

46/2012

Raport Badawczy
Research Report

RB/31/2012

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of a spatial air pollution
inventory with a statistical
inference approach (revised)**

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Warszawa 2012

Improving resolution of a spatial air pollution inventory with a statistical inference approach

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Abstract

This paper presents a novel approach for allocation of spatially correlated data, such as emission inventories, to finer spatial scales, conditional on covariate information observable in a fine grid. Spatial dependence is modelled with the conditional autoregressive structure introduced into a linear model as a random effect. The maximum likelihood approach to inference is employed, and the optimal predictors are developed to assess missing values in a fine grid. An example of ammonia emission inventory is used to illustrate potential usefulness of the proposed technique. The results indicate that inclusion of a spatial dependence structure can compensate for less adequate covariate information. For the considered ammonia inventory, the fourfold allocation benefited greatly from incorporation of the spatial component, while for the ninefold allocation this advantage was limited, but still evident. In addition, the proposed method allowed to correct the prediction bias encountered for the upper range emissions in the linear regression models.

Keywords: disaggregation methods; spatial inventory of emissions; statistical modelling.

1. Introduction

The development of high-resolution emission inventories is essential for designing suitable abatement measures. Spatial distribution of emissions can serve as an input for atmospheric dispersion models, which in turn may produce concentration maps of pollutants contributing to the adverse health effects, like ammonia emissions. For other air pollutants, such as greenhouse gasses (GHG), spatial patterns become helpful in improving identification of distributed emission sources.

Numerous issues underlying preparation of spatially resolved GHG inventory were discussed e.g. in Boychuk and Bun (this issue), Bun et al., 2010 or Thiruchittampalam et al., 2010. In general, the task crucially depends on availability of spatially distributed activity data. For instance, at present in Poland the activity data relevant to GHG emissions for 16 country regions (voivodships) can be obtained, and no more accurate spatial resolution is available. Information of higher spatial resolution can be often obtained only for some proxy data related to GHG emissions, such as land use and linear emission sources. Recently, also satellite observed nighttime lights have been used for more accurate estimation of spatial distribution of CO₂ emissions (Ghosh et al., 2010; Oda and Maksyutov, 2011).

Typically, the regression models have been applied for spatial allocation of emission data (Dragosits et al., 1998; Oda and Maksyutov, 2011). However, emissions in general tend to be spatially correlated, which gives rise to potential improvements. This idea motivated us to develop a more advanced approach for accurate disaggregation of air pollution data.

Making inference on variables at points or grid cells different from those of the data is referred to as the change of support problem (Gelfand, 2010). Several approaches have been proposed to address this issue. The geostatistical solution for realignment from point to areal data is provided by block kriging (Gotway and Young, 2002). Areal weighting offers a straightforward approach if the data are observed at areal units, and the inference is sought at a new level of spatial aggregation. Some improved approaches with better covariate modeling were also proposed e.g. in Mugglin and Carlin, 1998 and Mugglin et al., 2000.

In this study we propose to apply methods of spatial statistics to produce higher resolution emission inventory data, taking advantage of more detailed land use information. The approach resembles to some extent the method of Chow and Lin (1971), originally proposed for disaggregation of time series based on related, higher frequency series. Here, a similar methodology is employed to disaggregate spatially correlated data.

Regarding an assumption on residual covariance, we apply the structure suitable for areal data, i.e. the conditional autoregressive (CAR) model. Although the CAR specification is typically used in epidemiology (Banerjee et al., 2004), it was also successfully applied for modelling air pollution over space (Kaiser et al., 2002; McMillan et al., 2010). Compare also Horabik and Nahorski (2010) for another application of the CAR structure to model spatial inventory of GHG emissions. The maximum likelihood approach to inference is employed, and the optimal predictors are developed to assess missing concentrations in a fine grid.

The application part of the study concerns an ammonia (NH_3) emission inventory in a region of Poland. Ammonia is emitted mainly by agricultural sources such as livestock production and fertilized fields. Its high concentrations can lead to acidification of soils, forest decline, and eutrophication of waterways. Ammonia emissions are also recognized for their importance in contributing to fine particulate matter; hence its spatial distribution is of great importance. However, agricultural emission sources cannot be measured directly, and spatial emission patterns need to be assessed otherwise. This issue was addressed, among others, by Dragosits et al., 1998, where agricultural and land cover data were used to disaggregate the national NH_3 emission totals across Great Britain. We demonstrate that the straightforward approaches based on linear dependences might be improved by introducing a spatial random effect.

Nevertheless, the proposed approach is of wider applicability, and can be used in numerous situations where higher resolution of spatial data is needed. In the context of the greenhouse gasses, the method might be particularly adequate to improve resolution of these activity data which tend to be spatially correlated. The plausible sectors include agriculture, transportation and forestry. Improved resolution may in turn contribute to limitation of uncertainties underlying GHG inventories.

The format of the article is as follows. Section 2 describes the disaggregation model, its estimation in a coarse grid, and prediction of the value of interest in a fine grid. Section 3 presents the ammonia inventory case study. Here, the sensitivity of the proposed method is examined in various ways. We compare the models with different sets of covariates, the models with and without the spatial component, as well as instances of fourfold and ninefold disaggregation. Conclusions are given in Section 4.

2. Disaggregation framework

This section presents the statistical approach to the issue of spatial disaggregation. The goal of the method is as follows. We have available data on a spatially distributed variable (inventory emissions) integrated in a coarse grid. The aim is to estimate a distribution of this variable in a finer grid, conditional on some explanatory variables observable in the fine grid. It is assumed that the variable of interest is spatially correlated. Its residual covariance

structure is set and the conditional autoregressive model is applied. An additional important assumption of the method is that the covariance structure of the variable at a coarse grid is the same as that at a fine grid.

Below we specify the model and provide details on its estimation in the coarse grid as well as on prediction in the fine grid.

2.1. Model

Fine grid. We begin with the model specification in a fine grid. Let Y_i denote a random variable associated with a missing value of interest y_i defined at each cell i for $i=1, \dots, n$ of a fine grid (n denotes the overall number of cells in a fine grid). Assume that each random variable Y_i follows Gaussian distribution with the mean μ_i and variance σ_y^2

$$Y_i | \mu_i \sim \text{Gau}(\mu_i, \sigma_y^2) \quad (1)$$

Given the values μ_i and σ_y^2 , the random variables Y_i are assumed independent, thus the joint distribution of $\mathbf{Y}=(Y_1, \dots, Y_n)^T$ conditional on the mean process $\boldsymbol{\mu}=(\mu_1, \dots, \mu_n)^T$ is Gaussian

$$\mathbf{Y} | \boldsymbol{\mu} \sim \text{Gau}_n(\boldsymbol{\mu}, \sigma_y^2 \mathbf{I}_n), \quad (2)$$

where \mathbf{I}_n is the $n \times n$ identity matrix.

The mean $\boldsymbol{\mu}$ represents the true process underlying emissions, and the (missing) observations are related to this process through a measurement error with the variance σ_y^2 . The model for the mean process is formulated as a sum of the regression component with available covariates, and a spatially varying random effect. For this, the conditional autoregressive model is used. The CAR model is given through the specification of the full conditional distribution functions of μ_i for $i=1, \dots, n$ (Cressie, 1993; Banerjee et al., 2004)

$$\mu_i | \boldsymbol{\mu}_{-i} \sim \text{Gau} \left(\mathbf{x}_i^T \boldsymbol{\beta} + \rho \sum_{\substack{j=1 \\ j \neq i}}^n \frac{w_{ij}}{w_{i+}} (\mu_j - \mathbf{x}_j^T \boldsymbol{\beta}), \frac{\tau^2}{w_{i+}} \right), \quad (3)$$

where $\boldsymbol{\mu}_{-i}$ denotes all elements in $\boldsymbol{\mu}$ but μ_i , w_{ij} are the adjacency weights ($w_{ij} = 1$ if j is a neighbour of i and 0 otherwise, also $w_{ii} = 0$); $w_{i+} = \sum_j w_{ij}$ is the number of neighbours of area i ; \mathbf{x}_i is a vector containing 1 as its first element (for the intercept β_0) and k explanatory covariates of area i as the next elements; $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_k)^T$ is a vector of regression coefficients. The CAR structure follows an assumption of similar random effects in adjacent cells; this is reflected in the second summand of the conditional expected value of μ_i , which is proportional to the average values of remainders $\mu_j - \mathbf{x}_j^T \boldsymbol{\beta}$ for neighbouring sites (i.e. when $w_{ij} = 1$). This proportion is calibrated with the parameter ρ . Thus ρ reflects strength of spatial association. The variance of the full conditional distribution of μ_i is inversely proportional to the number of neighbours w_{i+} , and τ^2 is a variance parameter.

Given (3), the joint probability distribution of the process $\boldsymbol{\mu}$ is as follows, see e.g. Banerjee et al. (2004)

$$\boldsymbol{\mu} \sim \text{Gau}_n(\mathbf{X}\boldsymbol{\beta}, \tau^2(\mathbf{D} - \rho\mathbf{W})^{-1}), \quad (4)$$

where \mathbf{X} is the matrix whose rows are the vectors \mathbf{x}_i^T

$$X = \begin{bmatrix} I & x_{11} & \cdots & x_{1k} \\ \vdots & \vdots & \ddots & \vdots \\ I & x_{n1} & \cdots & x_{nk} \end{bmatrix};$$

D is an $n \times n$ diagonal matrix with w_{i+} on the diagonal; and W is an $n \times n$ matrix with adjacency weights w_{ij} . Equivalently we can write (4) as

$$\mu = X\beta + \varepsilon, \quad \varepsilon \sim \text{Gau}_n(\theta, \Omega), \quad (5)$$

where $\Omega = \tau^2(D - \rho W)^{-1}$.

Coarse grid. The model for a coarse grid (aggregated) observed data is obtained by multiplication of (5) with the $N \times n$ *aggregation matrix* C consisting of 0's and 1's, indicating which cells have to be aggregated together

$$C\mu = CX\beta + C\varepsilon \quad C\varepsilon \sim \text{Gau}_N(\theta, C\Omega C^T) \quad (6)$$

where N is the number of observations in a coarse grid. Now, suppose that the random variable $\lambda = C\mu$ is the mean process for random variables $Z = (Z_1, \dots, Z_N)^T$ associated with observations $z = (z_1, \dots, z_N)^T$ of the aggregated model

$$Z | \lambda \sim \text{Gau}_N(\lambda, \sigma_z^2 I_N). \quad (7)$$

Thus, random variables Z_i , $i = 1, \dots, N$ are conditionally independent

$$Z_i | \lambda_i \sim \text{Gau}(\lambda_i, \sigma_z^2) \quad (8)$$

where λ_i is the i -th element of the vector λ .

2.2. Estimation and prediction

Having available observations of Z_i in the coarse grid, we can estimate parameters $\beta, \sigma_z^2, \tau^2$ and ρ with the maximum likelihood (ML) method. First, from (6) and (7) the joint unconditional distribution of Z is derived

$$Z \sim \text{Gau}_N(CX\beta, M + C\Omega C^T), \quad (9)$$

where $M = \sigma_z^2 I_N$, I_N is the $N \times N$ identity matrix; see e.g. Lindley and Smith (1972). Next, we formulate the log likelihood function associated with (9)

$$\begin{aligned} L(\beta, \sigma_z^2, \tau^2, \rho) = & -\frac{1}{2} \log |M + C\Omega C^T| - \frac{N}{2} \log(2\pi) \\ & - \frac{1}{2} (z - CX\beta)^T (M + C\Omega C^T)^{-1} (z - CX\beta), \end{aligned}$$

where $|\bullet|$ denotes the determinant. With fixed σ_z^2, τ^2 and ρ , the above log likelihood is maximised for

$$\beta(\sigma_z^2, \tau^2, \rho) = \left[(CX)^T (M + C\Omega C^T)^{-1} CX \right]^{-1} (CX)^T (M + C\Omega C^T)^{-1} z,$$

which substituted back into the function $L(\beta, \sigma_z^2, \tau^2, \rho)$ provides the profile log likelihood

$$\begin{aligned}
L(\sigma_z^2, \tau^2, \rho) = & -\frac{1}{2} \log |\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T| - \frac{N}{2} \log(2\pi) \\
& - \frac{1}{2} \left[\mathbf{z} - \mathbf{C}\mathbf{X} \left[(\mathbf{C}\mathbf{X})^T (\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T)^{-1} \mathbf{C}\mathbf{X} \right]^{-1} (\mathbf{C}\mathbf{X})^T (\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T)^{-1} \mathbf{z} \right]^T \\
& \times (\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T)^{-1} \\
& \times \left[\mathbf{z} - \mathbf{C}\mathbf{X} \left[(\mathbf{C}\mathbf{X})^T (\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T)^{-1} \mathbf{C}\mathbf{X} \right]^{-1} (\mathbf{C}\mathbf{X})^T (\mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T)^{-1} \mathbf{z} \right].
\end{aligned}$$

Further maximisation of $L(\sigma_z^2, \tau^2, \rho)$ is performed numerically, including checks on ρ to ensure that the matrix $\mathbf{D} - \rho\mathbf{W}$ is non-singular, see Banerjee et al. (2004).

To obtain the standard errors of estimated parameters, one needs to derive the Fisher information matrix. The asymptotic variance-covariance matrix of the ML estimators is obtained by inverting the expectation of the negative of the second derivatives (the Hessian) of the log likelihood function, and the expectation is evaluated at the ML estimates. In other words, the expected Fisher information matrix is used to obtain the standard errors of parameters. Calculation of the Hessian with respect to the regression coefficients is relatively straightforward, but it becomes more burdensome for the covariance parameters. Detailed derivation of the explicit formulas for the expected Fisher information matrix will be provided elsewhere; here we report the standard errors of parameter estimators obtained in the case study.

To estimate the required values in a fine grid, we apply the following prediction procedure. Note that our primary interest is the underlying emission inventory process $\boldsymbol{\mu}$. The predictors optimal in the minimum mean squared error sense are given by $E(\boldsymbol{\mu} | \mathbf{z})$. The joint distribution of $(\boldsymbol{\mu}, \mathbf{Z})$ is given by

$$\begin{pmatrix} \boldsymbol{\mu} \\ \mathbf{Z} \end{pmatrix} \sim \text{Gau}_{N+n} \left(\begin{pmatrix} \mathbf{X}\boldsymbol{\beta} \\ \mathbf{C}\mathbf{X}\boldsymbol{\beta} \end{pmatrix}, \begin{pmatrix} \Omega & \Omega\mathbf{C}^T \\ \mathbf{C}\Omega & \mathbf{M} + \mathbf{C}\Omega\mathbf{C}^T \end{pmatrix} \right). \quad (10)$$

The distribution (10) allows for full inference, yielding both the predictor $\hat{\boldsymbol{\mu}} = \widehat{E}(\boldsymbol{\mu} | \mathbf{z})$ and its error $\hat{\sigma}_{\hat{\boldsymbol{\mu}}}^2 = \widehat{\text{Var}}(\boldsymbol{\mu} | \mathbf{z})$

$$\hat{\boldsymbol{\mu}} = \mathbf{X}\hat{\boldsymbol{\beta}} + \hat{\Omega}\mathbf{C}^T (\hat{\mathbf{M}} + \mathbf{C}\hat{\Omega}\mathbf{C}^T)^{-1} [\mathbf{z} - \mathbf{C}\mathbf{X}\hat{\boldsymbol{\beta}}] \quad (11)$$

$$\hat{\sigma}_{\hat{\boldsymbol{\mu}}}^2 = \hat{\Omega} - \hat{\Omega}\mathbf{C}^T (\hat{\mathbf{M}} + \mathbf{C}\hat{\Omega}\mathbf{C}^T)^{-1} \mathbf{C}\hat{\Omega}, \quad (12)$$

where $\hat{\cdot}$ denotes the estimated values.

3. Case study

3.1. Data

The proposed procedure is illustrated using a real dataset of gridded inventory of NH_3 (ammonia) emissions from fertilization (in tonnes per year) reported in a northern region of Poland (the Pomorskie voivodship). The inventory grid cells are of regular $5\text{km} \times 5\text{km}$ size, and the whole of cadastral survey compiles $n=800$ cells, denoted $\mathbf{y} = (y_1, \dots, y_n)^T$, see Figure 1. For explanatory information we use the CORINE Land Cover Map for this region, available from the European Environment Agency (2011). Specifically, for each grid cell we calculate area of these land use classes, which are related to ammonia emissions. The following CORINE classes were considered (the CORINE class numbers are given in brackets):

Non-irrigated arable land (211), denoted $x_1 = (x_{1,1}, \dots, x_{n,1})^T$;

Fruit tree and berry plantations (222), denoted $x_2 = (x_{1,2}, \dots, x_{n,2})^T$;

Pastures (231), denoted $x_3 = (x_{1,3}, \dots, x_{n,3})^T$;

Complex cultivation patterns (242), denoted $x_4 = (x_{1,4}, \dots, x_{n,4})^T$;

Principally agriculture, with natural vegetation (243), denoted $x_5 = (x_{1,5}, \dots, x_{n,5})^T$.

Performance of the proposed disaggregation framework depends on a few factors. Perhaps the most crucial ones are the following two: (i) explanatory power of covariates available in the fine grid, and (ii) an extent of disaggregation, which is connected with preservation of the spatial correlation. An impact of both these features will be evaluated in our case study.

Regarding the first factor, we will examine models with all the above land use classes (set 1), and compare the results with models including only two of them: non-irrigated arable land and complex cultivation patterns (set 2). This subset of land use classes was chosen on a basis of explanatory power. When limiting a number of explanatory variables, these two covariates provided the best results. Secondly, we compare a linear regression with independent (iid) errors versus spatially correlated errors modelled by the CAR process. We consider the following models:

Model CAR1: - CAR errors, set 1 of covariates;

Model LM1: - iid errors, set 1 of covariates;

Model CAR2: - CAR errors, set 2 of covariates;

Model LM2: - iid errors, set 2 of covariates.

This setting of four models is intended to enable the analysis of extent to which a limited number of explanatory information can be compensated by spatial modeling.

Regarding the second factor, we test the disaggregation from $10\text{km} \times 10\text{km}$ and $15\text{km} \times 15\text{km}$ (coarse) grids into a $5\text{km} \times 5\text{km}$ (fine) grid. To examine performance of the disaggregation procedure, first we aggregate the original fine grid emissions into respective coarse grid cells. Next, we fit the proposed model and predict ammonia emissions for a $5\text{km} \times 5\text{km}$ (fine) grid. Finally, we check the obtained results with the original inventory emissions of a $5\text{km} \times 5\text{km}$ (fine) grid. Thus, our simulation study tests the cases of a fourfold and ninefold disaggregation. The aggregated values of the two coarse grids as well as the actual inventory data in the fine grid are shown in Figure 1.

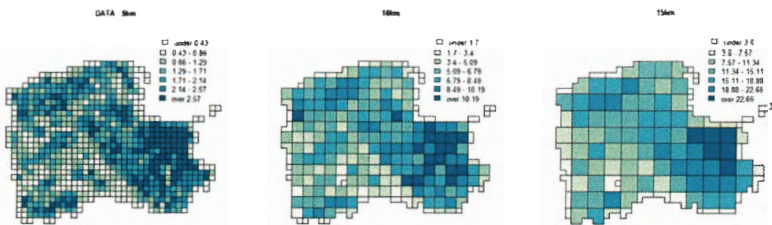


Figure 1. Ammonia emissions: inventory data in 5km grid, and aggregated values in 10km and 15km grids

3.2. Results of disaggregation from a 10km grid

This subsection presents the model testing results for disaggregation from a 10km grid. Table 1 displays the maximum likelihood estimates (denoted by Est.) and standard errors (denoted by Std.Err.) of the parameter estimators for each model. Note that in the models with set 1 of covariates (CAR1, LM1) the regression coefficient β_0 was dropped as it was statistically insignificant. In the table, we can observe that the ML estimates of the regression coefficients are similar for all the models. From the ratio of regression coefficients and its respective standard errors (i.e. the t-test statistic), we can roughly conclude that all the considered land use classes are statistically significant; in fact, in each case respective p -values proved to be less than 0.05 (not shown). Next, let us turn our attention to the error part of the models. Significantly lower values of σ_z^2 estimates under both the CAR models, as compared with their linear regression counterparts, indicate that greater variability is explained by the models with spatially correlated errors than by the corresponding models with independent errors. As expected, among the spatially correlated models, both variance parameters σ_z^2 and τ^2 are higher for CAR2 than for CAR1 model with five land use classes as explanatory variables. Furthermore, the parameter ρ reflects strength of the spatial correlation. Note that $\rho = 0$ corresponds to a model with independent errors, see also Banerjee et al. (2004) for more details. A value of parameter ρ is higher for CAR2 model, which illustrates that in the models of limited explanatory power, importance of spatial correlation becomes more pronounced.

Table 1. Maximum likelihood estimates for the 10km grid

	CAR1		LM1		CAR2		LM2	
	Est.	Std.Err.	Est.	Std.Err.	Est.	Std.Err.	Est.	Std.Err.
β_0	-	-	-	-	0.386	9.29e-02	0.452	5.45e-02
β_1	1.13e-07	3.26e-09	1.09e-07	2.46e-09	1.06e-07	5.03e-09	9.58e-08	4.43e-09
β_2	2.56e-07	1.94e-07	4.48e-07	1.97e-07	-	-	-	-
β_3	9.77e-08	1.19e-08	1.08e-07	1.08e-08	-	-	-	-
β_4	1.18e-07	2.13e-08	1.21e-07	1.76e-08	1.27e-07	2.72e-08	1.60e-07	2.22e-08
β_5	1.27e-07	1.32e-08	1.35e-07	1.11e-08	-	-	-	-
σ_z^2	0.334	0.073	1.165	0.109	0.522	0.111	1.95	0.184
τ^2	0.536	0.082	-	-	0.807	0.124	-	-
ρ	0.948	9.98e-04	-	-	0.972	9.98e-04	-	-

Results of the four models are also summarized using the Akaike criterion (AIC). The idea of AIC is to favour a model with a good fit and to penalize for a number of parameters; models with smaller AIC are preferred to models with larger AIC. Table 2 (the upper part) displays AIC for each model, and additionally it reports the negative log likelihood (-L). Naturally, the models with set 1 of covariates provide much better results than the models with another set. Among these respective sets, the models with the spatial structure considerably improve results obtained with the models of independent errors. Note, that this improvement is higher for the models with set 2 of covariates ($797.6-742.8 = 54.8$) than for the models with set 1 of covariates ($685.1-640.7 = 44.4$).

Table 2. Model comparison

Model	$-L$	AIC
10km grid		
CAR1	312.3	640.7
LM1	336.5	685.1
CAR2	365.4	742.8
LM2	394.8	797.6
15km grid		
CAR1	220.6	455.3
LM1	222.9	455.9
CAR2	240.4	492.8
LM2	248.1	504.4

The values of ammonia emissions predicted in a 5km×5km grid (y_i^*) are featured in Figure 2. Differences between the four models are negligible, although a visual comparison with the original emissions in Figure 1 (the left-hand-side plot) suggests that the both models based on set 1 of covariates (CAR1, LM1) provide slightly better results. Since the mapped emission values are classified into just 9 bins, therefore some features might not be easily distinguishable on the maps in Figure 2. To remedy this, Figure 3 presents the model residuals ($d_i = y_i - y_i^*$). Now the difference in prediction results among the models is evident – the best results are obtained for CAR1 model and the worst for LM2 model.

At this point we stress that the values predicted in a fine grid (y_i^*) are calculated with the formula (11) based on the aggregated values of 10 km grid; the calculations are made as if the true emissions were unknown. On the other hand, recall that these true emissions in fine grid (y_i) are available; see the left-hand-side map in Figure 1. From now on, our analysis is based on comparison between the prediction results obtained with the proposed technique and the original fine grid ammonia emissions (observations).

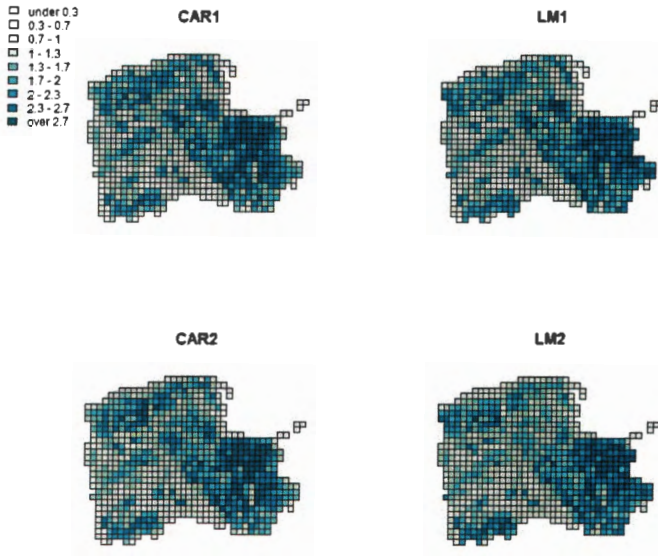


Figure 2. Ammonia emissions predicted in a fine grid – disaggregation from 10 km grid

Figure 4 presents, for each model, a scatterplot of predicted values y_i^* versus observations y_i . The straight line has slope 1, thus if the predicted values are close to the original data, points are close to the straight line. This setting, once again, illustrates much better explanatory power of models based on all the land use classes (set 1 of covariates). It also illustrates importance of the spatial structure component. In the case of models CAR2 and LM2, introduction of spatial dependence evidently improved accuracy of prediction. Whereas in the case of models CAR1 and LM1, the applied spatial structure allowed to considerably limit a number of highly overestimated predictions (points below the straight line). Furthermore, we note that the linear regression LM1 provides biased predictions (for the prevailing number of cases) of upper range emission values (emissions over 1.5 tonnes), while CAR1 model allows to overcome this deficiency. The dotted line for LM2 seems to have slightly higher slope than 1, while this effect is rather not visible for CAR2 model.

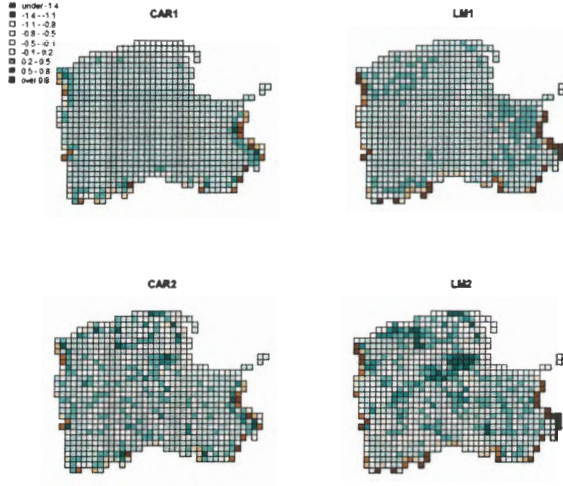


Figure 3. Residuals from predicted values – disaggregation from 10 km grid

The residuals d_i are further analysed in Table 3 (the upper part). Namely, we calculate the mean squared error (MSE)

$$MSE = \frac{1}{n} \sum (y_i - y_i^*)^2,$$

which should be as low as possible. The mean squared error reflects how well a model predicts data. In Table 3 we report also the minimum and maximum values of d_i , and the sample correlation coefficient r between the predicted y_i^* and observed y_i values. In terms of both the mean squared error and the coefficient r , the best model is CAR1 and the poorest one is LM2, following the previous assessments. Interestingly, the remaining two models changed their ranks compared with the AIC criterion. That is, CAR2 model has lower MSE = 0.158 and higher coefficient $r = 0.901$ than the linear model based on set 1 of covariates (LM1 model with MSE = 0.186 and $r = 0.882$). This proves that the model with a limited number of covariates but having a spatial component (CAR2) can provide better disaggregation results than the model based solely on a linear regression, even though its covariate information is richer (LM1). Note that the analysis based on residuals is more robust than the AIC rating, which basically tests a model fit to the aggregated data.

Table 3. Analysis of residuals ($d_i = y_i - y_i^*$)

Model	MSE	min(d_i)	max(d_i)	r
Disaggregation from 10km grid				
CAR1	0.064	-1.717	1.104	0.961
LM1	0.186	-2.544	0.268	0.882
CAR2	0.158	-1.917	1.362	0.901
LM2	0.291	-2.498	1.765	0.808
Disaggregation from 15km grid				

CAR1	0.136	-2.428	0.646	0.915
LM1	0.189	-2.600	0.516	0.880
CAR2	0.190	-2.132	1.446	0.880
LM2	0.295	-2.511	1.746	0.807

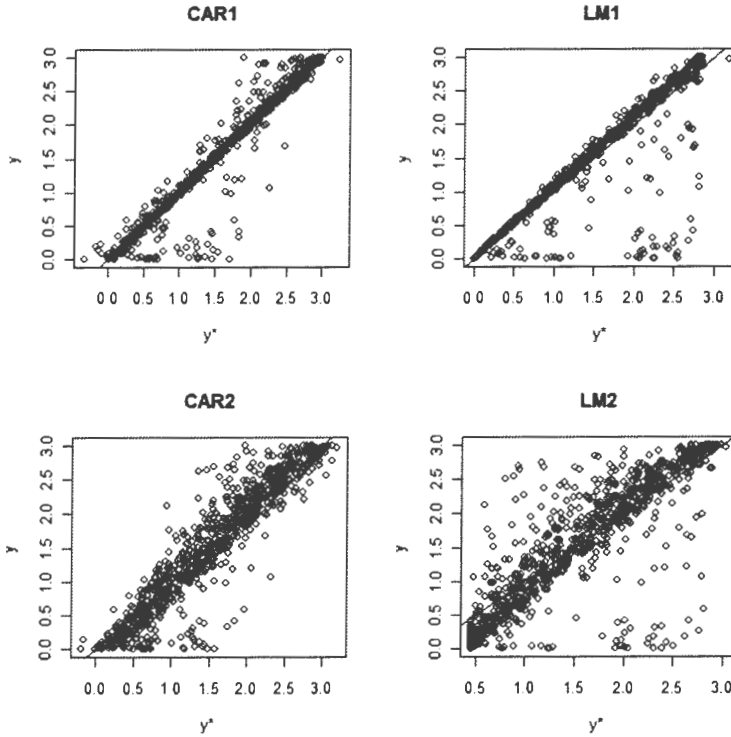


Figure 4. Predicted (\hat{y}) versus observed (y) values – disaggregation from 10 km grid

Following the formula (12), we calculate also the prediction error. Since in the present case study the correct values of predicted emissions are known, we are in a position to compare the prediction error with actual residuals (more precisely, with its absolute values). In Figure 5 these values are presented for CAR2 model. It is noticeable that the prediction error is significantly underestimated, and moreover, it does not reflect diversification of actual residuals properly. Note that in both the maps the highest errors are reported on the border of the domain; this fact is known as the edge effect in spatial modelling.

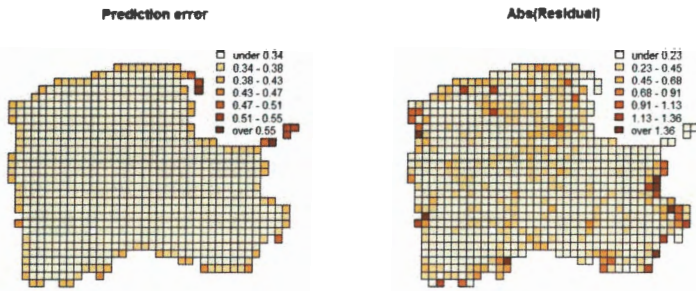


Figure 5. Prediction error and absolute values of residuals for CAR2 model. Note that the maps are drawn in different scales.

3.2 Results of disaggregation from a 15km grid

Next, the results of disaggregation from a 15km grid are presented. The conducted analysis is similar to the one of 10km grid, and, where appropriate, both settings are being compared.

Table 4 contains the maximum likelihood estimates for the 15km grid data. In the models with set 1 of covariates, again the regression coefficient β_0 was dropped. Moreover, in all the models at this level of aggregation land use class “Fruit tree and berry plantations” (β_2) was statistically insignificant, and thus it was also dropped from the considered models. The remaining land use classes were informative, with respective p -values lower than 0.05.

With regards to the error part of Table 4, all the comments reported for 10 km disaggregation (see Table 1) remain valid also here, although their degree is significantly lower. Both the CAR models provide lower values of σ_z^2 than their linear regression counterparts. However, the reduction of unexplained variability between the models, for instance, LM1 and CAR1 is only 1.5 (3.5/2.339), while it was over 3 (1.165/0.334) for respective models of 10 km disaggregation. This suggests that the spatial correlation strength of the 15km grid model is smaller than the 10km grid one. Thus, here the CAR models are less competitive than the LM models, as compared to the former grid.

Table 4. Maximum likelihood estimates for the 15km grid

	CAR1		LM1		CAR2		LM2	
	Est.	Std.Err.	Est.	Std.Err.	Est.	Std.Err.	Est.	Std.Err.
β_0	-	-	-	-	0.424	1.04e-01	0.476	6.82e-02
β_1	1.12e-07	3.95e-09	1.09e-07	3.42e-09	1.00e-07	7.01e-09	9.35e-08	5.79e-09
β_2	-	-	-	-	-	-	-	-
β_3	1.07e-07	1.84e-08	1.16e-07	1.55e-08	-	-	-	-
β_4	1.24e-07	2.77e-08	1.29e-07	2.34e-08	1.56e-07	3.65e-08	1.75e-07	2.79e-08

β_5	1.27e-07	1.65e-08	1.33e-07	1.49e-08	-	-	-	-
σ_z^2	2.339	0.424	3.50	0.474	2.681	0.548	5.55	0.753
τ^2	0.214	0.088	-	-	0.414	0.088	-	-
ρ	0.966	4.91e-04	-	-	0.982	5.55e-05	-	-

The values of AIC criterion and of the negative log likelihood (-L) are reported in the lower part of Table 2. Similarly as for the disaggregation from a 10km grid, also in this case the models based on set 1 of covariates provide better results. The CAR structure improves obtained linear regression results of both respective covariate sets. Note, however, that in the setting of 15km disaggregation, an impact of the spatial component is not that substantial anymore as it was previously. Again, a higher improvement is noted for the models with a limited number of covariates ($504.4 - 492.8 = 11.6$ in terms of the AIC criterion), and the gain from incorporation of the spatial component is only marginal for the models with set 1 of covariates ($455.9 - 455.3 = 0.6$).

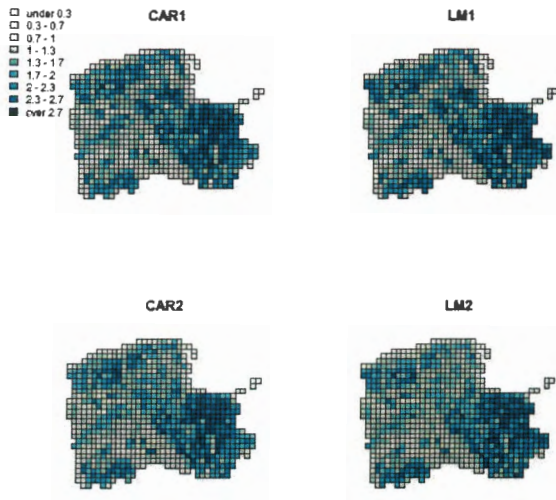


Figure 6. Ammonia emissions predicted in a fine grid – disaggregation from 15 km grid

The values of ammonia emissions disaggregated from 15 km cells and predicted in a fine grid are shown in Figure 6; respective residuals are featured in Figure 7. While for the 10 km disaggregation the residual maps clearly indicated discrepancies among the models, this is not so easily visible in Figure 7. The models based on set 1 of covariates (CAR1, LM1) provide smaller residuals. However, the differences between the spatial models and its linear regression counterparts seem to be negligible.

Table 3 (the lower part) provides further, more quantitative analysis of residuals. The mean squared error MSE and the correlation coefficient r yield a consistent ranking of the models. Obviously the best model is CAR1 with $r = 0.915$ and $MSE = 0.136$, while the poorest one is LM2 with $r = 0.807$ and $MSE = 0.295$. When it comes to the remaining two models, LM1 slightly outperforms CAR2 (only in terms of the mean squared error). Note that this order is reversed when compared with the results of 10 km grid disaggregation (the upper part of the table). Therefore, when disaggregating from 10 km grid, the spatial structure is more informative than some of the covariates, but this is not true anymore when disaggregating from 15 km grid. From this we conclude that in this particular case study, the proposed framework offers an efficient tool for a quadruple and nine-times disaggregation, but it may become less adequate for higher order allocations.

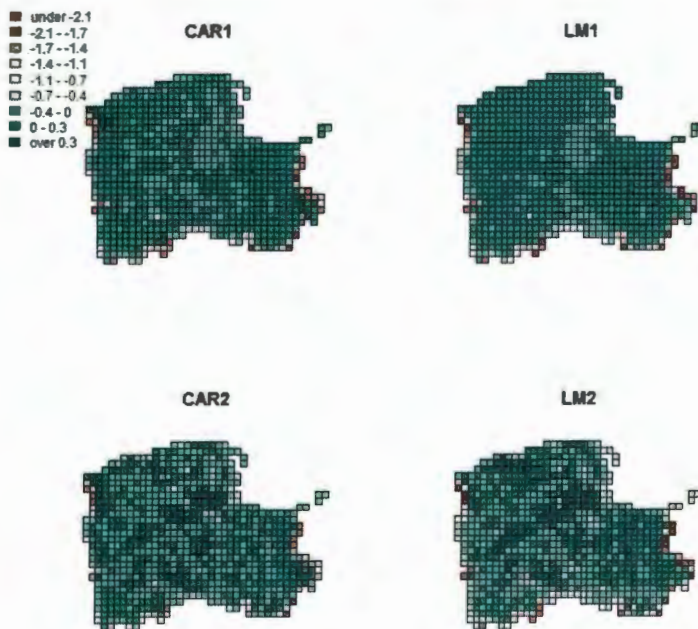


Figure 7. Residuals from predicted values – disaggregation from 15 km grid

The actual interplay among the four models is further illustrated on the scatterplots in Figure 8. We note that the 15 km disaggregation, in general, preserves the features reported previously - the performance of respective models is quite analogous as for the 10 km disaggregation. It means that for the models based on set 2 of covariates, the spatial correlation significantly improves prediction quality. Also for the other two models, introduction of spatial structure is still beneficial as it allows to correct the prediction bias and to slightly reduce a number of overestimates. We highlight the difference between the models

CAR2 and LM1, which yield almost the same MSE and coefficient r , but provide completely distinct plots, as shown in Figure 8. The residuals of CAR2 model are more dispersed owing to a limited set of explanatory covariates. On the other hand, improved covariate modeling of LM1 leads to the residuals gathered close to the diagonal, but a lack of spatial averaging result in much more overestimated values. Altogether, assessment of residuals of both the models, surprisingly becomes the same.

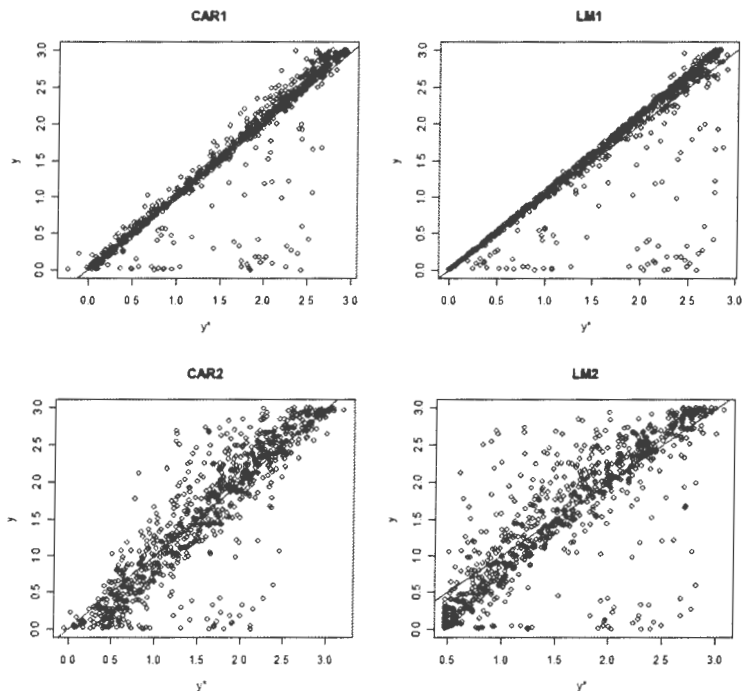


Figure 8. Predicted (y^*) versus observed (y) values – disaggregation from 15 km grid

A comparison of 10 km and 15 km disaggregation is presented in Figure 9, which shows the scatterplots for CAR1 models. As to be expected, performance of 10 km disaggregation is definitely better. This is especially visible for the overestimated emissions (points below the straight line) in the 15 km disaggregation model. In the left-hand-side plot, a number of overestimated predictions is significantly lower.

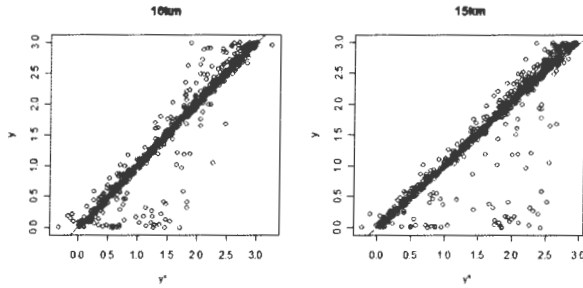


Figure 9. Predicted (y^*) versus observed (y) values for CAR1 model of disaggregation from 10 km and 15 km grids

4. Discussion and conclusions

The major objective of this study was to demonstrate how a variable of interest (e.g. emissions) available in a coarse grid plus information on some related covariates available in a finer grid can be combined together to provide the variable of interest in a finer grid, and therefore to improve its spatial resolution. We proposed a relevant disaggregation model and illustrated the approach using a real dataset of ammonia emission inventory. The idea is conceptually similar to the method of Chow and Lin (1971), originally designed for time series data; see also Polasek (2010). It was applied to the spatially correlated data, and a spatial dependence was modelled with the conditional autoregressive structure introduced into a linear model as a random effect.

The concept of the model lies in accounting for this part of spatial variation, which has not been explained by available covariates. Thus, if the covariate information do not correctly reflect a spatial distribution of a variable of interest, there is potential for improving the approach with a relevant model of spatial correlation. The underlying assumption of the method is that the covariance structures of the variable at a coarse grid and at a fine grid are the same. In the present study of ammonia emissions examined at 5 km, 10 km, and 15 km grids, this assumption proved to be reasonable.

Performance of the proposed framework was evaluated with respect to the following two factors: explanatory power of covariates available in a fine grid, and an extent of disaggregation. The results indicate that inclusion of a spatial dependence structure can compensate for less adequate covariate information. For the considered ammonia inventory, the fourfold allocation benefited greatly from an incorporation of the spatial component, while for the ninefold allocation this advantage was limited, but still evident. In addition, the proposed method allowed to correct the prediction bias encountered for upper range emissions in the linear regression models.

We note that in this case study we used the original data in a fine grid to assess the quality of resulting predictions. For the purpose of potential applications, we developed also a relevant measure of prediction error (the formula 12). Although not entirely faultless, it is the first attempt to quantify the prediction error in situations, where original emissions in a fine grid are not known.

It should also be mentioned that other approaches, such as a geostatistical model, might be potentially used for the problem of spatial allocation. Application of the geostatistical approach brings us to the concept of block kriging (Gelfand 2010). We stress, however, that

geostatistics is more appropriate for point referenced data, while our proposition is dedicated to the case of emission inventories which involve areal data. Thus, the choice between these two options should be considered on a case by case basis.

Another possibility to attack the issue of spatial disaggregation could be to use some expert knowledge and logical inference; compare Verstraete (this issue) for a fuzzy inference system to the map overlay problem.

The method of improving resolution opens the way to uncertainty reduction of spatially explicit emission inventories, hence the future work will also include testing the proposed disaggregation framework for inventories of greenhouse gasses.

Acknowledgements

The study was conducted within the 7FP Marie Curie Actions IRSES project No. 247645. J. Horabik acknowledges support from the Polish Ministry of Science and Higher Education within the funds for statutory works of young scientists. This contribution is also supported by the Foundation for Polish Science under International PhD Projects in Intelligent Computing; project financed from The European Union within the Innovative Economy Operational Programme 2007-2013 and European Regional Development Fund. Z. Nahorski was financially supported by the statutory funds of the Systems Research Institute of Polish Academy of Sciences.

The authors gratefully acknowledge the provision of data for the case study from Ekometria – Biuro Studiów i Pomiarów Proekologicznych in Gdańsk, Poland.

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the 1990s, the number of people in the world who are under 15 years of age is expected to increase from 1.1 billion to 1.5 billion (United Nations 1994).

There are a number of reasons why the number of children in the world is increasing. One of the main reasons is that the number of children who are surviving to adulthood is increasing. This is due to a number of factors, including improved medical care, better nutrition, and a decrease in child mortality.

Another reason why the number of children in the world is increasing is that the number of children who are being born is increasing. This is due to a number of factors, including a decrease in the age at which women are having children, and an increase in the number of children who are surviving to adulthood.

The number of children in the world is increasing, and this is a cause for concern. There are a number of reasons why this is a cause for concern, including the fact that the number of children who are living in poverty is increasing, and the number of children who are being abused is increasing.

There are a number of things that can be done to help reduce the number of children in the world. One of the most important things is to improve the health care system, so that more children are surviving to adulthood. Another important thing is to improve the nutrition of children, so that they are better able to survive.

It is also important to reduce the number of children who are being born. This can be done by providing women with better access to family planning services, and by educating women about the benefits of smaller families.

The number of children in the world is increasing, and this is a cause for concern. There are a number of things that can be done to help reduce the number of children in the world, and it is important that we take action now to help reduce the number of children who are living in poverty and being abused.

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