Derivative-based Global Sensitivity Analysis for Energy System Optimization Models via Implicit Differentiation

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Energy system optimization models (ESOMs) have emerged as valuable tools for guiding present-day decisions for the energy transition based on assumptions about the future. These future assumptions hold much uncertainty, which propagates to the model outputs. If not considered, this uncertainty can lead to unintended future outcomes. One way to address this uncertainty is by identifying the most influential parameters on the model output variability. With this information, we can refine the corresponding assumptions, or make present-day decisions more resilient to them.

Global sensitivity analysis (GSA) is a powerful tool for determining the most influential parameters on a model's output variability [1]. However, GSA can be challenging for computationally intensive models with thousands of parameters. ESOMs usually fall into this classification due to the required spatial and temporal resolution and the energy sectors they consider. GSA via variance decomposition for Sobol indices requires $N \cdot (p+2)$ model evaluations, with p being the number of model parameters (on the order of 10^2-10^3) and N a number greater than 500 [2]. The model evaluations required for GSA can significantly decrease via the Morris method, requiring $r \cdot (p+1)$ model evaluations with r being the number of trajectories (often between 5 and 50). However, the Morris method mainly serves for screening without quantitative information on uncertainty contributions from parameter interactions [1]. Due to these limitations, performing GSAs on large-scale ESOMs with quantified uncertainty contributions is a current challenge.

In this work, we propose an efficient method for GSA of computationally intense ESOMs. For this purpose, we employ derivative-based global sensitivity measures (DGSMs), derived from the expected square of the model derivatives with respect to each parameter. DGSMs are a promising GSA alternative, as calculation of the DGSMs requires a sample size, N, of model evaluations, independent of the number of model parameters, while providing an upper bound on the total Sobol indices [3]. DGSMs combine the quantitative benefits of Sobol index-based methods with the computational efficiency of the Morris screening method.

Calculating the DGSMs, however, requires derivatives of the model outputs with respect to the input parameters. Optimization problems don't have an analytical form relating the decision variables to the model parameters. Therefore, there's no analytical expression for the derivatives. However, derivatives can be calculated at the optimal point by implicit differentiation of the set of Karush-Kuhn-Tucker (KKT) conditions [4]. The KKT conditions provide a set of necessary and sufficient conditions for optimality. The KKT conditions take the form $K(\theta, z^*) = 0$, where θ are the optimization problem parameters and z^* is a vector containing the optimal decision variables x^* and the problem dual variables (λ^*, μ^*). Implicit differentiation stems from the implicit function theorem, which states that given an implicit system of equations, $F(x, y)$, and a point (x_0, y_0) at which $F(x_0, y_0) = 0$ and $J_y F(x_0, y_0) \neq 0$, there exists an explicit system of equations $y(x)$ on an interval containing x_0 such that $J_y F(x_0) = -[J_y F(x_0, y_0)]^{-1} \cdot J_x F(x_0, y_0)$. As long as the partial Jacobian of the KKT conditions, $J_z K(\theta, z^*)$ is non-singular, one can apply the implicit function theorem to the KKT conditions to obtain the sensitivities of the model decision variables to the model parameters, $J_\theta z^*(\theta)$ (Equation 1).

$$J_\theta z^*(\theta) = -[J_z K(\theta, z^*)]^{-1} \cdot J_\theta K(\theta, z^*) \tag{1}$$

Implicit differentiation of an optimization problem's KKT conditions has been applied in several disciplines such as process controls for determining on-line parameter sensitivities, machine learning for gradient-based neural network training, and energy systems optimization for calculating emissions factors. In this work, we use this technique to enable DGSM-based GSA for computationally intensive ESOMs for which calculation of Sobol indices is not feasible.

We carry out our DGSM-based GSA via implicit differentiation on a small ESOM and compare the resulting DGSMs to the total Sobol indices, S_T, calculated via variance decomposition using the SALib library in Python [5]. Our model minimizes the cost of n operating electricity generation technologies, x_i, with costs, c_i, subject to maximum generation constraints, G_i, and a total load, L, which must be satisfied.

Our preliminary results show that for most model parameters, DGSM-based GSA provides upper bounds for the total Sobol indices for with 78% less computation time (Table 1). The piece-wise constant nature of the decision variables of linear optimization problems with respect to objective function coefficients leads to zero-valued derivatives, highlighting a limitation of our method. We address this limitation by adding a quadratic penalty term to the objective function. Overall, we propose a method that enables GSA of computationally intense ESOMs, allowing to better-consider uncertainty in present-day decision-making.

Table 1: Computation time and sensitivity measure comparisons for total Sobol indices, S_T, calculated via variance decomposition, and DGSMs calculated via implicit differentiation.

		sensitivity of model decision variable, x_i to model parameters:				
method	computation time	L	$G_{j\neq i}$	$G_{j=i}$	$c_{j\neq i}$	$c_{j=i}$
DGSM	16 min	1.4	0.006	0.02	0	0
DGSM (+ penalty term)	18 min	1.1	0.003	0.02	0.2	0.8
S_T	72 min	0.5	0.004	0.01	0.1	0.6

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