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Emulation of simulations of atmospheric dispersion at Fukushima for Sobol' sensitivity analysis

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Polyphemus/Polair3D, from which derives IRSN's operational model ldX, was used to simulate the atmospheric dispersion at the Japan scale of radionuclides after the Fukushima disaster.
A previous study with the screening method of Morris had shown that
- The sensitivities depend a lot on the considered output;
- Only a few of the inputs are non-influential on all considered outputs;
- Most influential inputs have either non-linear effects or are interacting.
These preliminary results called for a more detailed sensitivity analysis, especially regarding the characterization of interactions.
The method of Sobol' allows for a precise evaluation of interactions but requires large simulation samples. Gaussian process emulators for each considered outputs were built in order to relieve this computational burden.
Globally aggregated outputs proved to be easy to emulate with high accuracy, and associated Sobol' indices are in broad agreement with previous results obtained with the Morris method. More localized outputs, such as temporal averages of gamma dose rates at measurement stations, resulted in lesser emulator performances: tests simulations could not satisfactorily be reproduced by some emulators. These outputs are of special interest because they can be compared to available observations, for instance for calibration purpose. A thorough inspection of prediction residuals hinted that the model response to wind perturbations often behaved in very distinct regimes relatively to some thresholds. Complementing the initial sample with wind perturbations set to the extreme values allowed for sensible improvement of some of the emulators while other remained too unreliable to be used in a sensitivity analysis. Adaptive sampling or regime-wise emulation could be tried to circumvent this issue.
Sobol' indices for local outputs revealed interesting patterns, mostly dominated by the winds, with very high interactions. The emulators will be useful for subsequent studies. Indeed, our goal is to characterize the model output uncertainty but too little information is available about input uncertainties. Hence, calibration of the input distributions with observation and a Bayesian approach seem necessary. This would probably involve methods such as MCMC which would be intractable without emulators.