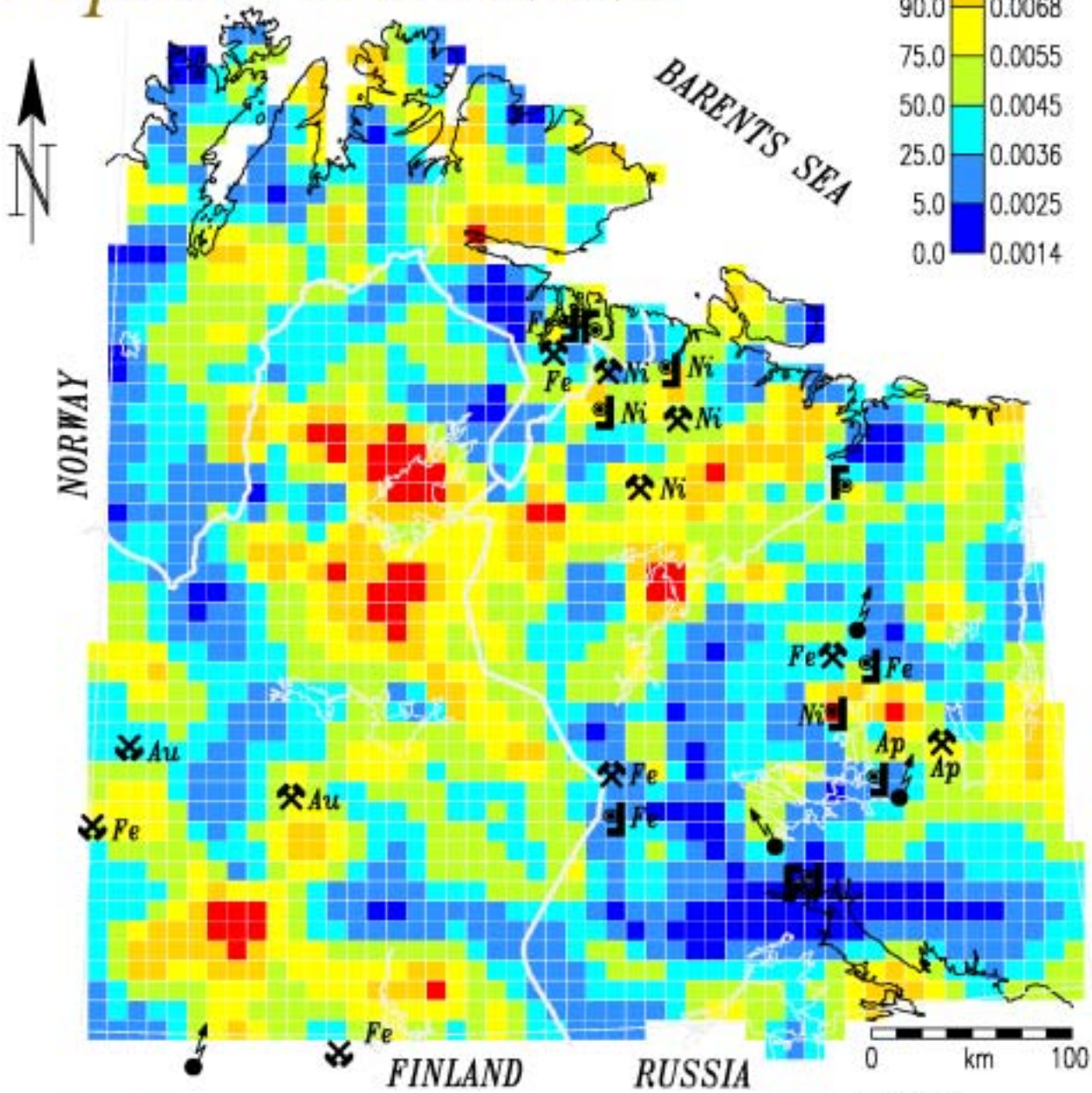


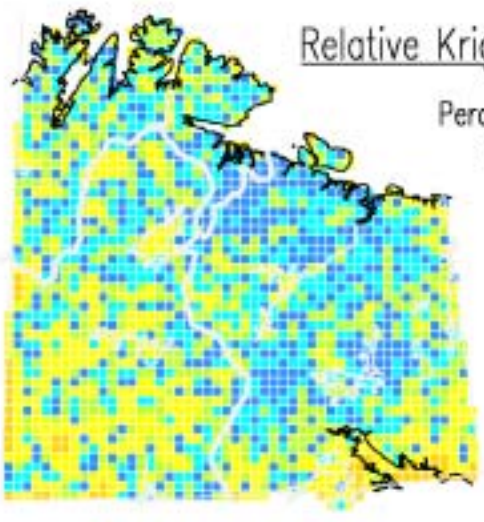
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

ARSENIC IN C-HORIZON

Au Topsoil 0–5 cm air dried, <2mm, INAA

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU



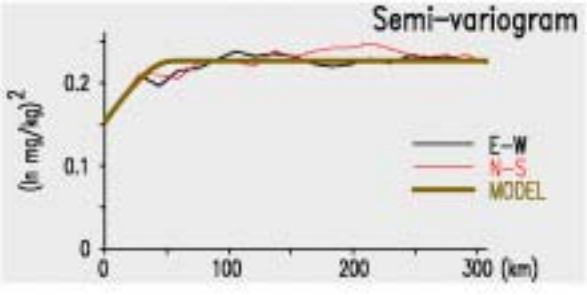


Relative Kriging Error

Percentile %
100.0 25
97.4 18
75.0 12
50.0 10
25.0 8
0.0 5

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



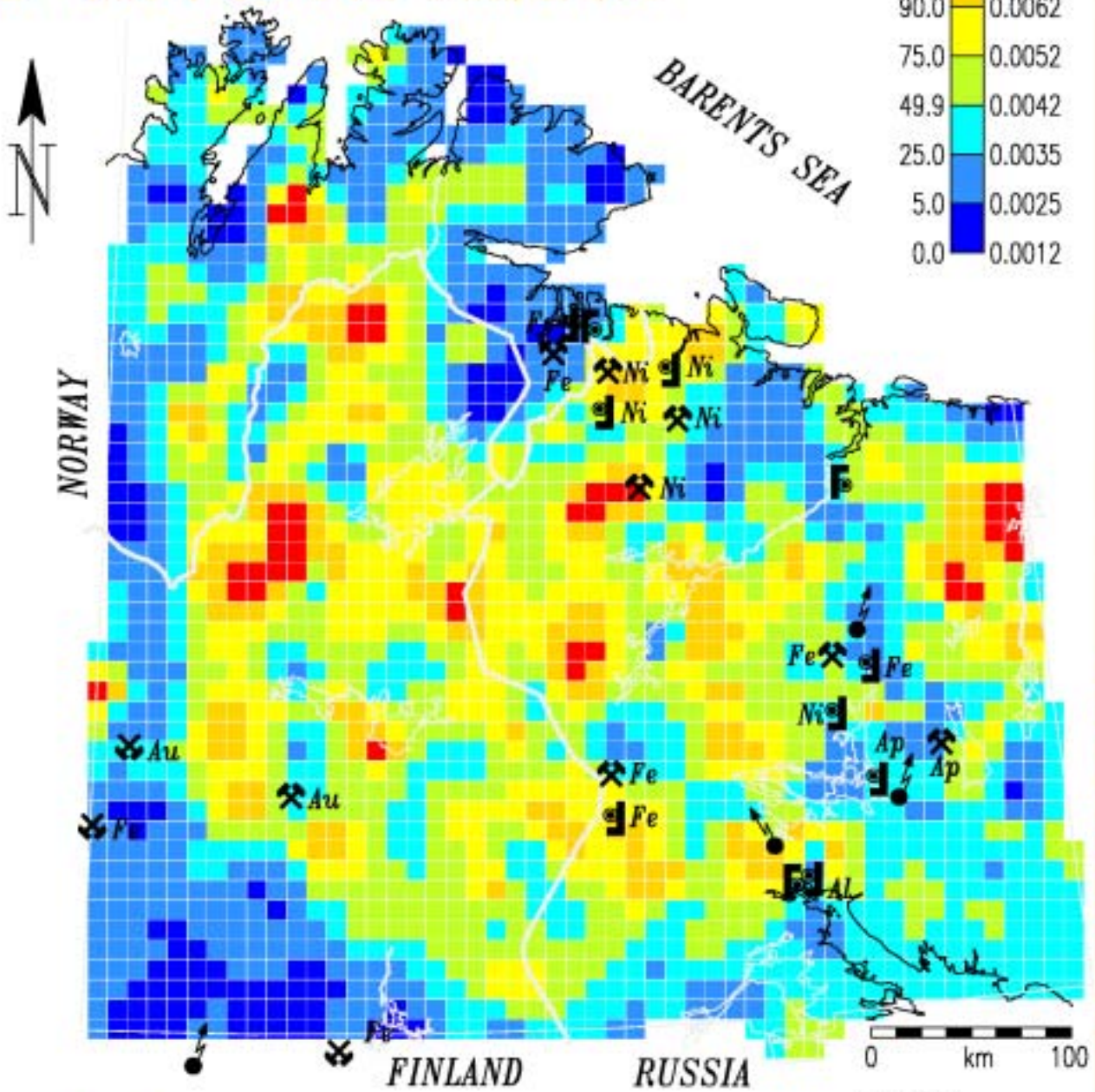
COLD IN TOPSOIL

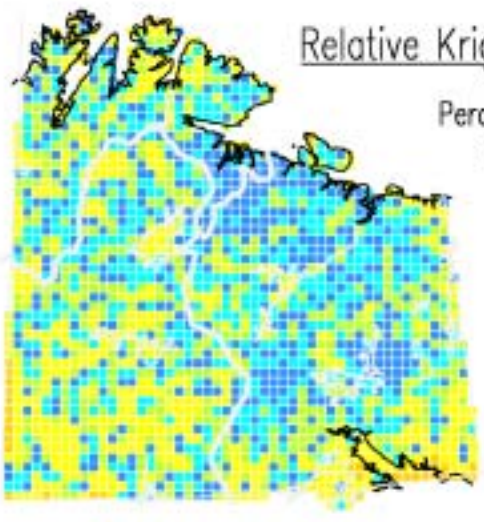
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

Au C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

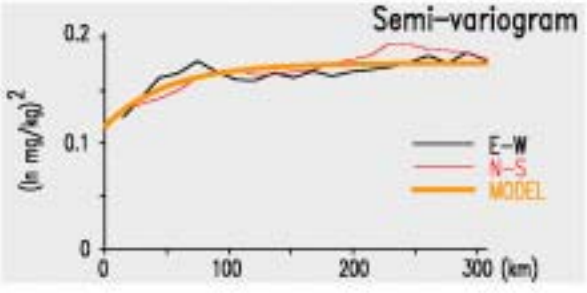
air dried, <2mm, INAA





Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



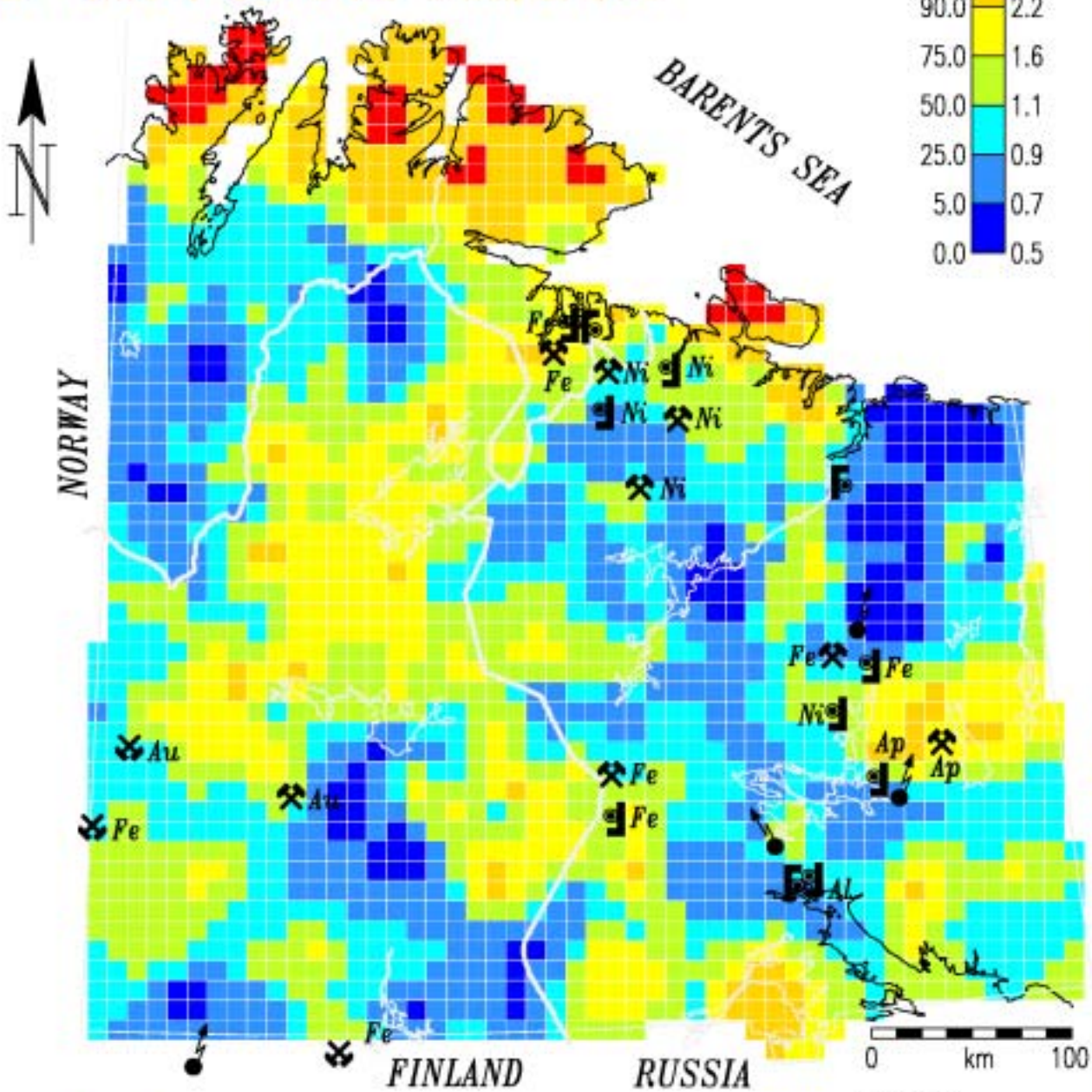
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

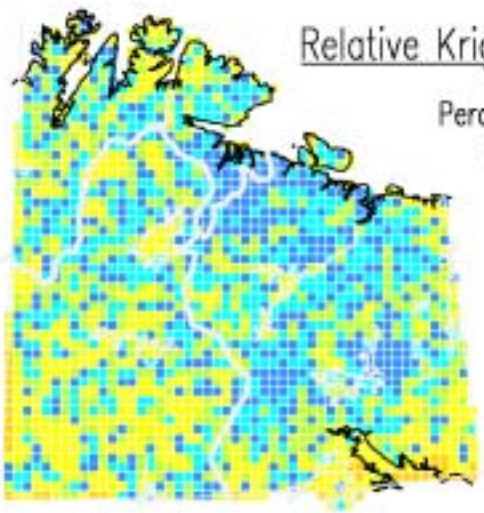
C-HORIZON

Cs
C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

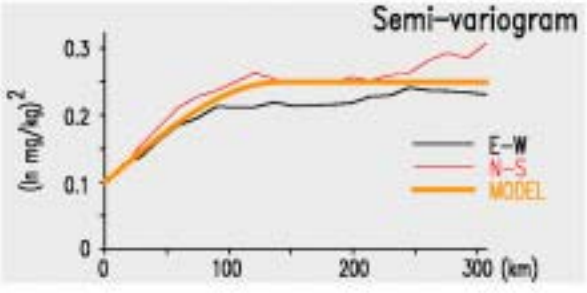
air dried, <2mm, INAA





Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



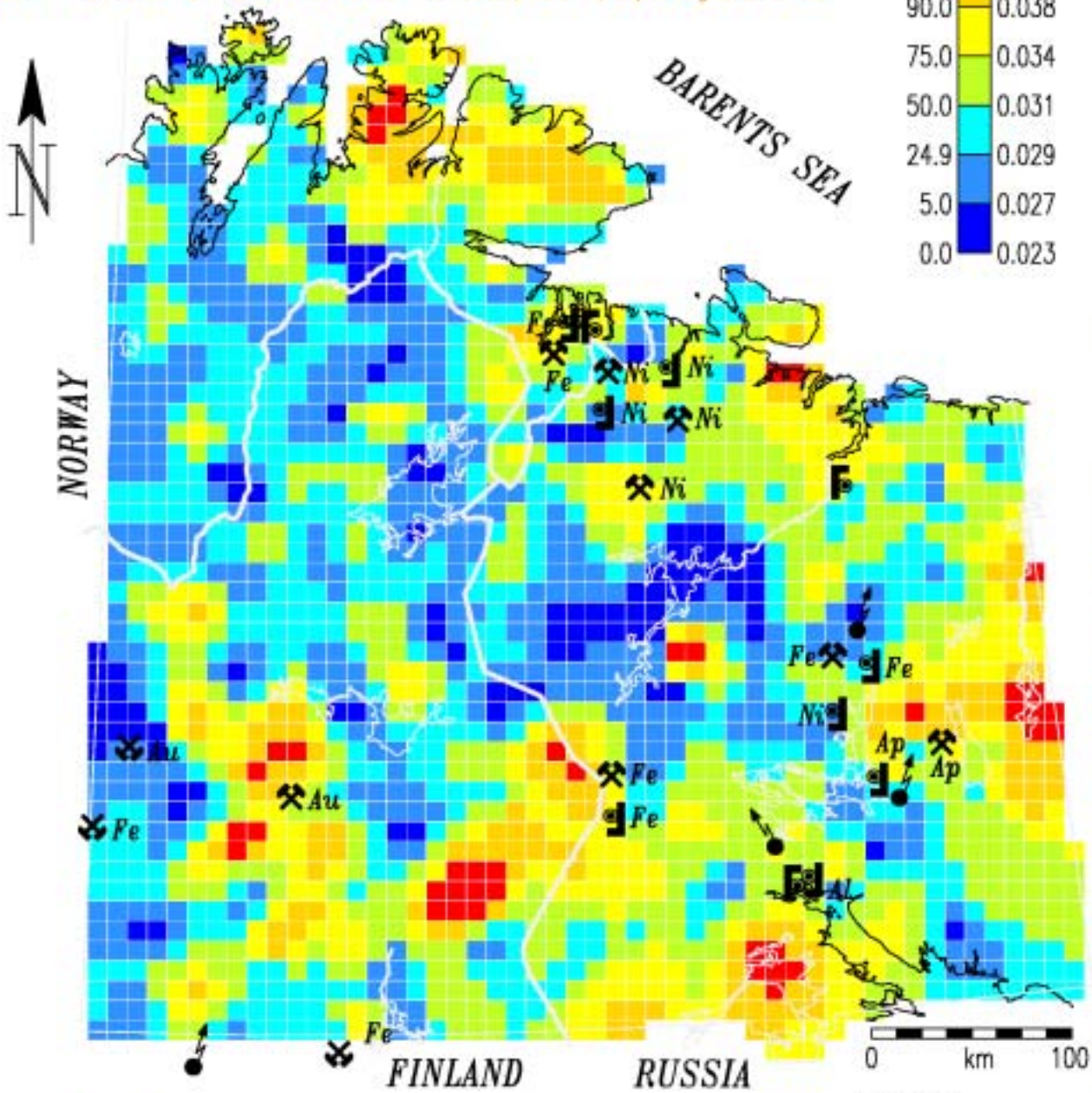
CESIUM IN C-HORIZON

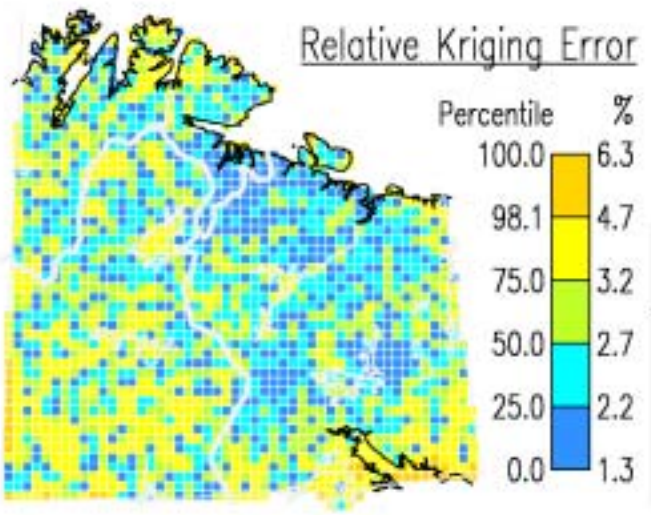
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

Hg
C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

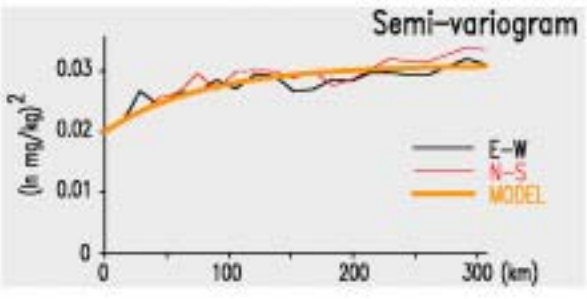
air dried, <2mm, aqua regia, CV-AAS





Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



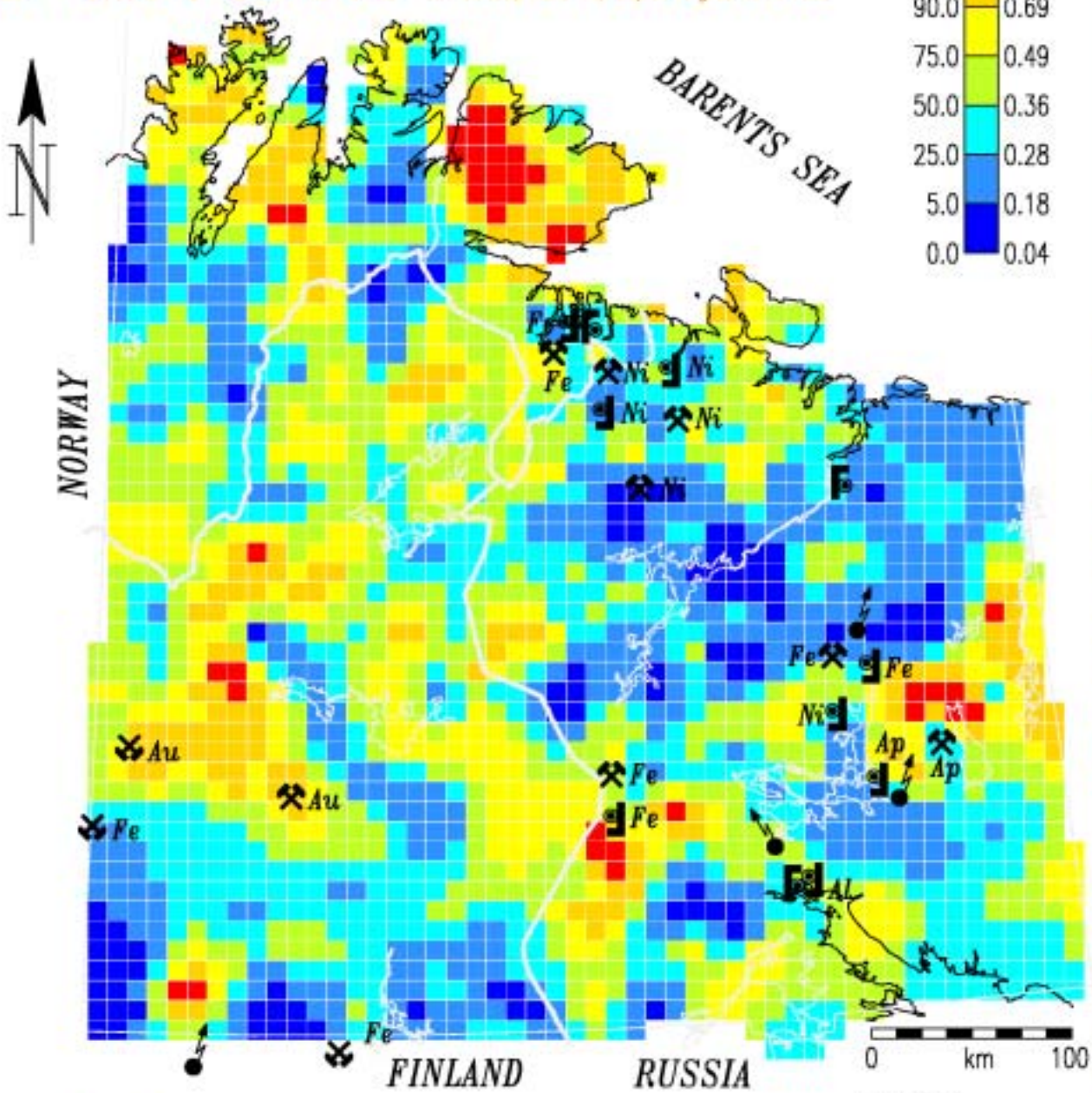
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

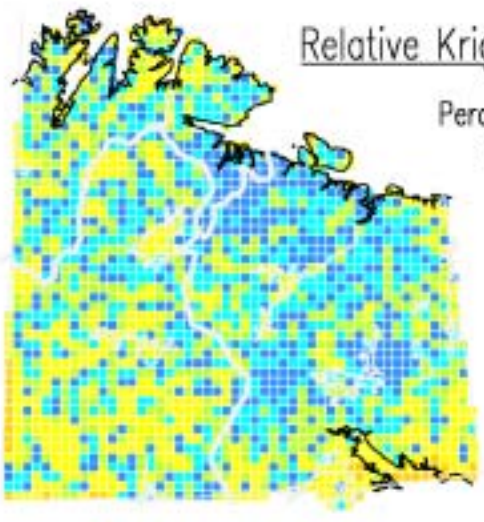
MERCURY IN C-HORIZON

Mo C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

air dried, <2mm, aqua regia, ICP-AES



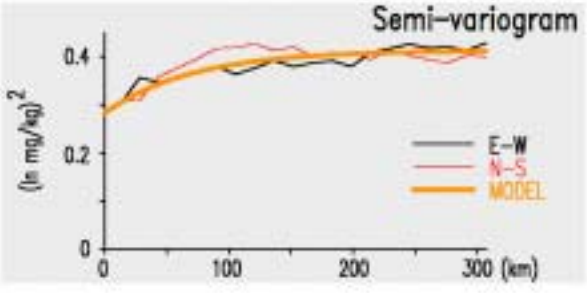


Relative Kriging Error

Percentile %
100.0 23
98.2 17
75.0 12
50.0 10
25.0 8
0.0 5

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper

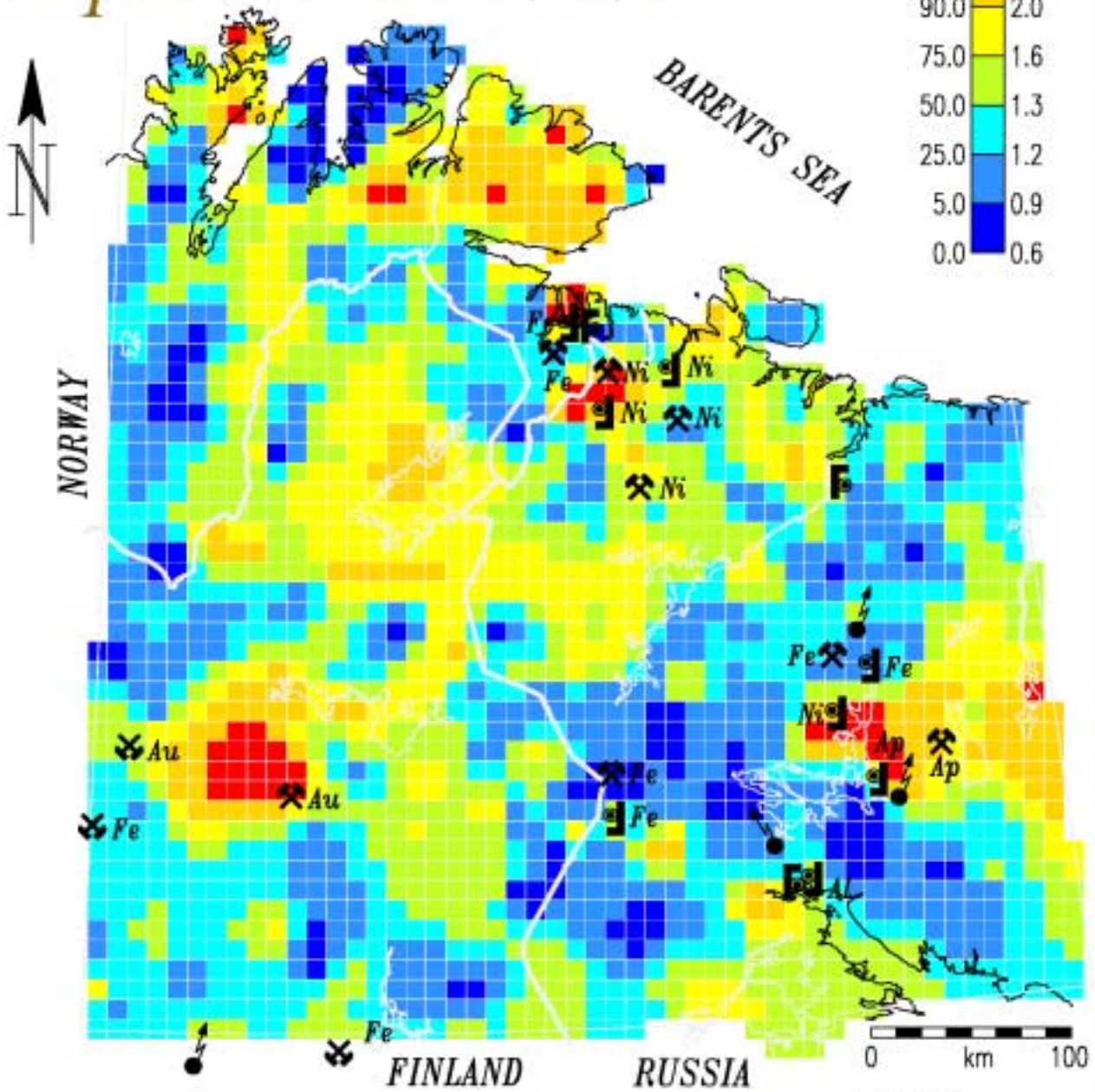


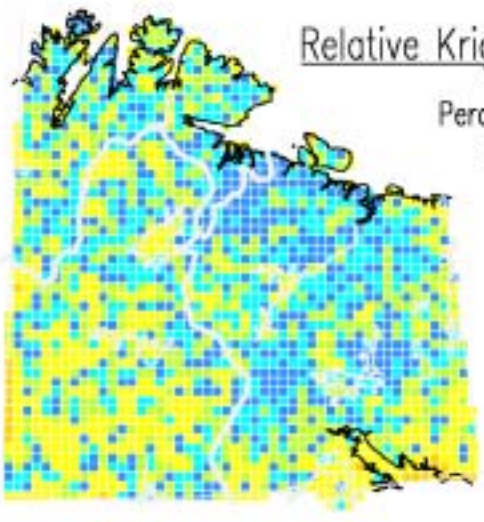
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

MOLYBDENUM IN C-HORIZON

Sb Topsoil 0–5 cm air dried, <2mm, INAA

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU



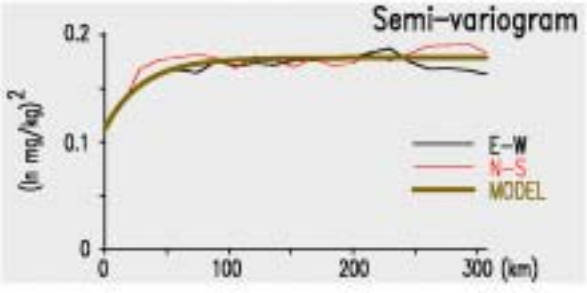


Relative Kriging Error

Percentile %
100.0 21
98.7 18
75.0 13
50.0 11
25.0 9
0.0 5

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



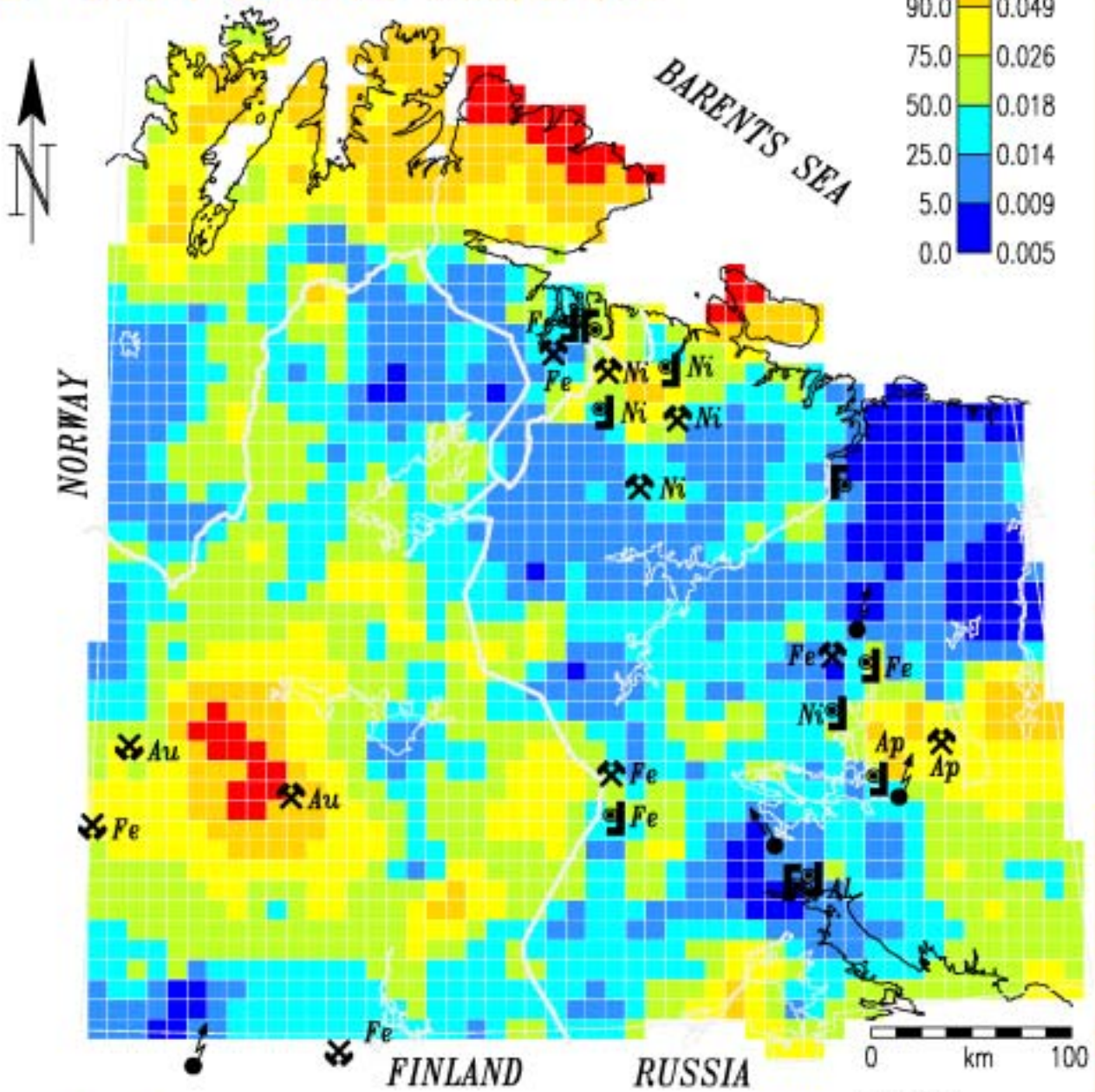
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

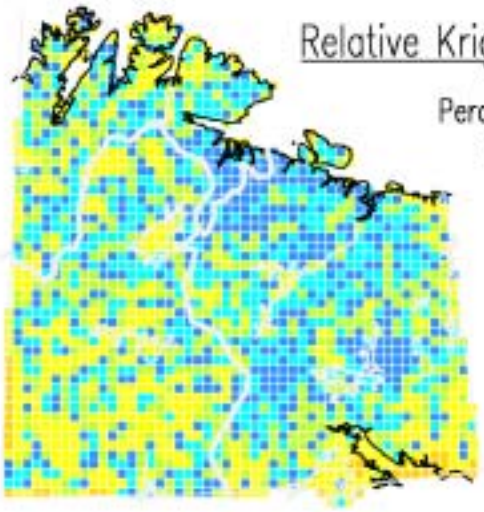
ANTIMONY IN TOPSOIL

Sb C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

air dried, <2mm, INAA



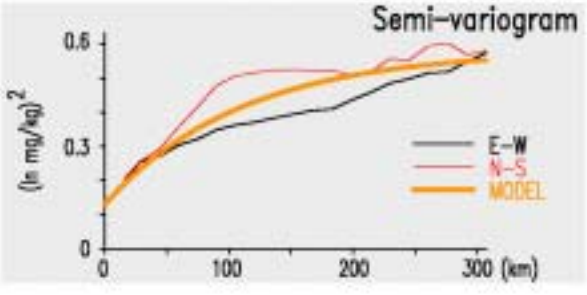


Relative Kriging Error

Percentile	%
100.0	36
97.9	26
75.0	18
50.0	15
25.0	12
0.0	7

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper

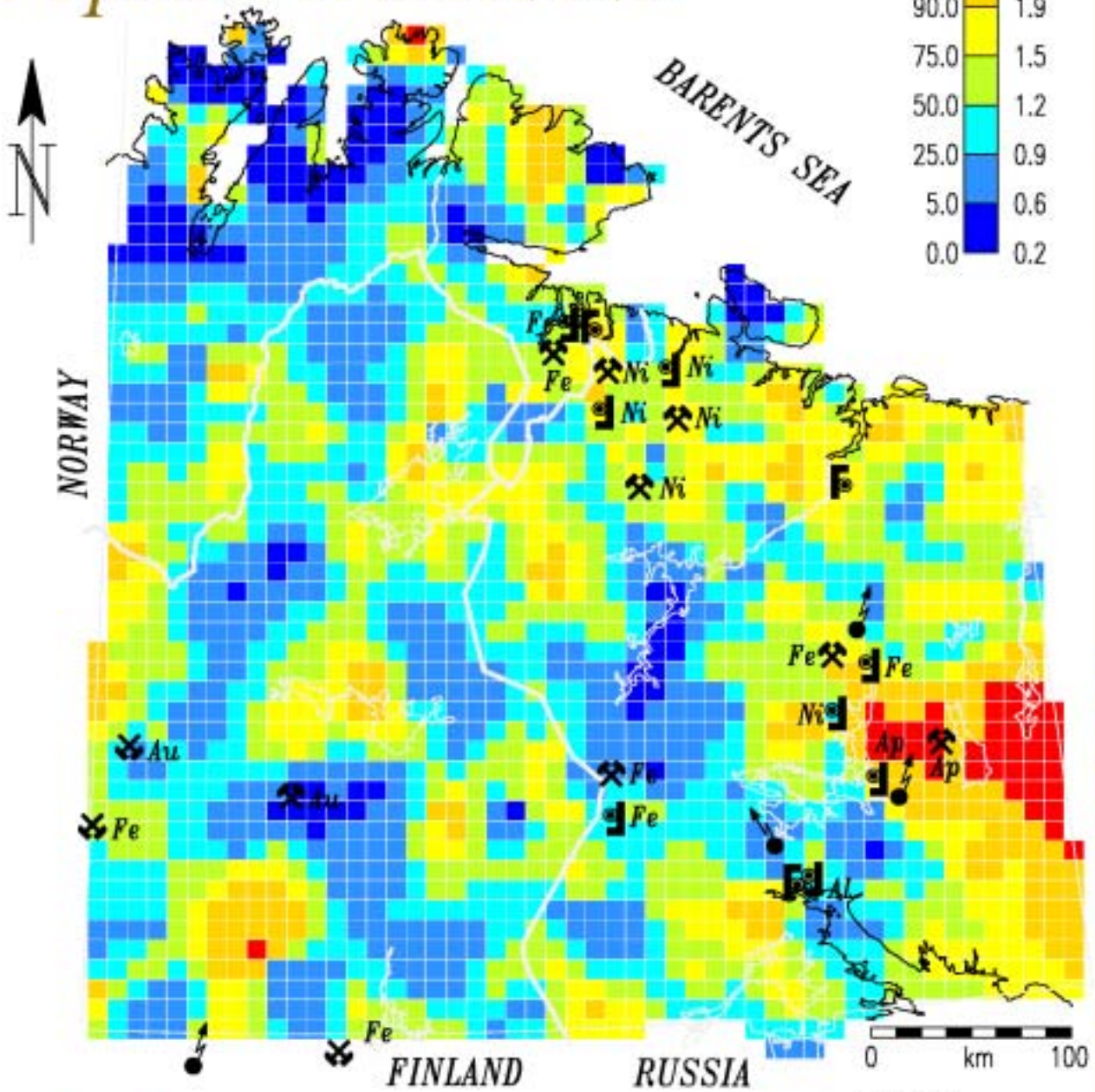


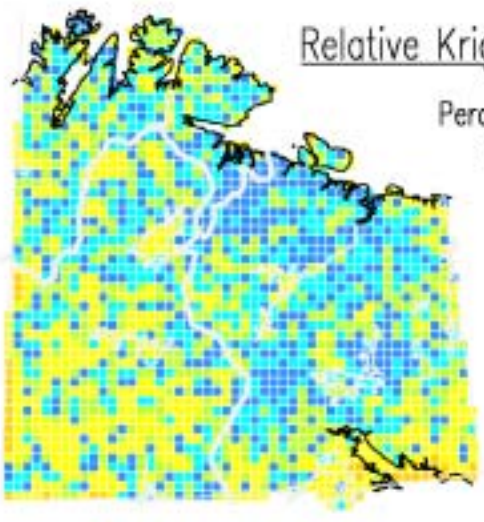
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

ANTIMONY IN C-HORIZON

Ta Topsoil 0–5 cm air dried, <2mm, INAA

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU



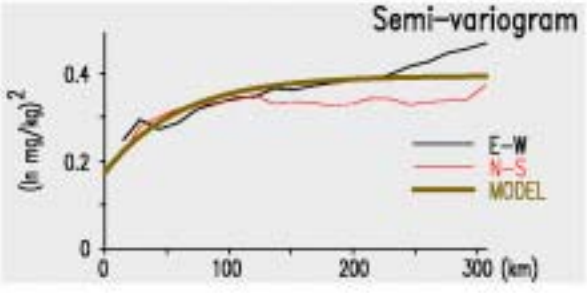


Relative Kriging Error

Percentile %
100.0 32
98.2 24
75.0 17
50.0 14
25.0 11
0.0 7

Smelter or production of mineral concentrates
Mining
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



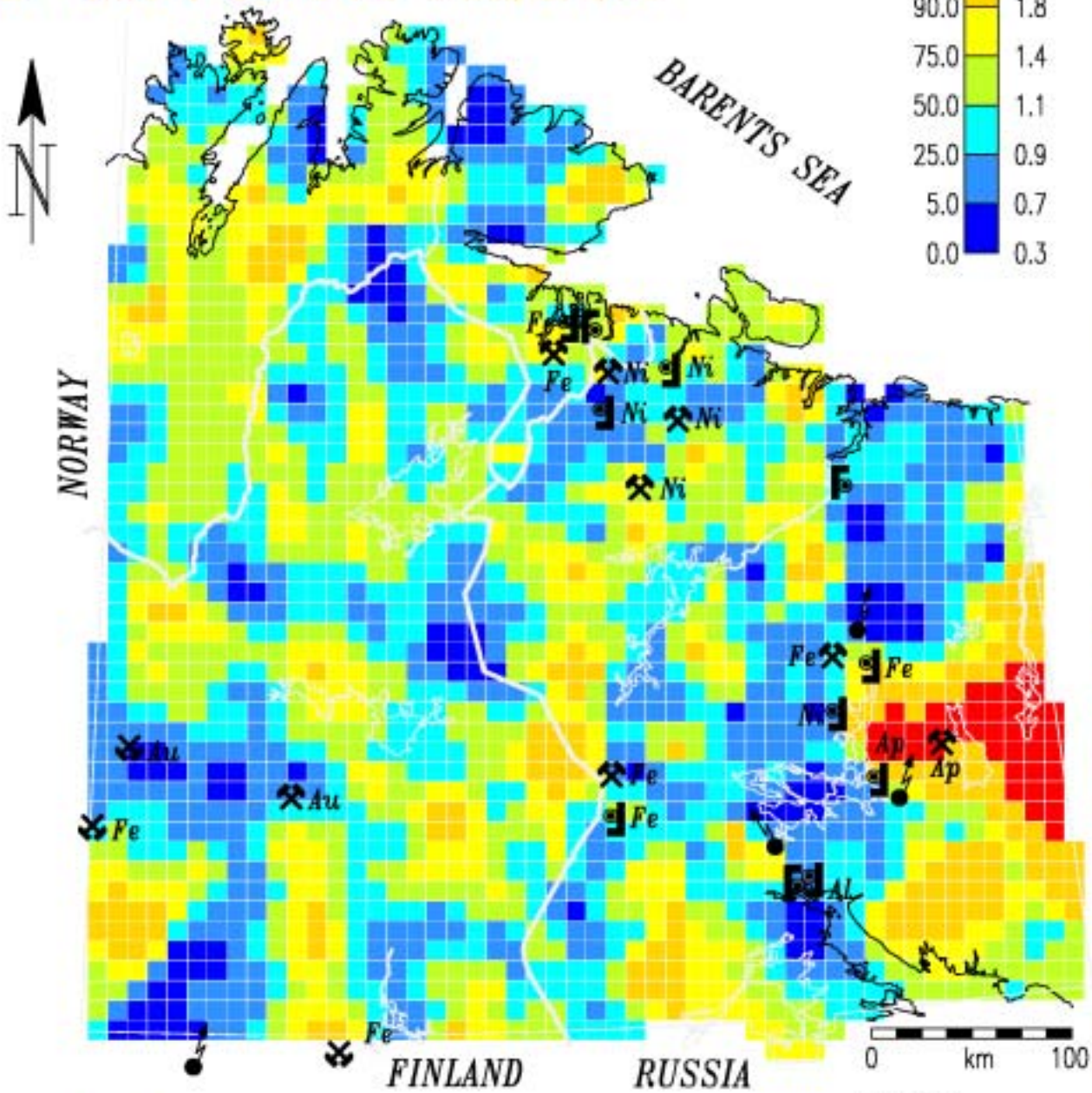
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

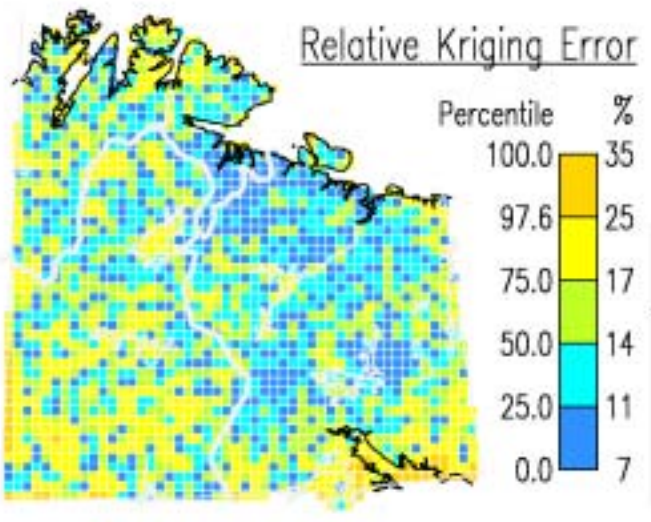
TANTALUM IN TOPSOIL

Ta C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

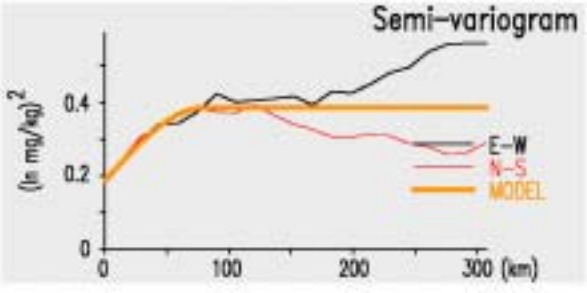
air dried, <2mm, INAA





Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper

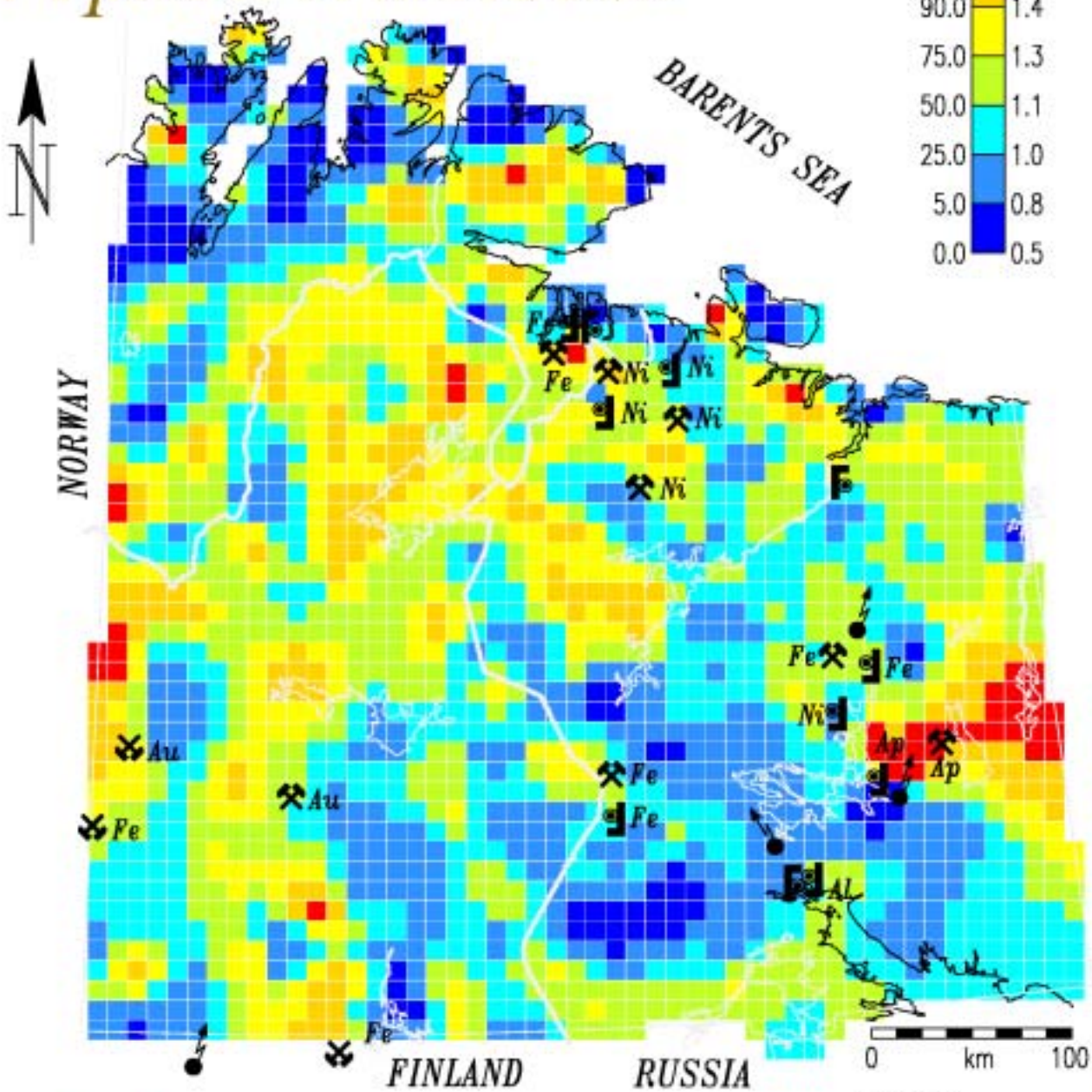


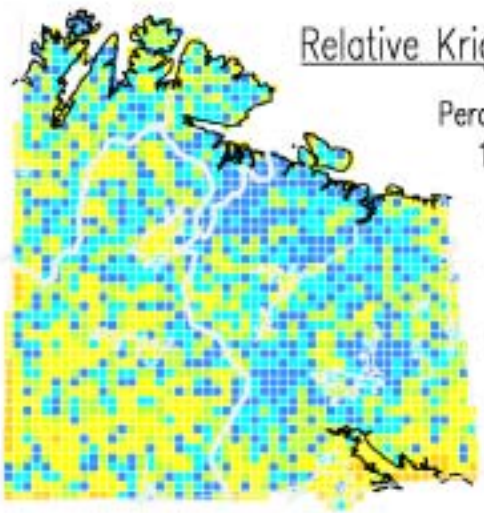
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

TANTALUM IN C-HORIZON

U Topsoil 0–5 cm air dried, <2mm, INAA

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU



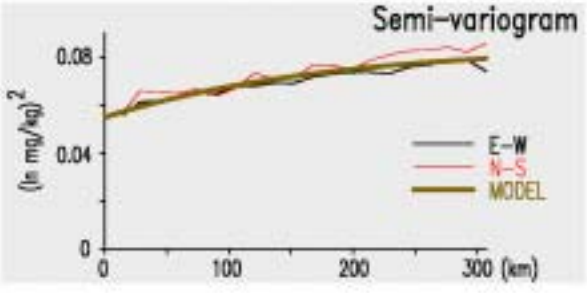


Relative Kriging Error

Percentile %
100.0 7.3
97.8 5.2
75.0 3.5
50.0 3.0
25.0 2.4
0.0 1.4

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

URANIUM IN TOPSOIL

U

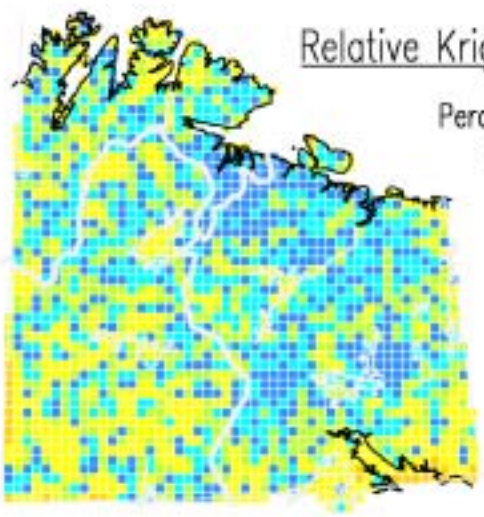
KOLA ECOGEOCHEMISTRY

Regional Mapping 1995

CKE-GTK-NGU

C-horizon

air dried, <2mm, INAA



Relative Kriging Error

Percentile	%
100.0	24
98.4	19
75.0	13
50.0	11
25.0	9
0.0	5

Mining

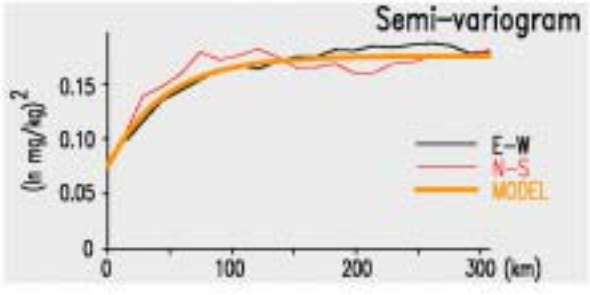
Smelter or production of mineral concentrates

Other metal industry

Thermal power station

Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper

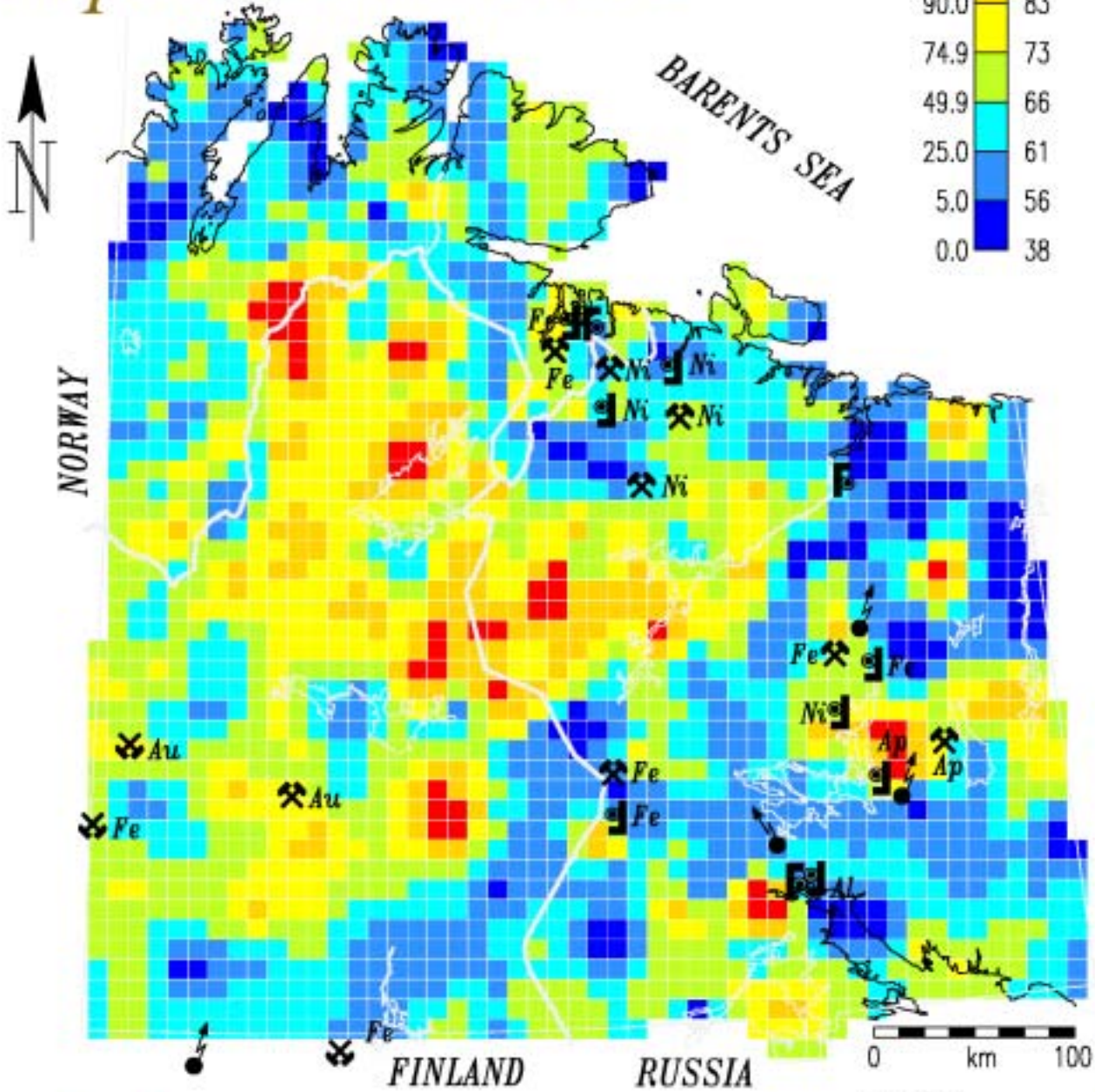


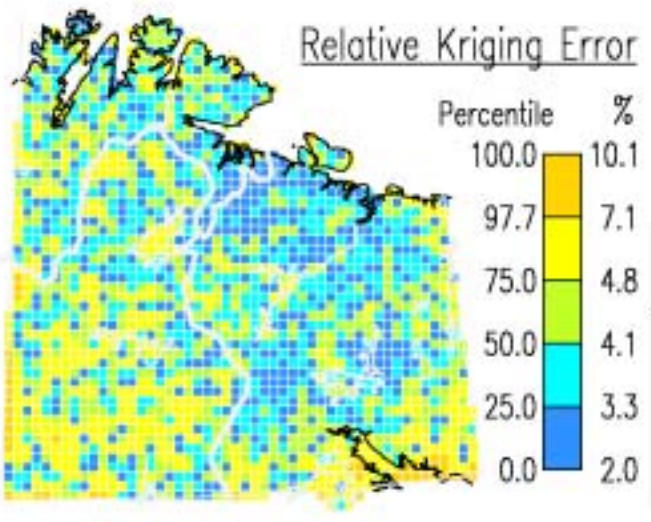
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

URANIUM IN C-HORIZON

Zn Topsoil 0–5 cm air dried, <2mm, INAA

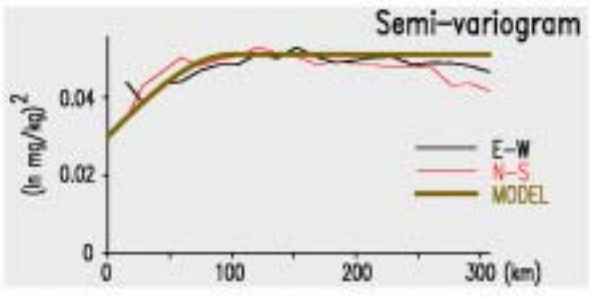
KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE–GTK–NGU





Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



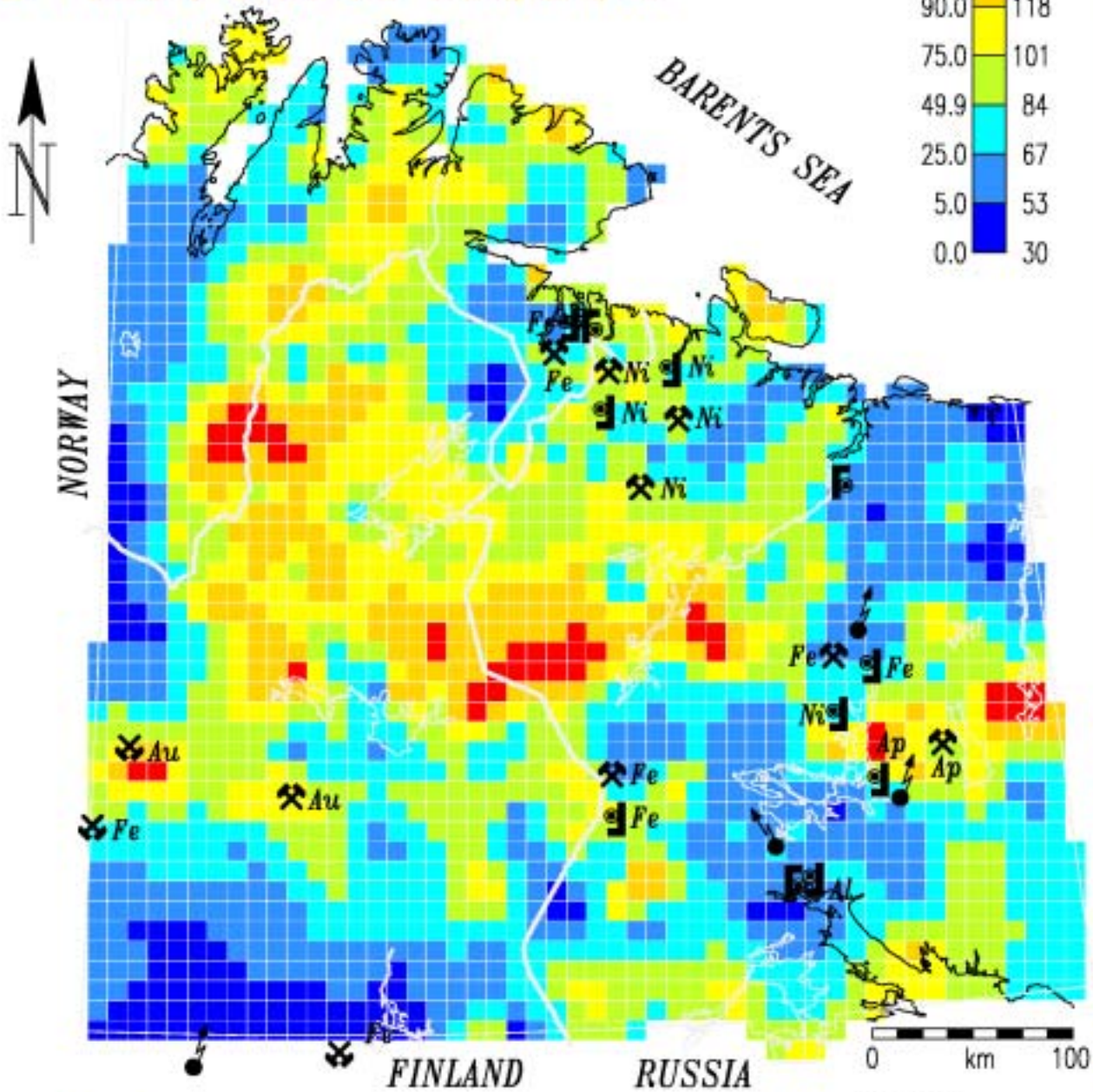
CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

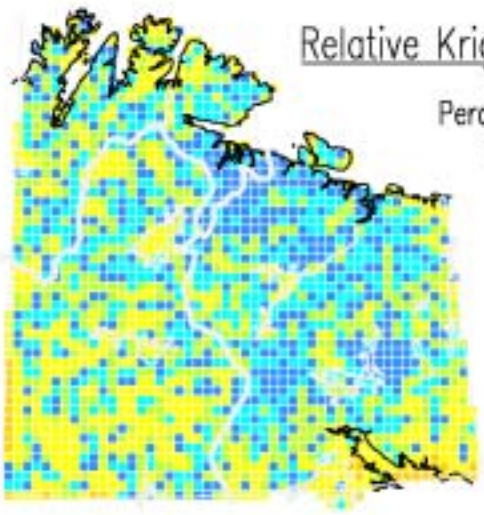
ZINC IN TOPSOIL

Zn
C-horizon

KOLA ECOGEOCHEMISTRY
Regional Mapping 1995
CKE-GTK-NGU

air dried, <2mm, INAA



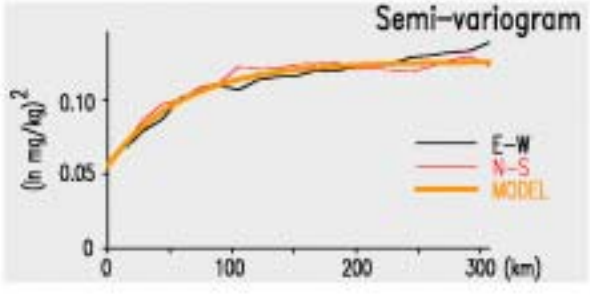


Relative Kriging Error

Percentile	%
100.0	18
98.2	14
75.0	9
50.0	8
25.0	6
0.0	4

Mining
Smelter or production of mineral concentrates
Other metal industry
Thermal power station
Nuclear power station

Al: Aluminium, Ap: Apatite, Au: Gold, Fe: Iron, Ni: Nickel/Copper



CENTRAL KOLA EXPEDITION (CKE), GEOLOGICAL SURVEY OF FINLAND (GTK), GEOLOGICAL SURVEY OF NORWAY (NGU)

ZINC IN C-HORIZON