Reduction and Emulation of ADMS Urban

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Introduction

- ADMS Urban is an air quality static model at urban scale.
- Input vector $p \in \mathbb{R}^K$: meteorological variables, background concentrations, hour of the day, Julian day.
- p varies from one simulated hour to the next.
- High-dimensional output concentration vector $y = \mathcal{M}(p)$.

But a full-year simulation of NO_2 concentrations over a city can take dozens of days of computation!

Objective

Replace ADMS Urban with an emulator.

Principle

- y is first projected onto a reduced subspace.
- The relations between the projection coefficients and the input vector p are then emulated.

Dimension reduction

- A reduced basis $[\Psi_1 \dots \Psi_N]$ must represent the variability of the concentration field and is determined by Principal Component Analysis over a training period.
- In practice just few principal components are enough to provide a good approximation.

$$y \simeq \sum_{j=1}^{N} \alpha_j \Psi_j$$

where $\alpha_j = y^T \Psi_j$ projection coefficient on j-th principal component.

Case study

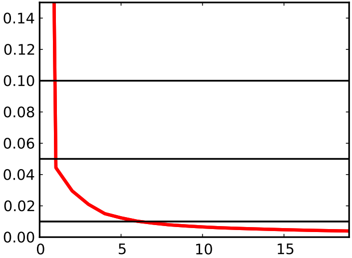
The application is the simulation of NO_2 concentrations every 3 hours across the city Clermont-Ferrand (France) for the full year 2008.

Input variables p contains $K = 10$ components.

- 5 meteorological input scalars from a meteorological station: wind speed, the wind direction, the temperature, the cloud coverage and the rain intensity.
- 3 background concentrations for NO_2, NO_x and O_3.
- 2 emission variables: emissions vary according to the Julian day and the hour of the day (spatial distribution of the emissions and emissions factors are part of the model).

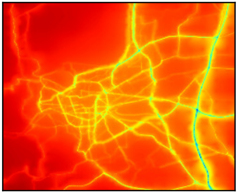
Dimension reduction

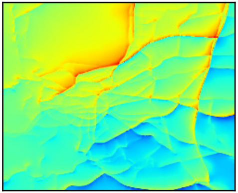
- We applied the principal component analysis to the full year 2008.
- Unexplained variance over the full year against the size of the projection basis N:



99% of the total variance with only $N = 8$ principal components.

$$y \simeq \sum_{j=1}^{8} \alpha_j \Psi_j$$





Ψ_1 and Ψ_3: effects of mean emissions and wind from south.

Scores

The simulation over the full year 2008 is compared to its projection on 8 principal components.

Mean $\mu g\,m^{-3}$	Bias $\mu g\,m^{-3}$	Corr. %	RMSE $\mu g\,m^{-3}$	Rel. RMSE %
23	0	99	2.37	10

Emulation

Every component $f_j(p) = \mathcal{M}(p)^T \Psi_j$ is replaced by a statistical emulator $\widehat{f}_j$ whose computational cost is negligible.

- M training samples $f_j(p^{(i)})$ by latin hypercube sampling.
- The emulator in p is made of two parts:

$$\widehat{f}_j(p) = \underbrace{\sum_{k=1}^{K} \beta_{j,k} p_k}_{\text{Regression}} + \underbrace{\sum_{i=1}^{M} w_{j,i}(p, \ldots, p^{(M)}) \left(f_j(p^{(i)}) - \sum_{k=1}^{K} \beta_{j,k} p_k^{(i)} \right)}_{\text{Interpolation of the residuals}}$$

- Interpolation of the residuals:
  - Interpolation with radial basis functions.
  - Mean of the closest neighbors.
  - Kriging (computationally intensive).

Case study

The components $\alpha_j = y^T \Psi_j$ of the projection are emulated, and the emulator is applied over a full year.

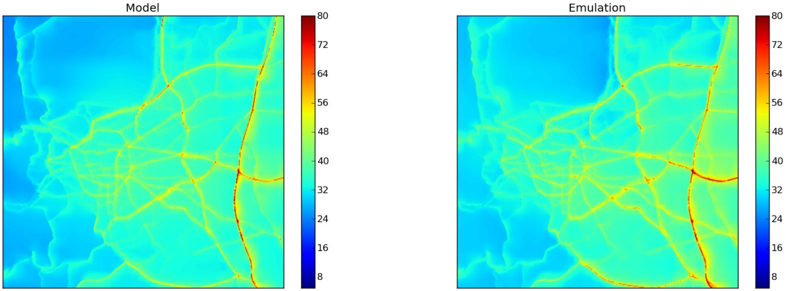
Emulation

- $M = 2000$ samples to build the 8 emulators.
- Linear regression.
- Interpolation of residuals : radial basis function (Python module Scipy).

Scores

	Bias $\mu g\, m^{-3}$	Corr. %	RMSE $\mu g\, m^{-3}$	Rel. RMSE %
Radial basis functions	-0.2	90	6.7	30

Comparison of ADMS Urban and the RBF emulator



200 frames over the year 2008

Demonstration of the RBF emulator

Conclusion

- The dimension reduction needs a 6-month simulation.
- Building the complete emulator requires the equivalent of a 8-month simulation.
- Then the prediction for any p is essentially instantaneous!

Perspectives

- Improve the interpolation part of the emulator, with error control: inverse distance weighting or even kriging.
- Generate an ensemble of simulations for uncertainty quantification (Monte Carlo simulation).
- Operational air quality forecast: Urban Air System by Numtech.
- Impact studies: focusing on yearly or monthly averages.
- All the new methods that were previously out of reach because of the computational cost of the model!

- $\widehat{f}_j(p) = \sum_{k=1}^{K} \beta_{j,k} p_k + \sum_{i=1}^{M} w_{j,i}(p, \ldots, p^{(M)}) \left(f_j(p^{(i)}) - \sum_{k=1}^{K} \beta_{j,k} p_k^{(i)} \right)$
- Let the residual be $r_j(p) = f_j(p) - \sum_{k=1}^{K} \beta_{j,k} p_k$, and the emulated residual be $\widehat{r}_j(p) = \widehat{f}_j(p) - \sum_{k=1}^{K} \beta_{j,k} p_k$
- $\widehat{r}_j(p) = \sum_{i=1}^{M} \alpha_{j,i} d(p, p^{(i)})$ where d is a distance, here d is a metric in K dimensions.
- We want to obtain the exact value at training points: $\widehat{r}_j(p^{(k)}) = r_j(p^{(k)}) = \sum_{i=1}^{M} \alpha_{j,i} d(p^{(k)}, p^{(i)})$
- We denote Δ_j the matrix whose element (k, i) is $d(p^{(k)}, p^{(i)})$, and $D_j(p)$ the vector whose ith component is $d(p, p^{(i)})$
- We get: $\alpha_j = \Delta_j^{-1} R_j$ if $R_j = (r_j(p^{(1)}), \ldots, r_j(p^{(M)}))^T$
- Note that $\widehat{r}_j(p) = \alpha_j^T D_j(p) = R_j^T \Delta_j^{-1} D_j(p) = D_j^T(p) \Delta_j^{-1} R_j$
- We therefore obtain: $w_j(p) = D_j^T(p) \Delta_j^{-1}$.