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Data-driven nonlinear optimisation of a simple air pollution dispersion model generating high resolution spatiotemporal exposure

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HIGHLIGHTS

- Fitting a simple dispersion model to high resolution air pollution monitoring data.
- Requires nonlinear regression to obtain the optimal model.
- The results are fully cross-validated.
- Providing pollution exposure estimates at a high resolution in both space and time.

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ABSTRACT

Spatially detailed estimation of exposure to air pollutants in the urban environment is needed for many air pollution epidemiological studies. To benefit studies of acute effects of air pollution such exposure maps are required at high temporal resolution. This study introduces nonlinear optimisation framework that produces high resolution spatiotemporal exposure maps. An extensive traffic model output, serving as proxy for traffic emissions, is fitted via a nonlinear model embodying basic dispersion properties, to high temporal resolution routine observations of traffic-related air pollutant. An optimisation problem is formulated and solved at each time point to recover the unknown model parameters. These parameters are then used to produce a detailed concentration map of the pollutant for the whole area covered by the traffic model. Repeating the process for multiple time points results in the spatiotemporal concentration field. The exposure at any location and for any span of time can then be computed by temporal integration of the concentration time series at selected receptor locations for the durations of desired periods. The methodology is demonstrated for NO_2 exposure using the output of a traffic model for the greater Tel Aviv area, Israel, and the half-hourly monitoring and meteorological data from the local air quality network. A leave-one-out cross-validation resulted in simulated half-hourly concentrations that are almost unbiased compared to the observations, with a mean error (ME) of 5.2 ppb, normalised mean error (NME) of 32%, 78% of the simulated values are within a factor of two (FAC2) of the observations, and the coefficient of determination (R^2) is 0.6. The whole study period integrated exposure estimations are also unbiased compared with their corresponding observations, with ME of 2.5 ppb, NME of 18%, FAC2 of 100% and R^2 that equals 0.62.

1. Introduction

Spatially accurate estimation of exposure to air pollutants in the urban environment is needed for most air pollution epidemiological studies (Jerret et al., 2005; Han and Naeher, 2006). Air pollution is emitted at many source locations, is dispersed and transformed by complex physical and chemical processes but is observed only at a limited sample of the locations where the population is exposed. As it is not feasible to distribute personal exposure monitors to a large number of people for long periods of time, epidemiological studies resort to various techniques to model the pollutants' concentrations. The large spatial variability in urban traffic-related pollutant levels requires estimation methods that can produce small scale exposure variations (Jerret et al., 2005). To benefit studies of acute effects of air pollution at the personal level (e.g., Maynard et al., 2007; Van den Hooven et al., 2012), the exposure features must be provided at high temporal resolution. The ideal model for estimating the full spatiotemporal concentration field of

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an air pollutant should attempt to simulate the emission, dispersion, transformation and removal processes and, due to the inherent difficulties involved and the inevitable errors, poses a built-in data-driven mechanism to adjust the model parameters based on the available observations. To the best of our knowledge none of the current schemes used for air pollution exposure estimation employs a data-driven model that incorporates a dispersion-based simulation of air pollutants.

Gaussian dispersion models (Cyrus et al., 2005; Beelen et al., 2010; Gulliver and Briggs, 2011) and the more comprehensive meteorological–photochemical ones (Astitha et al., 2008; Borrego et al., 2010) are designed to simulate air pollution concentrations given emission and meteorological inputs. However, unlike the current meteorological models, they do not adjust the model parameters in a closed loop controlled by available observations. For example, a recent paper by Beevers et al. (2012) demonstrated an impressive performance of a model coupling the photochemical CMAQ model (Byun and Ching, 1999) with the Gaussian ADMS model (McHugh et al., 1997) in estimating hourly NO_x, NO_2 and O_3 concentrations in London at a 20 × 20 m spatial grid resolution. Data from 80 monitoring stations were used for a comprehensive assessment of the model output. However, there was no attempt to incorporate any type of adjustment of the models using the simultaneous observations to lower the model errors and biases which were found. Various interpolation schemes (Son et al., 2010; Lee et al., 2012) take the opposite approach. The spatial air pollution exposure maps which they produce are based on observed values and statistical principles only. The sparse distribution of monitoring stations limits the ability of observed data interpolations to provide the detailed spatial exposure required for many epidemiological investigations (Yuval and Broday, 2006). In the last decade the modelling approach of Land Use Regression (LUR) has been extensively used in air pollution epidemiological studies (Ryan and LeMasters, 2007; Hoek et al., 2008). An LUR fits a suit of covariates (mainly metrics of urbanisation, topography and traffic) to observed concentrations and the recovered regression parameters are then used to produce detailed spatial exposure estimation. The LUR scheme is a data-driven method but it does not attempt to mimic the actual processes that associate the model covariates with the observations to which they are fitted. Moreover, in most cases the observations used by an LUR are integrated data over a period of a couple of weeks (or a few such periods at different seasons) so the short time scale processes governing air pollution dispersion are averaged out and only the chronic exposure is estimated.

Incorporating short time scale effects has been shown to improve the accuracy of chronic exposure to air pollution. Arain et al. (2007) used a vector average of hourly wind direction data to differentiate the effects of roads down and up the wind in their LUR model. Su et al. (2008) demonstrated improvement in LUR performance while considering the hourly emission fluxes along wedge–shaped boxes whose geometry was dictated by the hourly wind direction and speed. Wilton et al. (2010) incorporated in an LUR the impact of short term meteorological variation through adding hourly dispersion model outputs as covariates. A different approach by Szpiro et al. (2010) incorporated temporal trends in long–term exposure estimation as a linear combination of empirically derived temporal basis functions. Investigating the acute effects of particulate matter on mortality, Maynard et al. (2007) included various temporal covariates like day of the week, day of year and meteorology in assessing the black carbon exposure levels in a statistical scheme akin to universal kriging. A recent study by Van den Hooven et al. (2012) accounted for temporal variations by calculating spatial PM_{10} and NO_2 exposure patterns for eight different wind conditions and deriving hourly spatial patterns by means of interpolation between the eight characteristic spatial distributions. These patterns were subsequently adjusted for fixed temporal patterns of source activities to achieve the monthly, day of the week and time of the day concentrations at the home locations of pregnant women. None of those studies incorporated the covariates which they used in a scheme which was optimally adjusted to pollution observations at a temporal resolution close to the dominant frequency of the physical and chemical processes that govern air pollution levels.

This study introduces a new concept enabling production of detailed pollution concentration maps at very high temporal resolution. The main idea is formulating the study as an optimisation problem in which the parameters of a nonlinear scheme that simulates the spatial distribution of air pollution concentration are determined by fitting the scheme's output to observations. This requires the incorporation of meteorological and air pollution observations at a temporal resolution equal to or lower than the dominant time scales of the emission and dispersion processes. The methodology is demonstrated using very simple means but is shown to achieve spatial variability similar to that enabled by an LUR, at the high temporal resolution of the meteorological and monitoring data. The process is packaged in a closed mathematical form and can thus be run completely automatically. This enables a quantitative assessment of its performance using a true leave-one-out cross-validation scheme. The ability to provide both the short time scale acute exposure and the long term chronic exposure is demonstrated on real data from the monitoring network along the Israeli coast.

2. Data

2.1. Study area

The proposed method is demonstrated in a strip of land about 70 km long and 25 km wide along the Israeli coast that includes the metropolitan Tel Aviv area and the cities of Netanya and Ashdod north and south of it, respectively (see Fig. 1). The total population of the area is about 3.7 million. The area includes a dense road system to which feeds much of Israel's highway network, railway links, two airports and a seaport. The transportation fleet includes about 1.5 million private cars, 200,000 commercial vehicles, and 10,000 city and long distance buses. Industrial sources are relatively minor contributors to air pollution in the study area (Yuval and Broday, 2009). Two natural gas-powered electricity generation stations, a 450 MW station in Tel Aviv and a 1 GW station north of Ashdod, are the main industrial pollution sources.

2.2. Traffic model output

The traffic data is produced by the Metropolitan Tel Aviv Traffic Model developed by Cambridge Systematics (Cambridge Systematics, 2008) during 2005–2008 using the EMME/2 software platform (INRO, 2012). The model was applied and is maintained by an expert team employed by the Netivey Ayalon Company, a joint venture of the Israeli Government and the Tel Aviv municipality. The road network which the model uses includes 11,553 road segments (Fig. 1). Private car traffic is simulated by an activity based model. Bus tours follow the true bus network and the commercial fleet (trucks and pick-ups) is modelled by a separate module. The model output includes 23 traffic attributes produced for five periods during the day: morning, morning rush hour, middle day, afternoon rush hour and evening. For this work only the morning rush, middle day and afternoon rush outputs were available.