



A Model for Spatio-Temporal Prediction of Ground-Level Ozone Mixing Ratios

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Summary

Ground-level ozone is a secondary pollutant produced in the presence of sunlight by chemical reactions involving nitrogen oxides and a variety of volatile organic compounds. The ground-level ozone mixing ratios observed in any given setting depend on the atmospheric chemistry and meteorologic conditions and therefore display marked variability and covariability with location and time. We propose to model this process by first employing a generalized additive model that takes into account the key meteorological factors that influence ozone over time, and then fitting a flexible parametric space-time covariance model to the residual process. This covariance model does not require space-time separability and allows for asymmetries in the space-time process. This model is then used for spatio-temporal prediction and for estimation of the prediction error for surface ozone mixing ratios at locations without monitor data. A validation study shows that these predictions are more accurate than those obtained by using only spatial kriging and ignoring the space-time interactions. In ongoing work, the model will be used to generate neighborhood (ZIP-code) level predictions and standard errors of daily ozone mixing ratios in order to study health risks associated with air pollution at the ZIP-code level.

Keywords: space-time covariance models, ground-level ozone, generalized additive models

Motivation and Context

Multidisciplinary CISES project "Air Quality and Reported Asthma Incidence in Illinois"

- Develop and apply statistical models for spatio-temporal behavior of ozone and particulate matter
- Identify and characterize meteorological regimes which promote elevated air pollution levels
- Establish links between modeled air quality variables and the incidence of acute asthma at the neighborhood level

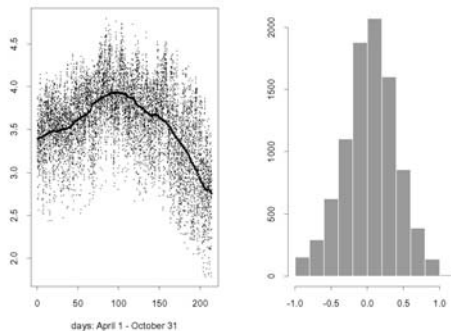
The Data

- Source: ILLINOIS EPA
- 11 monitors distributed throughout Chicago area with almost complete hourly ozone measurements (in ppb)
- Distance between monitors ranges from 5.7 to 52.1 km
- Period of interest: April 1 to October 31, 1995 - 1998

A Generalized Additive Model for Ozone

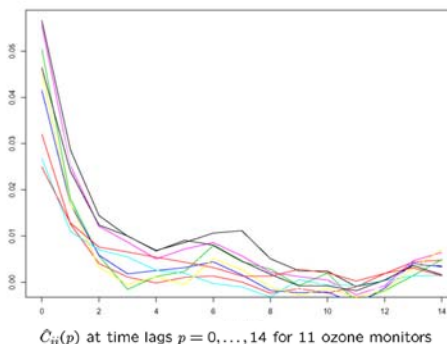
z_{ikl} = natural logarithm of maximum 8-hour-average ozone at station i , year k , day l

$$z_{ikl} = \beta_0 + \beta_1 l + g(l) + \beta^T X_{ikl} + e_{ikl}$$

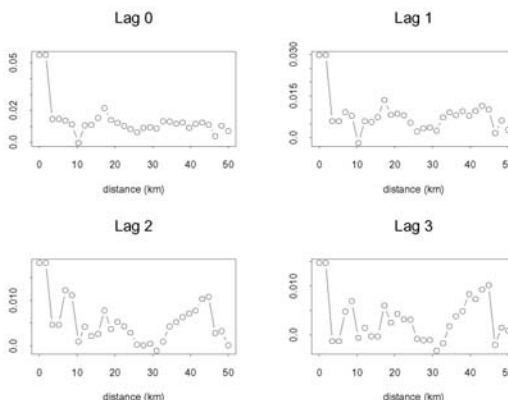


Empirical Measures of Space Time Variability

$$\hat{C}_{ij}(p) = \frac{1}{4n-p} \frac{1}{\sum_{k=1}^4 \sum_{l=1}^{n-p}} \hat{e}_{ikl} \hat{e}_{jk(l+p)}$$



$$\hat{C}(r, p) = \frac{1}{n_r \sum_{d_{ij} \sim r} \hat{C}_{ij}(p)}$$



Modeling The Space-Time Covariance Function

Assuming isotropy in space and short-memory in time, we use the Markov-Matern model introduced in Stein (2003). The space-time covariance function at distance r and lag p is given by

$$K(r, p) = \begin{cases} \frac{\pi^{\frac{d}{2}} \alpha^{\nu+\delta} |p| + d_r \nu + \delta |p| \mathcal{K}_{\nu+\delta}(\alpha r)}{2^{\nu+\delta} |p|^{-1} \Gamma(\nu + \frac{d}{2} + \delta |p|)} & \text{if } r > 0 \\ \pi^{\frac{d}{2}} \alpha^d \Gamma(\nu + \delta |p|) & \text{if } r = 0 \end{cases}$$

Because of the discontinuity of the empirical space-time covariance function at distance close to 0 that persisted for positive time lags, as in Gneiting (2002), we include another parameter to account for a component of the process with temporal but no spatial correlations. Thus we model the space-time covariance function of the residual process as

$$C(r, p) = K(r, p)(1 + \theta_0 1_{\{r=0\}}).$$

Future Work

- Simulation studies
- Exploit the observed asymmetries and use all the data at hand (107 monitors throughout the state of Illinois with variable number of records covering the period 1990-2000)
- Use models that incorporate information on emission sources and output from physical models accounting for the ozone chemistry and meteorological conditions
- Allow for spatial anisotropy, for example by generalizing the deformation approach

Main References

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