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Managing data diversity in air quality monitoring and dynamical mapping

by

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Abstract

In the last decades, air quality monitoring networks have been increasingly installed around the world, with designs which are developed often on a local basis. For example, the European Community gives general rules for the member states which demand local governments to design and manage such local networks.

As a result, even if modern instruments are rather precise, the EC monitoring network is very expensive and appears rather heterogeneous from the point of view of spatial representativeness, human risk exposure etc.. Thickening the network at the global scale is an unaffordable task.

Satellite measurements are then an interesting data source because of homogeneity over time and space and fixed cost.

Along these lines, in this paper, we discuss statistical issues in air quality indexes and spatio-temporal modelling for merging ground level data, computer simulation outputs and satellite data.

1 Introduction

The perspective of defining a European "common monitoring methodology" for air quality is developing in these years from the level of "common measurements methods" to the level of "common interpretation methods".

In particular, the European Community started by regulating measurement instruments (e.g. European norm (EN 12341)) in the 1990's and recent projects (CiteAir, Interreg IIIC) consider common index methodology. Moreover *Directorate General - Environment of European Commission* [4] envisaged a common assessment methodology, which makes air quality fully comparable in time and across different countries.

This paper is then focussed on the level of *"common interpretation methods"*, which means here, discussing statistical issues related to data diversity in air quality with special reference to *"common spatio-temporal modelling"* aimed at understanding important relations by means of parametric models and dynamical mapping. Moreover, we discuss *"common air quality indexes"* assessing the network heterogeneity around the European Community.

To this considering data from three diffeerent sources is important. The first, more traditional data source, is based on ground level air quality monitoring networks which have been increasingly installed around Europe and the world. Since they are designed and managed mainly on a local basis difficulties of comparisons may arise.

The second data source isa based on simulation models both at the regional and continental scale which are increasingly used, and give regularly spaced data both in time and space. Bias often arises and call for statitsical calibration.

The third more promising data source is abased on satellite data which are very interesting because of homogeneity over time and space and fixed cost. Nevertheless, optical data are subject to meteorological conditions.

In this frame, spatio-temporal modelling is concerned with a number of statistical issues which first are related with spatial correlation among the observations in different locations. Moreover data are usually correlated over time so we have serial correlations. In order to manage complexity an important assumption to be considered is that of separability that is spatial correlation is constant over time and serial correlation is constant over space.

Since we are going to consider multiple responses, we need multivariate model machinery which can be managed by hierarchical models. Thanks to the state space model representation we also manage data with systematic missingness, arising from sensitivity to meteorological conditions of satellite data.

The remaining part of the paper is divided in four case studies which discuss data diversity in environmental monitoring.

The first case study is related to instruments heterogeneity and calibration and arise from Northern Italy air quality pollution networks in the early $2000's$. It show that air quality modelling and calibration of different instruments may be performed ex-post. This is important not only in day by day monitoring but also in retrospective trend and time series analysis.

The second case study considers design heterogeneity of air quality networks at the European level. It is especially focussed on the effects of this kind heterogeneity on air quality indexes which are a very useful tool for communicating to wide audience, in a simple way the complex, multidimensional and spatially dispersed concept of "air quality". Since air quality indexes are often used for comparisons, we focus on network design which may influence the index in various countries.

The third case study covers spatio-temporal modelling of computer output data and the EM algorithm. It show estimation and dynamical mapping by using the freely available software `STEM`.

The forth case study considers satellite data and coregionalization and large problem EM algorithm. This level of complexity is often tackled by the Bayesian approach. In this paper we use the classical likelihood approach by resorting extensively to the EM algorithm, here developed at various levels of the hierarchy and coupled with coregionalization.

2 Instrumental heterogeneity

Measurement heterogeneity may arise both over space and/or time because of relevant instrumental differences and biases. For example, European general rules for the member states demand local governments to design, install and manage local monitoring networks, as a result, considering Italy, this is accomplished separately by the 20 local governments "Regioni".

Particulate matters (PM_{10}) monitors have been greatly improved in the last years. In the 1990 monitors based on a tapered element oscillating microbalance (TEOM) were popular in EU because of the low cost, automatic operations and high frequency sampling. After they revealed to be biased with bias size depending on climate conditions, European Community directives asked to move to the method of reference for sampling and measuring PM_{10} concentrations. This is given by the European norm (EN 12341) and is based on the collection of the particulate matters on a filter and the determination of its mass following the gravimetric principle: the high- and low-volume gravimetric samplers (HVG and LVG) comply with the above mentioned regulation. Moreover, the norm suggests standardizing the measurements coming from other samplers that don't respect the gravimetric method and allows also for so-called $\beta-TEOM$. We may then have time series with structural changes because of the change in instruments and/or different stations equipped with different instruments.

2.1 Calibration

Considering the data in Po Valley, 2003, the linear dynamical calibration model of [5] is given by a random intercept and a constant slope

$$\begin{pmatrix} y_G\left(s,t\right) \\ y_T\left(s,t\right) \end{pmatrix} = \begin{pmatrix} u\left(s,t\right) \\ \alpha\left(t\right)+\beta u\left(s,t\right) \end{pmatrix} + \begin{pmatrix} \varepsilon_G\left(s,t\right) \\ \varepsilon_T\left(s,t\right) \end{pmatrix}$$

where the "true value" $u\left(s,t\right)$ is based on a $k-$dim EOF decomposition:

$$u\left(s,t\right) = \Phi\left(s\right) z\left(t\right)$$

The common pollution factor $z(t)$ has a stable Markovian dynamics over time:

$$z_t = Az_{t-1} + \eta_t$$

Information on $\alpha(t)$ and β is accumulated around the map, thanks to the spatial correlation of the errors ε which is covered by the empirical covariance.

The hidden component z is estimated by $\hat{z}(t) = E_{j-1}(z(t)|Y)$ which is given by the Kalman smoother.

Maximum likelihood estimates are obtained by Newton Raphson algorithm, giving

$\bar{\alpha}$	β	A	$log(\sigma_\varepsilon^2)$
2.32	0.34	0.996	-1.28
0.03	0.007	0.002	0.01

$log(\sigma_{\eta_1}^2)$	$log(\sigma_{\eta_2}^2)$	$log(\sigma_{\eta_3}^2)$	$log(\sigma_{\eta_4}^2)$
2.16	-0.38	-0.52	-4.35
0.08	0.15	0.16	0.12

MLE parameters and standard errors for $k = 4$.

2.2 Conclusions

In the perspective of defining a European *"common model based monitoring methodology",* which makes air quality comparable in time and across different countries, ex post calibration based on stochastic modelling may be used to reconstruct comparable time series and improve with respect to those situations where fixed rules for calibration are used.

3 Network heterogeneity

In this section, we consider some issues related to the influence of network heterogeneity with respect to air quality indexes and comparisons at the European level.

In particular, we consider an example of three important regions around Central and Southern Europe, which are subject to different climate, different industrialization and different administrative rules.

Following [1], we consider the North West side of Po Valley, Italy, of Fig. 1, which is heavily polluted and subject to reduced air circulation caused by the C-shaped mountain structure. Using data from 2005, we compare this with two regions from the European central plane, namely Berlin-Brandenburg in Germany, Fig. 2, and Masovia in Poland, Fig. 3, which are subject to Atlantic air circulation.

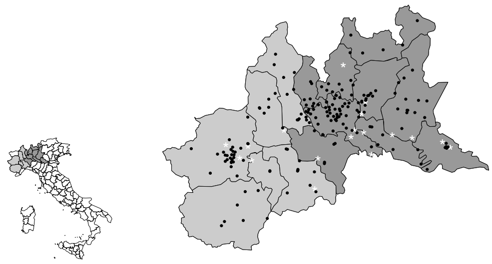

Figure 1: Italian Region of Piedimont-Lombardy.

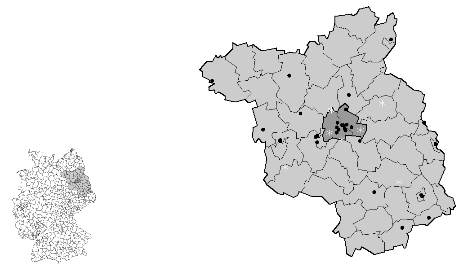

Figure 2: German Region of Berlin-Brandeburg.

The network heterogeneity arises here because station density around the land and monitor type per station are markedly different in the three regions considered. In particular Tab. 1 shows that the three networks are country unbalanced and sensor unbalanced.

3.1 Air quality indexes

Bruno and Cocchi [2] and [3] introduced a general technique for building air quality indexes related to

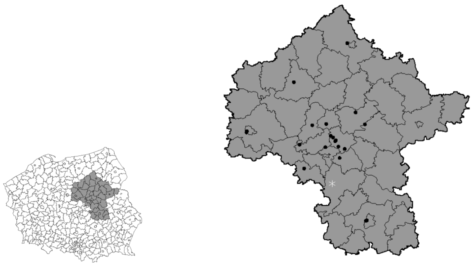

Figure 3: Polish Region of Masovia.

	Italy: Piedimont-Lombardy	Germany: Berlin-Brandeburg	Poland: Masovia
Benzene	21	6	2
CO	124	20	7
NO_2	184	36	12
PM_{10}	79	31	18
O_3	86	26	8
SO_2	75	20	11
N. Stations	199	41	21
Area	49'000 km^2	30'000 km^2	35'000 km^2

Table 1: Year 2005 $-$ Number of stations according to the sensor.

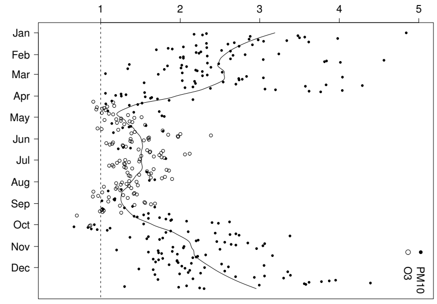

Figure 4: Maxmax index for Italian region, 2005.

the well known air quality index (AQI) from USEPA and European research projects known as CityAir and Interreg III. We consider here the severe exposure daily index commonly denoted by *Maxmax*:

$$I\left(SP.MM\right) = \max_s \left[\max_p \left(\frac{X_{spd}}{u_p}\right)\right]$$

where the symbol p stands for pollutants; namely Benzene, carbon oxide (CO), Nitrogen dioxides (NO_2), particulate matters (PM_{10}), Ozone (O_3) and Sulphur dioxides (SO_2). Hence the quantity X_{spd} is the concentration of pollutant "p" at station "s" on day "d". The denominator u_p is the standard limit value for pollutant "p".

The *Maxmax* index is useful for characterizing critical situations and may be plotted by pointing out the critical pollutant which is the index maximizer for each day. For example, it is clear from Fig. 4-6 that the Italian pollution is much higher and obeys to a stronger seasonality pattern. In summer Ozone is the critical pollutant while in winter the critical pollutant is PM_{10} as a consequence of the climatic stability and lowering of the mixing boundary layer.

3.2 Spatial averaging

As long as *Maxmax* is a measure of severe exposure and should be used by decision makers for ad hoc measures, milder indexes are sometimes required by

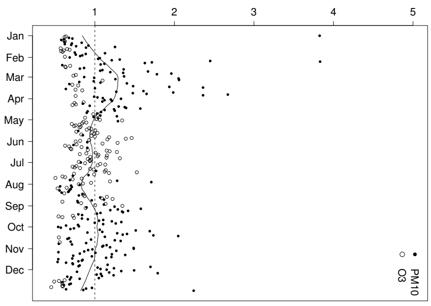

Figure 5: Maxmax index for the German region, 2005.

policy planners. We consider here two different ways of spatial averaging based on the median operator.

The first one is the *spatial median of the worst pollutant*, which is given by

$$I\,(SP.mM) = \underset{s}{median}\left[\max_{p}\left(\frac{X_{spd}}{u_p}\right)\right]$$

This index is shown below to be appropriated for assessing the spatial or network variability. The second one is the *worst median pollutant*, which is given by

$$I\,(PS.Mm) = \max_{p}\left[\underset{s}{median}\left(\frac{X_{spd}}{u_p}\right)\right]$$

and is a valid alternative to the *Maxmax* index for air quality assessment and comparisons..

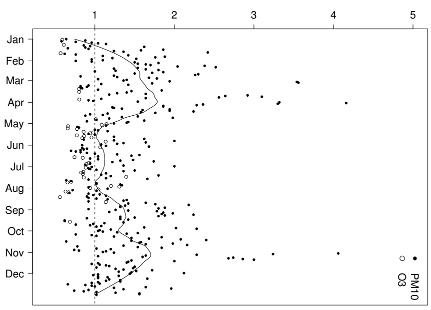

Figure 6: Maxmax index for the Polish region, 2005.

In order to appraise network heterogeneity, [1] proposed the following proper dispersion index, which is given by the one's complement of two indexes ratio as follows

$$V = 1 - \frac{I_d\,(SP.mM)}{I_d\,(SP.MM)}$$

For example Tab. 2 shows the differences in average and dispersion of the considered regions.

	Italy	Germany	Poland
$I\,(SP.MM)$	1.91	1.01	1.33
$I\,(PS.Mm)$	1.04	0.70	0.78
$V = 1 - \frac{I(SP.mM)}{I(SP.MM)}$	0.72	0.31	0.48

Table 2: Annual average of considered indexes.

3.3 Conclusions

Simple indexes like above BC index may be used for synthetic communication of daily health risk related to air pollution and regional comparisons.

In the perspective of defining a European *"common index methodology"*, which makes air quality comparable in time and across different countries, we suggest using companion indexes which can be used for "diagnostics" as shown by index V above.

4 Simulation models

4.1 Model structure

Computer model outputs are particularly useful for mapping because they are available on fine and regular grids and do not have missing values.

The final output considered here is given by daily concentration fields of some primary and secondary pollutants defined on a regular $4Km$ by $4Km$ grid and given by the computer model chain of Fig. 7, which is composed by

1. A *meteorological module* based on *Minerve* and *Surfpro* models (developed, respectively, by Aria Technologies and Arianet) with inputs on geographical information from *Corine Land Cover* project.

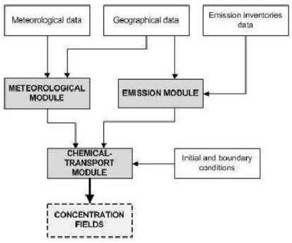

Figure 7: ARPA Piemonte model chain.

2. An *emission module* based on *Emission Manager* model (developed by Arianet) with inputs from the regional and national Emission Inventories.

3. A *chemical-transport module* based on *FARM* (Flexible Air Quality Regional Model by Arianet).

Although the quality and the reliability of such computer-based data is an important point, this issue is not taken into consideration here, and the covariates to be used in the trend $X_t\beta$ are chosen among a set of gridded variables that are the intermediate or final output of the EMCT deterministic model chain. In particular, the set of daily variables under consideration includes meteorological fields, particulate primary emissions (PPM in $g/s/Km^2$) and concentrations (SimPM in $\mu g/m^3$) for year 2004.

4.2 Modelling

We use a measurement error equation

$$y(s,t) = u(s,t) + \varepsilon(s,t)$$

The underlying "true" local pollution level $u(s,t)$ has the following structure

$$u(s,t) = X(s,t)\beta + z_t + \omega(s,t)$$

where X comprises both computer model outputs and other covariates (e.g. altitude)

The purely geostatistical component ω has a Matern correlation structure given by

$$Cov[\omega(s,t), \omega(s',t)] = \sigma_\omega^2 C_\theta(|s-s'|)$$

Moreover, z_t has a stable Markovian temporal dynamics given by

$$z_t = Az_{t-1} + \eta_t$$

The parameter vector

$$\Psi = \left(\beta, \sigma_\varepsilon^2, A, \Sigma_\eta, \theta, \sigma_\omega^2\right)$$

is estimated by Fassò et al. 2008a and by the G-EM algorithm and bootstrap confidence intervals.

Remark 1 *The results are much more stable then NR likelihood optimization because most parameters are updated by closed form formulas.*

Remark 2 *`STEM` software is an R library, developed by Cameletti, available at CRAN repository of R-project.*

Remark 3 *Bootstrap SE have been computed using a cluster based on 10-pentium PC's and `snow` library for distributing the job in R language.*

4.3 EM algorithm

The EM algorithm is a numerical technique for maximizing complex likelihood functions which is particularly suitable for hierarchical models. It is based on iterating an $E-step$ and an $M-step$.

Using a provisional value of the parameter vector Ψ, say Ψ_{j-1}, the $E-step$ gives the expected loglikelihood conditional on all observed data:

$$Q_{j-1}(\Psi) = E_{\Psi_{j-1}}(\log L(\Psi)|Y)$$

The $M-step$ is an update step:

$$\Psi_j = \arg\max Q_{j-1}(\Psi)$$

Thanks to hierarchical modelling we have a simplified optimization problem. To see this partition

$$\Psi = (\Psi_X, \Psi_z, \Psi_\omega)$$

and, accordingly,

$$Q_{j-1}(\Psi) = Q_{j-1}(\Psi_X) + Q_{j-1}(\Psi_z) + Q_{j-1}(\Psi_\omega)$$

Moreover, the first two quantities have closed form formulas and only θ requires numerical optimization.

Applying this algorithm EM to PM_{10} data for 2004, described in [6], one would get the parameter estimates of Tab. 3 and 4 where some coefficients are constant over seasons and others different winter and summer values.

	Winter			
	Estimate	SE	95% CI bounds	
Intercept	3.237	0.046	3.147	3.325
PPM	0.040	0.012	0.017	0.062
SimPM	0.239	0.019	0.203	0.275
Mixing height	-0.133	0.108	-0.364	0.072
Altitude	-0.822	0.060	-0.948	-0.701
	Summer			
	Estimate	SE	95% CI bounds	
Intercept	2.417	0.071	2.185	2.649
PPM	0.093	0.008	0.080	0.109
SimPM	0.233	0.016	0.204	0.268
Mixing height	0.191	0.076	0.047	0.335
Altitude	-0.252	0.052	-0.348	-0.146

Table 3: Seasonal component estimates.

	Estimate	SE	95% CI bounds	
σ_ω^2	0.078	0.001	0.075	0.080
θ	0.023	0.002	0.019	0.026
σ_ε^2	0.078	0.002	0.074	0.082
G	0.747	0.038	0.651	0.806
Σ_η	0.054	0.004	0.045	0.062
μ_0	-0.434	1.074	-2.544	1.551

Table 4: Nonseasonal component estimates.

4.4 Mapping

Using the estimated, the map is computed by the dynamical Kriging equation

$$\hat{Y}(s,t) = E_{j-1}\left(Y(s,t)\,|Y\right)$$

for every s. This gives the dynamical map of Fig. 8 with standarda errors assessing the mapping uncertainty as in Fig. 9.

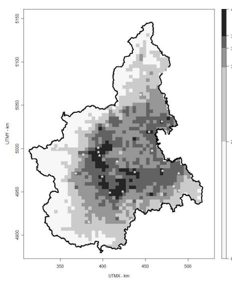

Figure 8: Jan. 30, 2004 - PM_{10} - log scale.

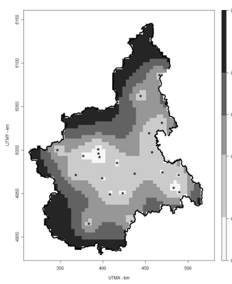

Figure 9: Jan. 30, 2004 - Bootstrap SE of PM_{10} - log scale.

4.5 Conclusions

On the one side computer model outputs may effectively be used to increase the spatial representativeness of ground level monitoring networks. On the other side integrating network data and simulated data may be used for validation and understanding of the computer model behavior.

The EM algorithm is a useful tool for separable spatio-temporal model estimation as it reduces the dimensionality of the related numerical optimization problems.

5 Satellite data

Satellite measurements are an interesting data source because of homogeneity over time and space and fixed cost. For example, MODIS satellites, known as Terra and Aqua give, twice a day, the so-called aerosol optical thickness (AOT) which is reported at 10×10 km^2 resolution and may be used to get information on airborne particulate matters PM_{10} and $PM_{2.5}$ (Chu et al., 2003). AOT are less precise than ground-level measurements of particulate matters based on gravimeters, but can be calibrated using ground-level data on PM_{10} and $\mathrm{PM}_{2.5}$ (Koelemeijer et al. 2006, Wang & Christopher, 2003). Unfortunately AOT depends on cloud free sky. So missing data are the rule rather than the exception and using the previous regression-type approach does not work.

Hence we move to a multivariate spatio-temporal model which covers missing data in the response and data from the various components are not necessarily co-located. Candidate covariates are boundary layer height (BLH), land altitude, land use, wind, humidity. Since relevant correlation of PM and $\frac{AOT}{BLH}$, we use relative AOT, that is $rAOT = \frac{AOT}{BLH}$ for mapping oriented modelling.

5.1 Modelling

The calibration model is now defined using the measurement vector given by

$$y(s,t) = \begin{pmatrix} y_{PM}(s,t) \\ y_{rAOT}(s,t) \end{pmatrix}$$

and a two dimensional vector measurement error equation which is given by

$$y(s,t) = u(s,t) + \varepsilon(s,t)$$

Now, the two-dimensional underlying "true" local pollution level $u(s,t)$ has the following structure

$$u_A(s,t) = X_A(s,t)\beta_A + z_t + W(s,t), \quad {\scriptstyle \mathrm{A=PM,rAOT}}$$

In this equation, the hidden component W is defined by a two-dimensional coregionalization model, i.e.:

$$W(s,t) = \sum_{j=1}^{c} W_j(s,t)$$

and the W_j are the coregionalization components. That is $W_1, ..., W_c$ are independent and white noise with spatial Matern covariance matrices given by

$$Cov\left[W_j(s,t), W_j(s',t)\right] = V_j C_\theta\left(|s-s'|\right)$$

5.2 EM algorithm

The EM algorithm used here extends both results of section 4.3 and the Zhang algorithm introduced for the co-located coregionalization without replications.

The parameter vector is now enlarged to include the coregionalization components

$$\begin{aligned}\Psi &= \left(\beta, \sigma_\varepsilon^2, A, \Sigma_\eta, \theta_1, V_1, ..., \theta_c, V_c\right) \\ &= \left(\Psi_X, \Psi_z, \Psi_{W_1}, ..., \Psi_{W_c}\right)\end{aligned}$$

Thanks to the hierechical structure and parameter partitioning the EM algorithm keeps the nice additive form. Accordingly, the $E - step$ gives:

$$Q_{j-1}(\Psi) = Q_{j-1}(\Psi_X) + Q_{j-1}(\Psi_z) + \sum_{i=1}^{c} Q_{j-1}(\Psi_{W_i})$$

Note that only $\theta_1, ..., \theta_c$ require numerical optimization and all other parameters are update by (high dimensional) closed form formulas.

In practice at j^{th} EM-step, we need to compute the Gaussian expectations conditional on all observed data Y which are given y the following high dimensional (HD) linear and Schur computations

$$\begin{aligned}\hat{z}(t) &= E_{j-1}(z(t)|Y) \\ &= \text{HD Kalman smoother} \\ \hat{W}(\circ,t) &= E_{j-1}(W(\circ,t)|Y) \\ &= \text{HD Gaussian linear computation} \\ \hat{\Omega}(t) &= Var_{j-1}(W(\circ,t)|Y) \\ &= \text{HD Gaussian Schur computation} \\ \hat{Y}(s,t) &= E_{j-1}(Y(s,t)|Y) \\ &= \text{HD Dynamic Kriging computation}\end{aligned}$$

5.3 Estimation and mapping

Preliminary results for model estimation are given in Tab. 5 and 6.Using these estimates, we get both

	Ψ_X			Ψ_z	
	BLH	$altitude$	σ_ε^2	A	σ_η^2
PM_{10}	-0.08	-0.17	1.3	0.74	0.18
$rAOT$		-0.21	1.1		

Table 5: STEM2 model estimates

	Ψ_{W_1}			Ψ_{W_2}		
	θ_1	V_1		θ_2	V_2	
PM_{10}	10.7	0.94	0.7	0.22	0.95	0.81
$rAOT$			0.72			0.75

Table 6: STEM2 model estimates

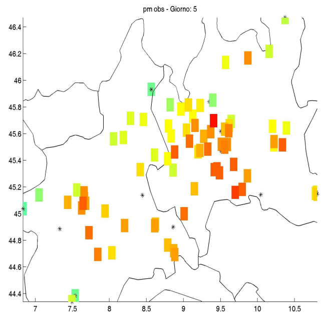

Figure 10: Observed PM_{10} - Ground level network. January 5, 2006.

missing values for AOT and $rAOT$ and dynamical mapping of PM_{10} far away from the original grdound level network. This is done by the dynamical Kriging formula, that is

$$\hat{Y}(s,t) = E_{j-1}(Y(s,t)|Y)$$

As an example, we perfomed these computations for Jan 5, 2006, when PM measurements are as in Fig. 10 and missing values of $rAOT$ are estimated as in Fig. 11. Finally the reconstructed map for $PM_{10} is$ shown in Fig. 12.

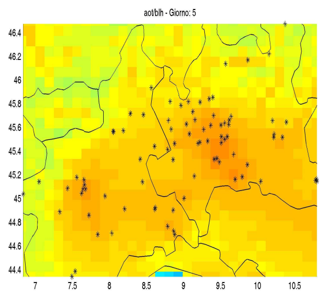

Figure 11: Relative AOT - missing estimated. January 5, 2006.

5.4 Conclusions

Integrating data from satellites and ground level networks at a sub-continental level gives rise a statistical estimation problem which can be fully estimated by the EM algorithm without the need of those oversimplifying and subjective assumptions which are extensively used in most of meteorological and geographical approaches.

The EM algorithm, implemented via Matlab or R language (CRAN) on medium and relatively cheap computer clusters, seems an adequate tool for performing the required likelihood optimization.

The need of bootstrap for computing uncertainty is not simply a computer time costly operation. As a matter of fact, bootstrap simulation is an important step for understanding the model behavior at the identification and validation stage.

6 General Conclusions

In the perspective of defining a European common monitoring methodology, which makes air quality comparable in time and across different countries, the statistical approach may be used together with satellite data to integrate data coming from different networks and to conform monitoring around EU.

On the one side spatio-temporal modelling with ex post calibration may be used to improve air quality mapping capability both at the EU level and at the smaller local scales and giving uncertainty measures of reconstructed values.

On the other side air quality indexes may be completed with diagnostic indicators useful to qualify network heterogeneity.

6.1 Acknowledgements

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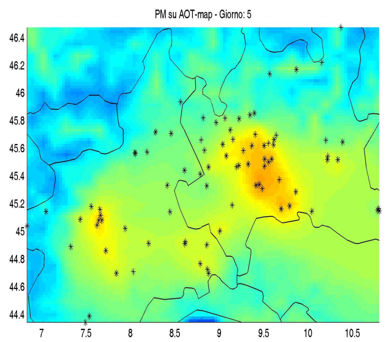

Figure 12: Final Map for PM_{10}. January 5, 2006.

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