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Global Sensitivity analysis of atmospheric chemistry models using emulator-based and emulator-free methods

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Carrying out global sensitivity analysis (GSA) for a numerical model is critical in determining which inputs (e.g. parameters, driving data) most affect the model output. This informs us of which inputs to include: (i) for model calibration; (ii) when quantifying the uncertainty in the output given the uncertainty in the inputs. It is also used to diagnose differences in outputs between models. GSA quantifies the sensitivity index (SI) of a particular input – the percentage of the total variability in the output attributed to the changes in that input – by averaging over the other inputs, rather than fixing the other inputs at particular values as done in one-at-a-time sensitivity analysis. Traditional means of computing the SIs involve running the model thousands of times, but this becomes infeasible when the computational cost is high. GSA methods which use a surrogate of the model, called an emulator, are popular as they typically require far fewer runs of the model. Here we consider methods that would further reduce the computational burden of sensitivity analysis.

When the output of a model is non-scalar, it is standard practice with an emulator-based GSA method to build a separate emulator for each dimension of the output space. An alternative is to apply principal component analysis (PCA) to reduce the output dimension and then build an emulator for each of the transformed outputs. We consider here a global map of methane lifetimes from our chemistry models. This requires $\sim$2000 emulators for the emulator-based GSA methods, but only 10-50 emulators for the PCA-emulator hybrid approach, reducing the computation of the SIs from 1 hour to 3 minutes on a desktop computer. The other benefit of PCA is that the transformed outputs are orthogonal, and thus building separate emulators is appropriate. Results show that very similar maps of SIs are produced whether the emulator-only or emulator-PCA hybrid approach is used.

Another avenue to reducing the computational burden is to consider emulator-free methods. These only require $\sim$100 runs of the model, whereas the emulator-based methods typically need 100-300 runs depending on the number of inputs. For our chemistry models, the SIs computed from the emulator-free method are very similar to those computed using the emulator-based method. Thus emulator-free methods can provide a good approximation of the SIs.