Urban air quality simulation

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Quick introduction to urban air quality simulation

Simulation of pollutant concentrations over a city with street resolution.
Objectives

1. Evaluating the air concentrations of NO$_2$, PM$_{10}$, O$_3$, ...
   - Analyzing: exposure of population for one or several past years
   - Forecasting: for the next few days

2. Supporting decision making
   - Characterizing: emission sources, local versus regional pollution
   - Testing: scenarios of emissions reduction, new roads or industrial facilities
Simulation tools: numerical models with street resolution

Classical model: ADMS Urban

1. Computing the stationary solution of the reactive transport equation
   - Every point source creates a plume, with Gaussian shape crosswind
   - Parameterization for the standard deviations depending on meteorological variables
   - Special treatment within the streets

2. Inputs
   - Time-dependent: spatial distribution of emissions, background pollutant concentrations, meteorological variables (one value for the whole domain)
   - Time-independent: street network

3. High computational costs
   - $\sim 10 \text{ min of computations for a single date}$, i.e., $\sim 4 \text{ h for a full day}$
Simulation tools: numerical models with street resolution

Output points of ADMS Urban for Paris (east part)
An important source of information: observations
Merging model outputs and field observations

Data assimilation classical assumptions

- The error on the simulated concentration vector \( x^b \) has mean 0 and variance \( B \)
- The observation vector \( y \) can be compared with \( H x^b \) where \( H \) is called the observation operator
- The error on the observation vector \( y \) has mean 0 and variance \( R \)
- No correlation between simulation and observational errors

BLUE: best linear unbiased estimator

- BLUE is the linear estimator \( x^a = L x^b + K y \) whose error has mean 0 and variance \( A \), so that \( A \) has minimal trace
- BLUE reads

\[
x^a = x^b + K(y - Hx^b), \text{ with } \quad K = BH^\top (HBH^\top + R)^{-1}
\]
Parameterization for the error variances

Observational error

- Observational error variance: \( R = rI \)

Simulation error

- Simulation error covariance: \( B_{ij} = b \exp \left(-\frac{d_{ij}}{L_d}\right) \exp \left(-\frac{|P_i - P_j|}{L_p(i,j)}\right) \)

- \( d_{ij} \): distance, along the network, between the projections on the network of the output points \( i \) and \( j \)
- \( P_i \): distance to the road network
- \( L_d \) and \( L_p(i,j) = L_p + \alpha \min(P_i, P_j) \): decorrelation lengths

Determination of the parameters

- Statistical study of \( y - Hx^b \), whose variance should be \( HBH^T + R \)
- Leave-one-out cross-validation
Simulation error covariances

With respect to a traffic station
Simulation error covariances
With respect to a background station
Before and after assimilation (preliminary result)
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[Two maps showing air quality before and after assimilation with color scales and data points.]
Before and after assimilation (preliminary result)
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### Leave-one-out cross-validation (preliminary result)

<table>
<thead>
<tr>
<th>Station</th>
<th>Error change (%)</th>
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<tbody>
<tr>
<td>AUB</td>
<td>-8</td>
</tr>
<tr>
<td>BAGN</td>
<td>+15</td>
</tr>
<tr>
<td>BASC</td>
<td>-44</td>
</tr>
<tr>
<td>BONA</td>
<td>-45</td>
</tr>
<tr>
<td>CELE</td>
<td>-33</td>
</tr>
<tr>
<td>ELYS</td>
<td>-44</td>
</tr>
<tr>
<td>ETU6</td>
<td>-44</td>
</tr>
<tr>
<td>HAUS</td>
<td>-56</td>
</tr>
<tr>
<td>IVRY</td>
<td>-44</td>
</tr>
<tr>
<td>PA12</td>
<td>-50</td>
</tr>
<tr>
<td>PA13</td>
<td>-7</td>
</tr>
<tr>
<td>PA18</td>
<td>-42</td>
</tr>
<tr>
<td>PA4C</td>
<td>-49</td>
</tr>
<tr>
<td>PERA</td>
<td>-51</td>
</tr>
</tbody>
</table>

![Map of stations with error changes indicated](image-url)
Standard deviation of the analysis (preliminary result)
Reduction of the standard deviation (preliminary result)
Data assimilation at urban scale

Running operationally since June 2011
- See http://votreair.airparif.fr/
- Real-time traffic → emission model → ADMS Urban → real-time observations → data assimilation
- Still a prototype, but will be extended to Paris or Paris region by Airparif

Part of Numtech products
- For air quality agencies and cities
- Might need to assimilate new type of observations

Need for a better uncertainty estimation.
Reduction strategy

Dimension reduction

- Projection of inputs $p$ (when necessary) and outputs $x$ into a reduced subspace
- E.g., for outputs, application of principal component analysis on outputs of a one-year simulation
  - 99% of total variance explained with just 8 modes
  - $x \simeq \sum_{j=1}^{8} \alpha_j \Psi_j = \Psi \alpha$

Relative part of unexplained variance against number of modes
Projection modes
Example for Clermont-Ferrand
Reduction strategy

Reduced model

- Complete model: \( x = M(p) \)
- Reduced model: \( \alpha = \Psi^\top M(p) \); note that \( x \simeq \Psi \Psi^\top M(p) \)
- \( p \in \mathbb{R}^{10} \) and \( \alpha \in \mathbb{R}^{8} \) are low-dimensional vectors

Emulation

- Components of \( \alpha \) show a smooth dependence on the components of \( p \)
- Emulation consists in finding a surrogate function \( m \) for \( \Psi^\top M \)
- We can always reconstruct the full output: \( x \simeq \Psi m(p) \)
Building the emulator

Training values

- Let us consider the $j$th component of $\Psi^\top M$, and its emulator $m_j$
- We draw $M$ samples $p^{(i)}$, possibly by latin hypercube sampling
- We apply the reduced model to constitute the learning set: $\Psi_j^\top M(p^{(i)})$

Emulator formulation

- The emulator is made of two parts:
  
  $$m_j(p) = \sum_{k=1}^{10} \beta_{j,k} p_k + \sum_{i=1}^{M} w_{i,j}(p, p^{(1)}, \ldots, p^{(M)}) \left( \Psi_j^\top M(p^{(i)}) - \sum_{k=1}^{10} \beta_{j,k} p^{(i)}_k \right)$$

  - Regression
  - Interpolation of the residuals

- Different options for the interpolation of the residuals:
  
  - Kriging (particular case of Gaussian processes), which also provides an uncertainty estimation;
  - Interpolation in high dimension with radial basis functions
  - Even the closest neighbor(s)
Model reduction applied to urban simulations

Computational costs: dimension reduction, emulator training and prediction

- About 6 months of simulation to determine the reduced subspace spanned by the columns of $\Psi$
- $M = 2000$ samples for the emulator training, i.e., less than 3 months of simulation
- Full ADMS Urban cost: $\sim 10$ min on 12 cores for one date (i.e., one hour)
- Emulator prediction cost: 50 ms
Summary and perspectives

Data assimilation

- Merging model outputs and observations
  1. Strongly improves the evaluation of air quality across the city
  2. Provides insights on the best locations for the monitoring stations
- Requires better uncertainty estimation

Model reduction

- Dimension reduction is very efficient on outputs
- Emulation is possible and is so fast that it dramatically changes the perspectives

A few perspectives

- Propagation of inputs PDFs through the emulator
- Inverse modeling: computing the a posteriori PDFs on the inputs