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Space-time model to predict tropospheric ozone concentration levels in an industrial region

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The main goal of this work was to develop a space-time model to predict tropospheric ozone (O_3) concentration levels in the surroundings of an industrial Portuguese region, Sines. Regional air quality monitoring network is composed by three conventional monitoring stations, which register hourly O_3 concentrations levels on a high temporal resolution but with very low spatial resolution. To overcome the lack of spatial data to characterize ozone dispersion, O_3 spatial patterns were obtained through several field campaigns of passive samplers (Radiello diffusive tubes) performed over time. This passive sampler allows collecting data on a high spatial density sampling design but for periods of time between 1 to 2 weeks for each campaign, obtaining O_3 mean concentrations over this period.

The proposed space-time model is based in a two steps methodology:

- 1. Time prediction of O_3 concentration levels on monitoring stations location using Multilayer perceptron (MLP) networks.
- 2. Spatial prediction of O₃ concentration levels for the Sines region using block simulation.

The main advantages of applying MLP networks to predict pollutant concentrations are that MLP models do not need exhaustive information about measured pollutant concentrations, reaction mechanisms, meteorological parameters or emission pollutant concentrations, identifying and reproducing nonlinear relationships between the different predictor variables. The developed MLP models presented good performances with values reaching up to 78% of prediction success of O₃ hourly concentrations levels. In the second step Block Sequential Simulation (BSSIM) algorithm is applied to predict spatial pattern of O₃ concentration levels. This simulation method is based on direct sequential simulation (DSS) (Soares, 2001), which does not require a non-linear transformation of the main variable; hence, data with different supports can be jointly used in the same model. In this study we considered O₃ concentrations measured/predicted in point locations but in different time supports. Hence, BSSIM algorithm allowed the integration of hourly O₃ concentration predictions at monitoring station locations and block data such as O₃ mean ozone concentrations over the passive samplers exposure period of time on their locations. Block data error was set for different weather conditions, based on the field campaigns exposed data periods. Preliminary results are quite satisfactory since Block simulation seems able to reproduce the relation between real and predicted values, guaranteeing that the implementation conditions of the stochastic simulation algorithm (variograms, histograms and correlation coefficient of each pair of variables) are reproduced in the final results.