

Extreme learning machines for variance-based global sensitivity analysis

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Collaborators



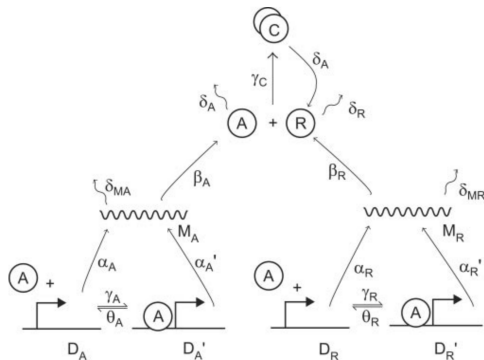
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Motivating example - genetic oscillator

Biochemical model describing circadian rhythm regulation:



Which rate constants need to be measured most accurately so we can determine the concentration of R ?

Image credit¹

¹J.G. Vilar, H.Y. Kueh, N. Barkai, S. Leibler. Mechanisms of noise-resistance in genetic oscillators. 2002.

Introduction: Variance-based global sensitivity analysis

- Consider a model $y = f(\mathbf{x})$ where $y \in \mathbb{R}$, and $\mathbf{x} \sim \pi(\mathbf{x})$ has independently distributed entries
- Sobol' indices are invaluable tools for GSA which measure the contribution of each input to variance in model output:

$$S_k := \frac{\text{var}[f_k(x_k)]}{\text{var}[f(\mathbf{x})]}, \quad S_k^T := 1 - \frac{\text{var}[\mathbb{E}(f(\mathbf{x})|x_j, j \neq k)]}{\text{var}[f(\mathbf{x})]}$$

- $f_k(x_k) := \int f(\mathbf{x}) d\mathbf{x}_{-k} - \mathbb{E}(f\mathbf{x})$, where $d\mathbf{x}_{-k}$ denotes integrating over all inputs **except** x_k
- First order Sobol' index S_k measures influence of x_k **outside of** interactions
- Total Sobol' index S_k^T measures influence of x_k **including** interactions with other inputs

Introduction: Computing Sobol' indices

- Monte Carlo (MC) methods generally used to estimate Sobol' indices
- However this is intractable when f is costly to evaluate
- Instead can construct surrogate model $\hat{f} \approx f$ which is cheap to evaluate
- Some surrogate models (e.g. polynomial chaos², Gaussian processes³) admit analytic formulas for Sobol' indices

²B. Sudret. Global sensitivity analysis using polynomial chaos expansions. 2008.

³A. Marrel, B. Iooss, B. Laurent, O. Roustant. Calculations of Sobol indices for the gaussian process metamodel. 2009.

Neural network-based GSA tools

- Let $y = f(\mathbf{x})$, where $\mathbf{x} \in [0, 1]^d$ has independent uniformly distributed entries
- f is computationally expensive to evaluate and/or input dimension d is large
- Can we develop a neural network-based surrogate method which admits analytic formulas for Sobol' indices?

Background: Single layer neural networks

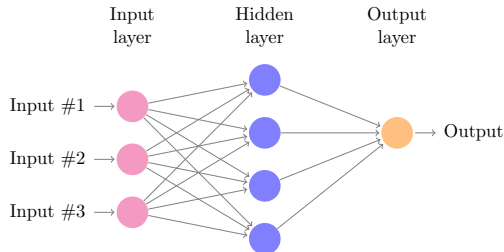
A single layer neural network has the form $\hat{f}(\mathbf{x}) = \boldsymbol{\beta}^\top (\phi(\mathbf{W}\mathbf{x} + \mathbf{b}))$

\mathbf{W} -hidden layer weight matrix

\mathbf{b} - hidden layer biases

$\boldsymbol{\beta}$ - output weights

ϕ - activation function



We train the neural network by solving the nonlinear least squares problem for training points $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)$, where $y_i = \hat{f}(\mathbf{x}_i)$

$$\arg \min_{\mathbf{W}, \mathbf{b}, \boldsymbol{\beta}} \sum_{i=1}^m (\hat{f}(\mathbf{x}_i; \mathbf{W}, \mathbf{b}, \boldsymbol{\beta}) - y_i)^2$$

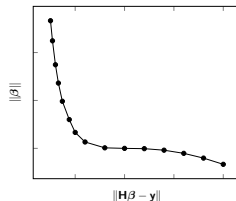
Background: Extreme learning machines

- \mathbf{W} , \mathbf{b} independently sampled randomly (e.g. from standard normal distribution)⁴
- Solve the L_2 regularized linear least squares problem to find output weights

$$\arg \min_{\boldsymbol{\beta}} \frac{1}{2} \|\mathbf{H}\boldsymbol{\beta} - \mathbf{y}\|_2^2 + \frac{\alpha}{2} \|\boldsymbol{\beta}\|_2^2$$

- $\mathbf{y} = [y_1 \ \cdots \ y_m]^\top$ and $H_{ij} = \phi(\mathbf{w}_j^\top \mathbf{x}_i + b_j)$
- Computationally quick and easy to use but requires more hidden layer neurons

We determine the regularization parameter α
by the L-curve method⁵



⁴G.-B. Huang, Q.-Y. Zhu, C.-K. Siew. Extreme learning machine: Theory and applications. 2006.

⁵P. C. Hansen. Getting Serious: Choosing the Regularization Parameter 2010.

Variance-based GSA with ELMs

- Analytically integrating ELM surrogate should be easy if we want Sobol' index formulas
- Common ML activation functions (e.g. sigmoid) do not make integration easy
- However, activation function can be any smooth non-polynomial function⁶
- Set $\phi(t) = e^t \rightarrow$ we derive analytic formulas in terms of \mathbf{b} , \mathbf{W} , and β
- After training ELM, **obtain Sobol' indices for free**⁷

$$S(\hat{f}) = S(\mathbf{b}, \mathbf{W}, \beta), \quad S^T(\hat{f}) = S^T(\mathbf{b}, \mathbf{W}, \beta)$$

⁶G.-B. Huang, Q.-Y. Zhu, C.-K. Siew. Extreme learning machine: Theory and applications. 2006.

⁷J. Darges, A. Alexanderian, P.A. Gremaud. Extreme learning machines for variance-based global sensitivity analysis. 2022.

Genetic oscillator

- Stiff ODE system (expensive to solve)
- 16 reaction rate parameters are uncertain
- Each parameter uniformly distributed in interval $\pm 5\%$ of respective nominal value
- Study average concentration in time of species R as QoI:

$$f(\mathbf{x}) = \frac{1}{T} \int_0^T R(t; \mathbf{x}) dt$$

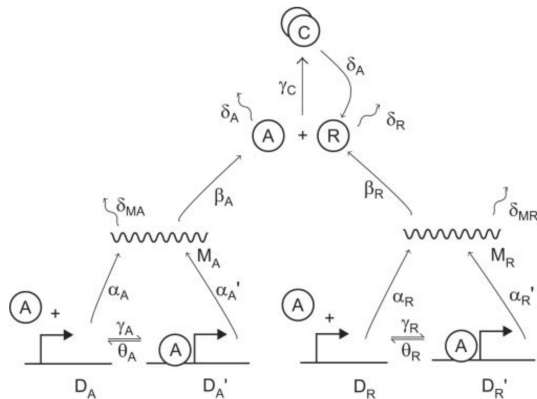
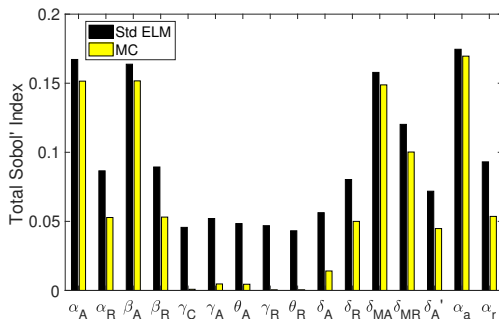
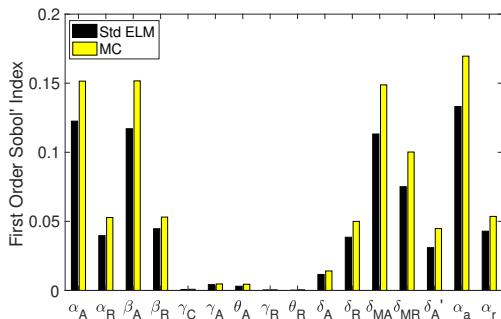


Image credit⁸

⁸J.G. Vilar, H.Y. Kueh, N. Barkai, S. Leibler. Mechanisms of noise-resistance in genetic oscillators. 2002.

GSA for genetic oscillator using ELM surrogate

Experimental setup: 3000 training size, 1000 hidden layers, $\alpha = 10^{-4}$



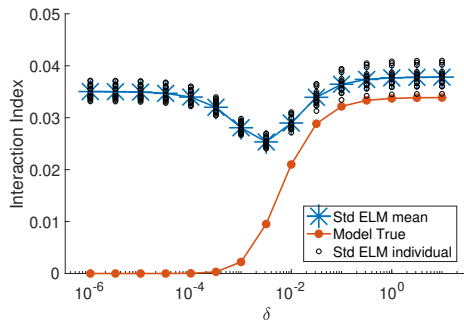
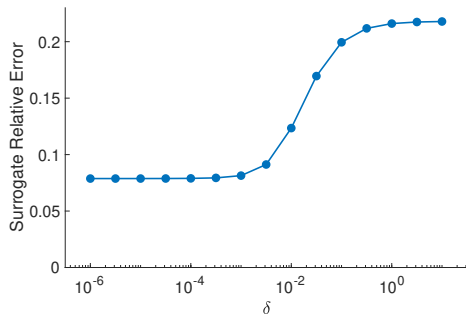
ELM surrogate overestimates higher-order indices compared to MC⁹

⁹M. Merritt, A. Alexanderian, P.A. Gremaud. Multiscale global sensitivity analysis for stochastic chemical systems. 2021.

ELM and variable interactions

Consider $f_{\delta}(\mathbf{x}) = \sum_{k=1}^{15} x_k + \delta \prod_{j=1}^d (1 + x_j)$, $\mathbf{x} \in [0, 1]^{15}$ where δ controls variable interactions

Note: Interaction indices $S_i^{\text{int}} = S_i^T - S_i$ are the same for all inputs

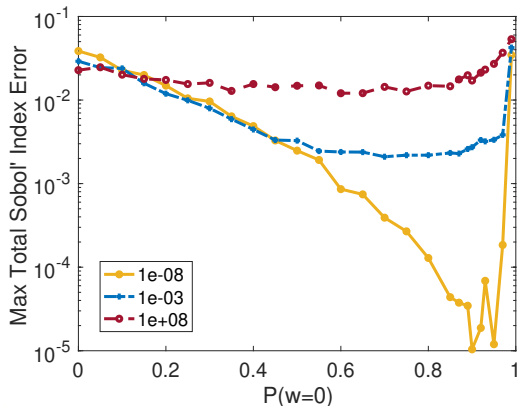
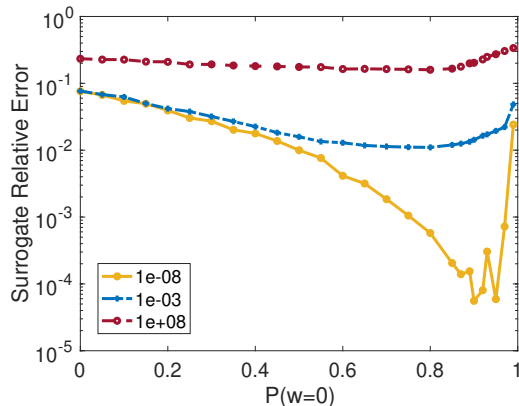


ELM surrogate overestimates higher-order indices when interactions are negligible

Sparsification

- **Issue:** ELM may overestimate higher order Sobol' indices
- Higher order Sobol' indices correspond to influence of interactions
- **Idea:** We can reduce influence of interaction terms by making inner weight matrix sparse
- Sparse weight matrix $\mathbf{W}_s = \mathbf{B} \circ \mathbf{W}$, where $\mathbf{B}_{ij} = \begin{cases} 0 & \text{with probability } p, \\ 1 & \text{with probability } 1 - p \end{cases}$
- How do we know which p to use?

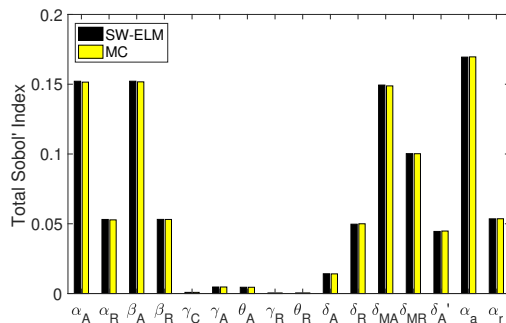
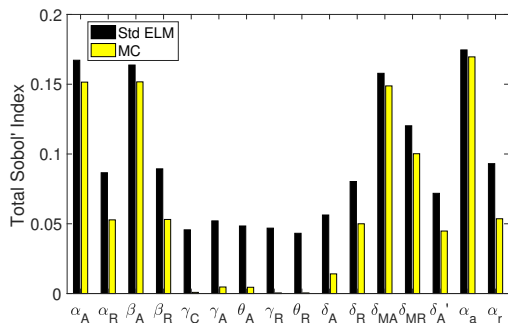
Sparse weight ELM



Sparse Weight ELM: Choose p by testing which value gives the best surrogate error on a validation set

GSA for genetic oscillator using SW-ELM

Standard ELM surrogate (left) compared to SW-ELM (right) with $p = 0.9$



Note: SW-ELM also performs well with FAR fewer training points

Summary and future work

- We use ELM as a quick and easy tool for variance-based GSA¹⁰
- With exponential activation function, we derive analytic expressions of Sobol' indices for uniformly and normally distributed inputs
- After training surrogate, we obtain Sobol' indices for no additional cost
- Sparse weight ELM improves GSA performance without sacrificing speed and simplicity of ELM
- Can we develop measures or heuristics to give information about variable interactions of black box functions?

¹⁰J. Darges, A. Alexanderian, P.A. Gremaud. Extreme learning machines for variance-based global sensitivity analysis. 2022.

References I