Global Sensitivity Analysis (GSA) for a MACRO meta-model for Swedish drinking water abstraction zones

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Introduction

In Sweden farmers are legally obliged to apply for permits for pesticide use if their land lies within a drinking water abstraction zone. The standalone modelling tool MACRO-DB 4 developed by SLU is available for risk assessment and decision support. MACRO-DB 4 is used by local authorities, farmers and consultants, and is based on the well-established leaching model MACRO 5.2 (Larsbo and Jarvis, 2003). Recently, a robust meta-model of MACRO-DB 4 was developed and integrated in a web-based tool (MACRO DB Steg2 v.5).

The meta-model (Reichenberger et al., 2021) is based on 583200 MACRO simulations for the whole agriculturally relevant area of Sweden. The simulations comprised 18 climates (Fig. 1), 72 soils, 1 typical crop, 3 application seasons, and 150 dummy compounds consisting of a grid of normalized Freundlich coefficient Koc, degradation half-life at reference conditions DT50 and Freundlich exponent nf. The meta-model performs a trilinear interpolation (in the space of Koc, DT50 and nf) for log10 of Predicted Environmental Concentrations (PEC) in groundwater or surface water, respectively.

The objective of this study was to determine the most important factors influencing predicted pesticide concentrations in drinking water resources in Sweden. For this aim, a Global Sensitivity Analysis (GSA) was conducted for the MACRO meta-model.

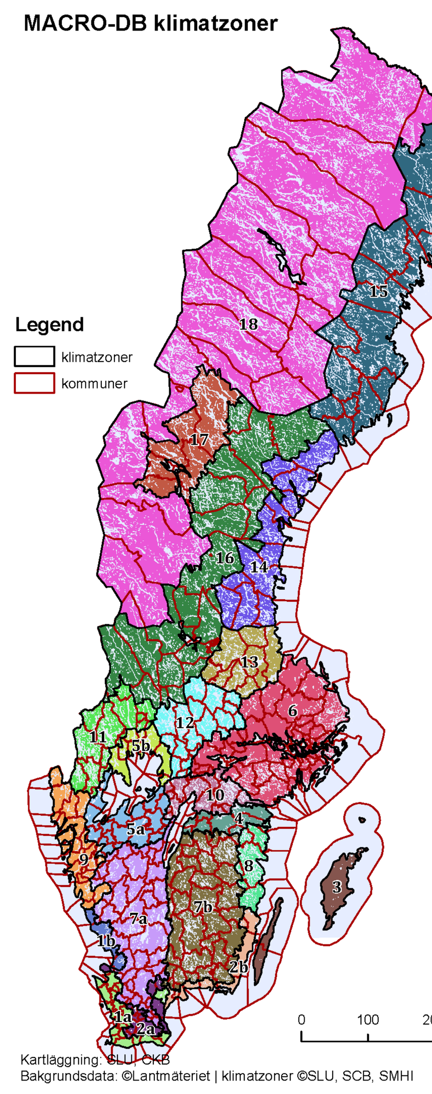

Fig. 1: Swedish climate zones

Materials and Methods

- A variance-based Global Sensitivity Analysis (GSA) was performed using the Sobol' method (Sobol', 1993; Gatel et al., 2019). This method works also for non-linear, non-monotonic and non-additive models and allows i) identification of first-order (direct) and higher-order (interaction) effects for each input factor, and ii) a ranking of the input factors according to their importance.
- All calculations were done in R.
- Sobol' quasi-random sampling was done using the script sobol_sensitivity (Zambrano-Bigiarini, 2013).
- For calculating sensitivity indices three different methods were tested
  - JRC Sobol: the script sobol_sensitivity.R from JRC (Zambrano-Bigiarini, 2013)
  - the function sobolshap_knn from the R package sensitivity (Iooss et al., 2021)
    - deals explicitly with categorical variables
    - calculates newly proposed alternative sensivity measure (Shapley effect; Owen, 2014.)
  - the R package BASS (Bayesian Adaptive Spline Surfaces; Francom and Sansó, 2020))
    - categorical predictor variables included as factors.
    - BASS first fits a meta-model and then calculates the Sobol' indices

Constant factors

- application rate: 1000 g/ha
- application frequency: 1 application every year
- proportion of arable land in the catchment: 100 %
- pesticide interception fraction: 0

Independent variables

Table 1: Input factors included in the GSA and their distributions

factor	description	type of distribution	range of values
lgKoc	logarithmic normalized Freundlich coefficient	uniform	min = $\log_{10}(3)$; max = $\log_{10}(10000)$
lgDT50	logarithmic degradation half-life in soil at ref. conditions	uniform	min = $\log_{10}(3)$; max = $\log_{10}(200)$
nf	Freundlich exponent	uniform	min = 0.75; max = 1
Soiltype	soil type	discrete uniform	72 soils for SW; 57 for GW
HSG	hydrological class	discrete uniform	4 values for SW (L, W, U, Y); 3 for GW (L, W, Y)
TXT	texture class	discrete uniform	5 values (1, 2a, 2b, 3, 4)
HR	presence of hard rock in subsoil	discrete uniform	2 values (presence, absence)
OMC	organic matter class	discrete uniform	3 values (low, normal, high)
Season	application season	discrete uniform	3 values (spring, summer, autumn)
Climate	climate zone	discrete uniform	18 climates

Target variables

- Groundwater: 20-year mean leaching flux concentration at 2 m depth
  PECgw = (total pesticide leaching)/(total percolation)
- Surface water: 20-year mean concentration in water entering surface water
  PECsw = (total losses via drainage and leaching)/(total drainflow and percolation)

Method comparison

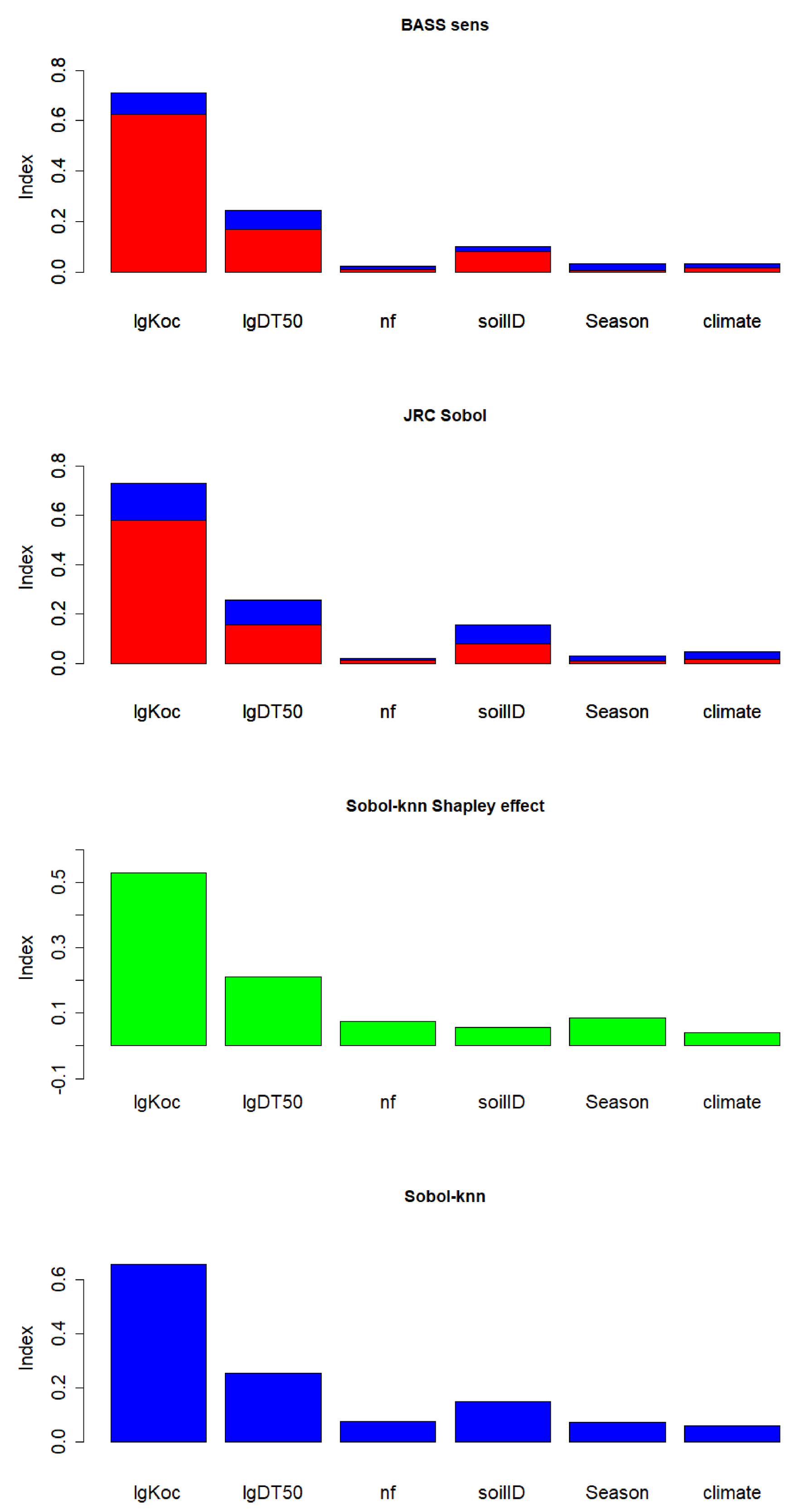

Fig. 2: Comparison between different methods to calculate sensitivity indices for target variable lgPECsw. Blue: total sensitivity index STi; red: first-order sensitivity index Si; green: Shapley effect. For Sobol-knn Si were nonsensical (> STi) and are thus not shown.

- Si and especially STi obtained with JRC Sobol and BASS very similar (Fig. 2)
- Sobol STi obtained with sobolshap_knn similar to the above two methods
- However, Sobol' Si and Shapley effect obtained with sobolshap_knn not reliable:
  - Si usually > STi, and sometimes also negative
  - Shapley effect sometimes negative

→ Base interpretation on JRC Sobol

Sensitivity indices using soil IDs

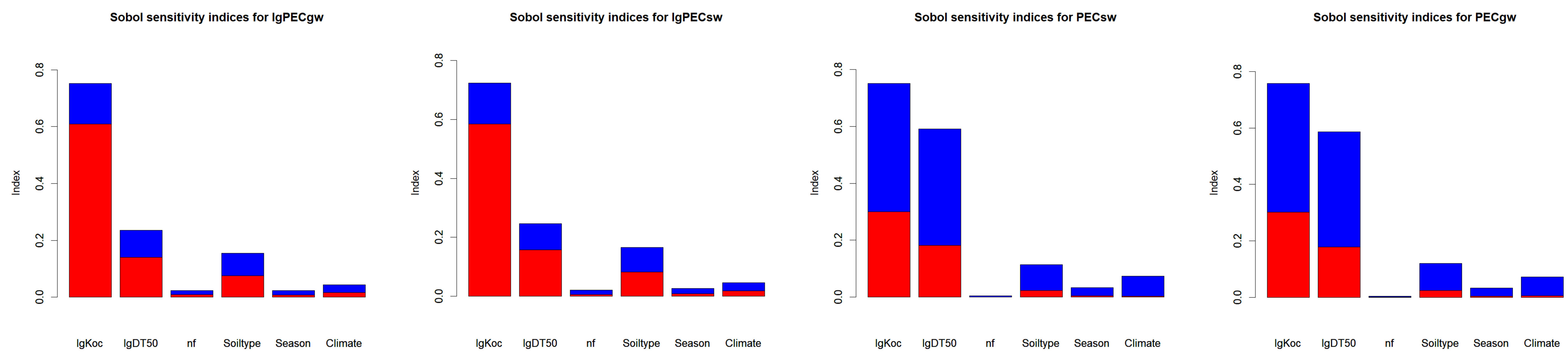

Fig. 3: Sensitivity indices using soil IDs. Left: logarithmic target variable; right: non-logarithmic target variable. Blue: total sensitivity index STi; red: first-order sensitivity index Si

Sensitivity indices using soil variables

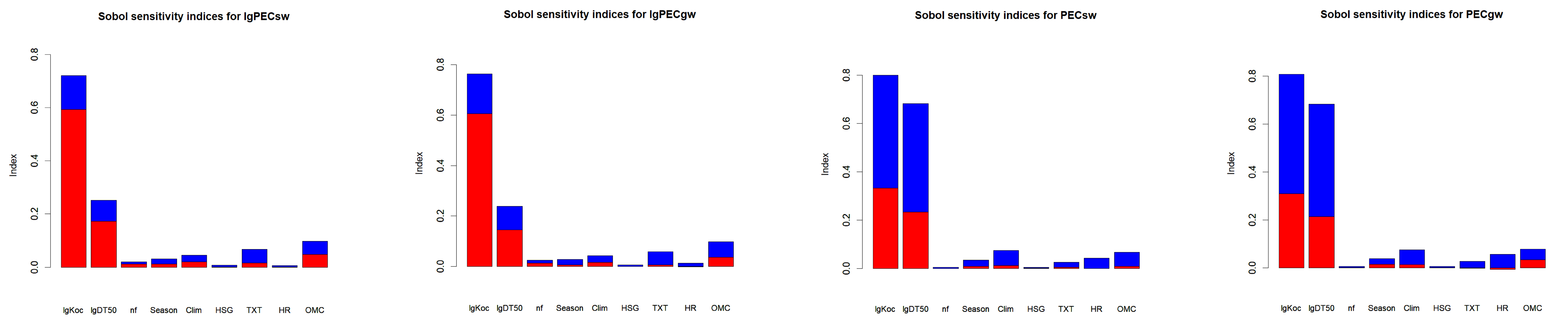

Fig. 4: Sensitivity indices using soil variables. Left: logarithmic target variable; right: non-logarithmic target variable. Blue: total sensitivity index STi; red: first-order sensitivity index Si

Discussion

- Notable difference in Sobol' indices between logarithmic and non-log PEC, but little difference between PECsw and PECgw.
- Non-additivity (interactions beween input factors) higher for non-log PEC than for logarithmic PEC: Sum of first-order indices Si < 0.58 for non-log PEC, but > 0.82 for log PEC.
- The most important factors are lgKoc > lgDT50 > soil > climate.
- When the soil ID is split into four variables, the organic matter class (affecting sorption) is the most important of them.
- Influence of hydrological class HSG very small. Explanation:
  - The hydrological class mainly affects the proportion of excess water routed to SW vs. GW, not so much concentrations in leachate and drainflow
  - Dilution (mixing) with water originating from other soils not taken into account in calculation of target variables

Conclusions

- The Global Sensitivity Analysis of the MACRO meta-model revealed that substance sorption and degradation parameters were the most important factors influencing Predicted Environmental Concentrations in Swedish drinking water resources.
- Soil type, climate zone and application season were much less important than compound parameters
- However, the effects of soil hydrology and climate may be underestimated because in this analysis we did not account for mixing with water from other sources, and hence absolute water and solute fluxes are less important than concentrations in leaching and drainflow.
- Global Sensitivity Analysis combined with meta-modelling is a very useful tool for analyzing complex, non-linear, non-monotonic and non-additive environmental models.

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