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Elementary Effects: on general models and trajectory generation

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Introduction

Elementary effects is a popular choice for sensitivity analysis in the environmental and biological sciences, but the current formulation is not suitable for most real-life models. Furthermore, it is not clear which of the commonly used trajectory generation methods is best.

Traditional EE

- Effect for input i, output j: $ee_{ij}^n = \frac{Y_j(\mathbf{X^n}+\delta_i \mathbf{e}_i)-Y_j(\mathbf{X^n})}{\delta_i}$;
- Assumed that $X_i \in [0,1] \subset \mathbb{R}$; $[X_i] = [Y_j] = 1$.

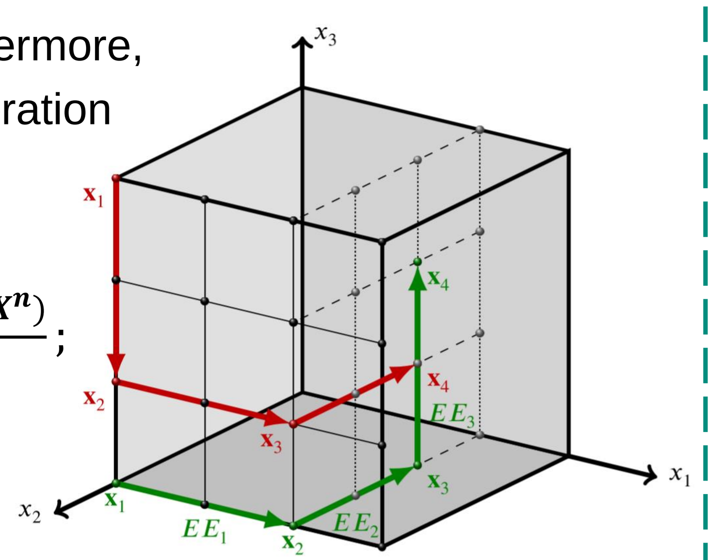
Fig. 1: Traditional winding design.

Problems with traditional EE

- Real-life models are dimensional & $X_i \notin [0,1]$;
- Sensitivity measures depend on input dimensions;

→ This can lead to erroneous ranking results.

- Current trajectory generation methods are not compatible with integer/Boolean inputs.

Methods

Scaling effects

- Essential to ensure results are in line with notion of sensitivity (relative contribution of input variability to total variance in output); must be function of input range;
- We propose: $EE_{ij}^n = ee_{ij}^n \cdot c_i$; where $c_i = max(X_i) - min(X_i)$.
- Drawback: $min(X_i)$, $max(X_i)$ are typically uncertain.

Identify (un)important inputs

1. Sensitivity measure: dimensionless & normalized median (χ) of absolute effects (based on [1,2]): $S_\chi(i,j) = \frac{\chi_{ij}\, c_i}{\sum_{l=1}^{k} \chi_{lj}\, c_l}$;
2. Sort: $\underbrace{S_\chi(i_1,j) < S_\chi(i_1,j) < \cdots < S_\chi(i_q,j)} < \cdots < S_\chi(i_k,j)$;
3. Unimportant $= \{X_{i_1}, X_{i_2}, \ldots, X_{i_q}\}$ (q follows from threshold set by modeller);
4. Important = X_i for which $S_\chi(i,j) > \mu(S_0) + 3\sigma(S_0)$, where $S_0 = \{S_\chi(i_1,j), \ldots, S_\chi(i_q,j)\}$.

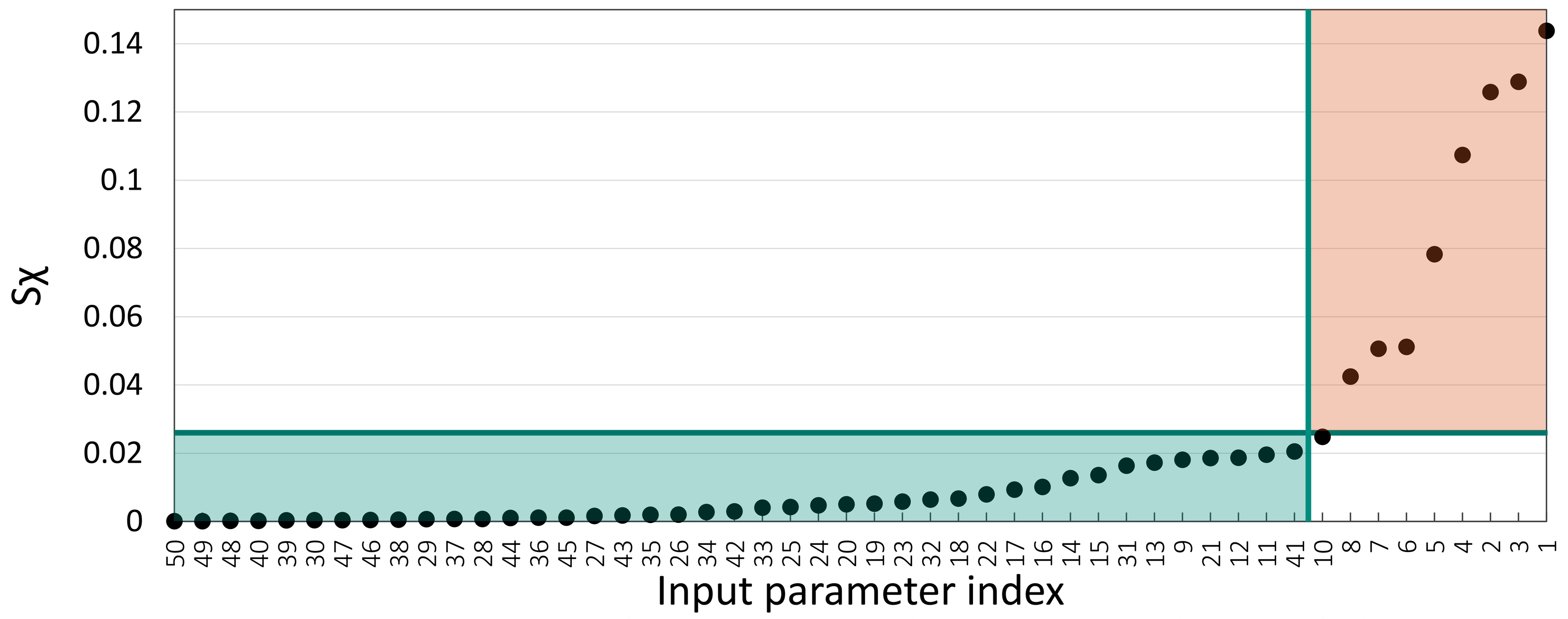

Fig. 2: Given some threshold, unimportant: left of vertical line (teal shader); important: above horizontal line (orange shader).

Trajectory generation methods

- Compared: Optimized Trajectories (OT), Sobol QR radial & winding stairs, and novel R_d QR radial & winding;
- R_d sequence $\{\boldsymbol{x}_n\}_n$ in d dimensions [3]:

$$\boldsymbol{x_n} = \frac{1}{2} + n\left(\frac{1}{\phi_d}, \frac{1}{\phi_d^2}, \ldots, \frac{1}{\phi_d^d}\right) \bmod 1;$$

$$\phi_d = \sqrt[d+1]{1+\sqrt[d+1]{1+\sqrt[d+1]{1+\cdots}}}.$$

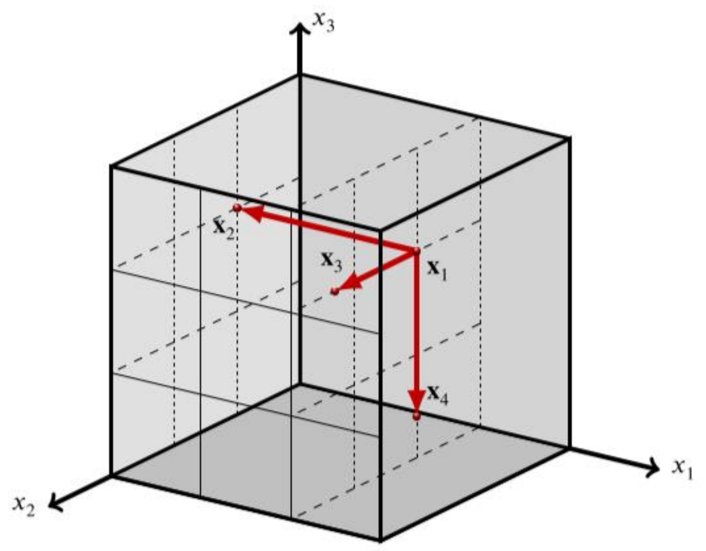
Fig. 3: Radial design.

Trajectory generation for integer/Boolean inputs

- QR sequences give non-integer input values. To ensure integer/Boolean values, we propose the following version of QR sampling designs:

  'Standard': double inputs → use QR sequence; integer/Boolean → transform QR base point to one of p_i discrete values and use fixed step size $|\delta_i|$ for perturbed point, where p_i satisfies: $max(X_i) - min(X_i) = m(p_i - 1)$ for some $m \in \mathbb{N}$ and $|\delta_i|$ is a multiple of $1/(p_i - 1)$.
- As an efficient alternative to OT, we also considered:

  'Pinned': all inputs → transform QR base point to one of p_i discrete values and use fixed step size $|\delta_i|$.

Results

Experiment 1: estimating Sobol total sensitivity indices S_{T_i} (Fig. 4)

Extended experiment in [4] for K- and G^*-functions (included higher dimensions & more sampling approaches); compared radial vs. winding sampling designs.

We found:

- Small step sizes ('standard') better than large step sizes ('pinned');
- Radial equal or better than winding, but difference not significant in K-function.

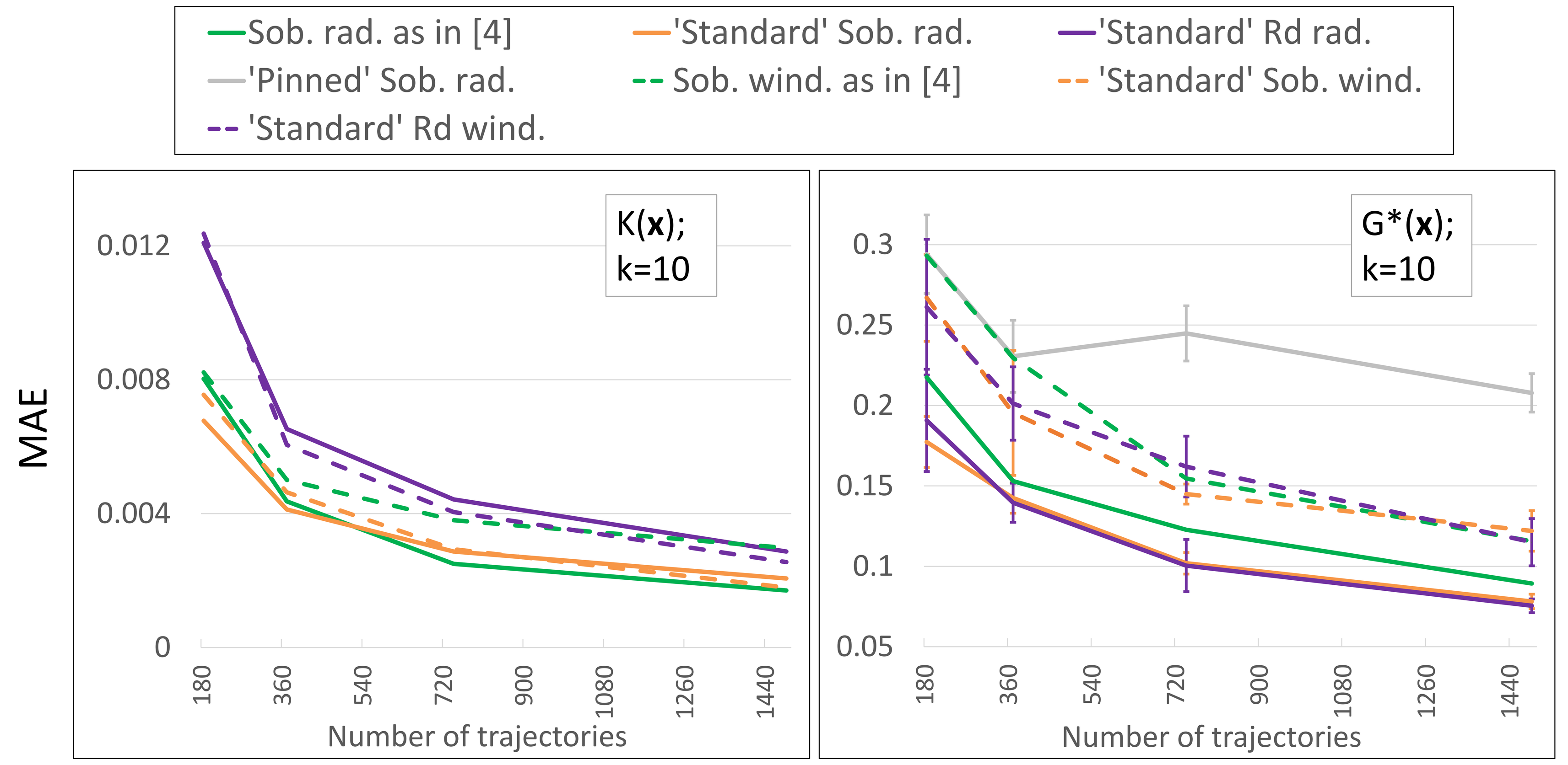

Fig. 4: Mean absolute error $\text{MAE} = \frac{1}{50k}\sum_{j=1}^{50}\sum_{i=1}^{k}|\hat{S}_{T_i} - S_{T_i}|$. Full lines show radial designs, dotted lines show winding designs. Left: MAE for 'Pinned' Sob. rad. was larger than plot range shown here. Right: mean ±1 std is shown over 5 calculations of MAE.

Experiment 2: ranking parameters using Elementary Effects (Fig. 5)

Kendall $\tau - a$ correlation between analytical and estimated rankings. Estimated rankings based on $S_\chi(i,j)$. Included OT wherever computationally feasible.

We found:

- 'Standard' R_d radial overall top performer, slightly outperforming 'standard' Sobol radial.
- For more complex output functions, #trajectories ≳ 20 beneficial;

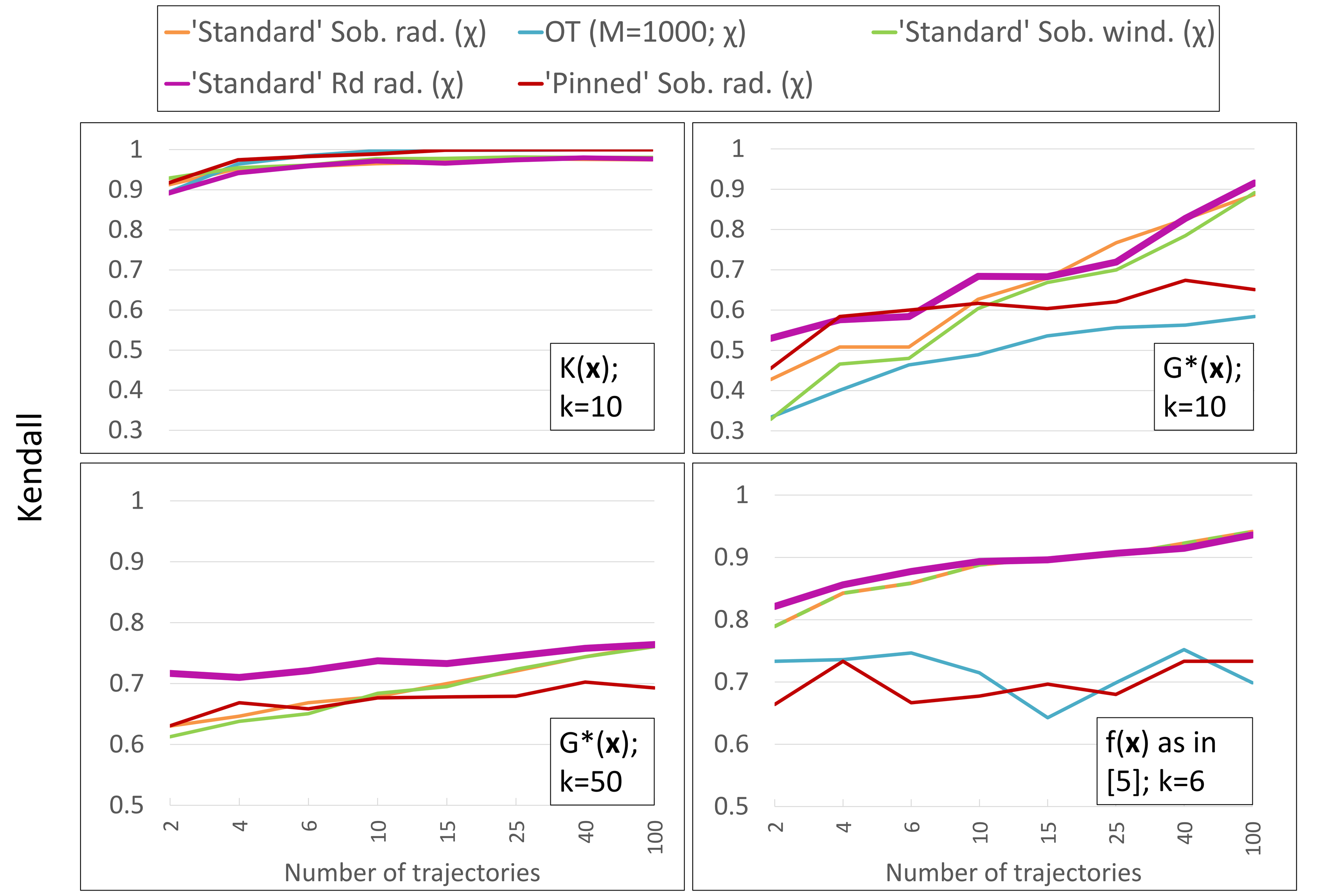

Fig. 5: Lines depict the mean over 50 calculations of the Kendall correlation coefficient. Uniqueness of replicates was ensured by taking different sections of the QR sequence (K- and f-functions) or by randomly sampling the δ-parameter in the G^*-function (as in [4]). Note: different vertical axis ranges.

Conclusion

To apply EE to a typical real-life - thus dimensional - model one must scale the effects and use a dimensionless sensitivity measure. We propose to scale by $c_i = max(X_i) - min(X_i)$ and use the scaled & normalized median of absolute effects $S_\chi(i,j)$.

Our results on ranking inputs (Fig. 5) suggest 'standard' R_d radial is the best sampling strategy for EE. Both Fig. 4 and Fig. 5 imply OT and 'pinned' methods are not advisable.

Further research

- Incorporate standard deviation of effects (non-linearity/interactions);
- Spread and discrepancy of sampled simulation points are poor proxies of performance (not shown here);
  → What characteristic should sampling designs be based on?
- Adapt method to deal with inherent randomness in model.

References

[1] Menberg et al., *Energy and Buildings*, 2016; [2] Wu, *Applied Math. Modelling*, 2020; [3] Roberts, http://extremelearning.com.au/unreasonable-effectiveness-of-quasirandom-sequences/, accessed 02-07-21;
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