A Unified Framework for Uncertainty and Sensitivity Analysis of Computational Models with Many Input Parameters

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Outline

- Introduction
  - Uncertainty Analysis
  - Sensitivity Analysis
- Framework
  - Latin Hypercube Sampling
  - Generalized Polynomial Chaos Expansions
- Hierarchical Variable Selection Approach
- Examples

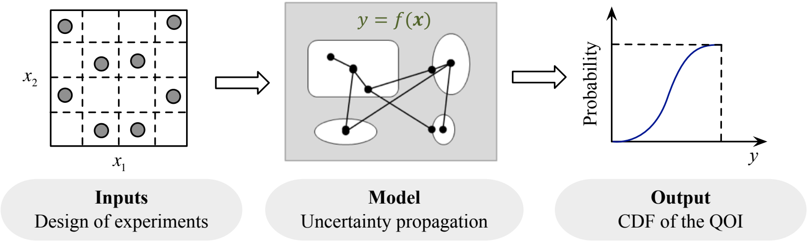
Uncertainty Analysis

Identifying and analyzing the uncertainties on complex systems are important.

Identification of uncertainties

Uncertainty Analysis (UA) studies how the uncertainties in the input parameters can be mapped to the uncertainties in the outputs.

- Monte Carlo methods (Helton and Davis, 2003).



Sensitivity Analysis

Analysis of uncertainties

Sensitivity Analysis (SA) studies how the total output uncertainty can be attributed to the uncertainties in each input parameter.

Direct computation:

- Fourier Amplitude Sensitivity Test (FAST, Cukier *et al.*, 1973);
- Sobol' indices (Sobol', 1993).

Metamodeling:

- Linear regression model (Saltelli *et al.*, 2001);
- Gaussian process model (Oakley and O'Hagan, 2004);
- Generalized polynomial chaos expansions (Sudret, 2008);
- Smoothing spline (Touzani and Busby, 2013).

SA on High Dimensions

Based on the effect sparsity principle (Wu and Hamada, 2009), only a few (but unknown) parameters are significant among many candidates. When the number of input parameters is large, variable selection is necessary.

Screening design:

- Elementary effect method (Morris, 1991).

Model-based variable selection:

- Bayesian variable selection on Gaussian process models (Linkletter et al., 2006);
- Bayesian variable selection on smoothing spline ANOVA models (Reich et al., 2009).

Potential Problems

One can choose the aforementioned methods to sequentially conduct UA, variable selection, and SA.

- Too many function evaluations due to *three different* methods and *three separate* designs.
- Variable selection is computational intensive when the number of parameters is large and the computational model is complex.

Computational Model

Consider the computational model

$$y = f(\boldsymbol{x}),$$

where f is the computer code, $\boldsymbol{x}$ is the p-variate input, and y is the output.

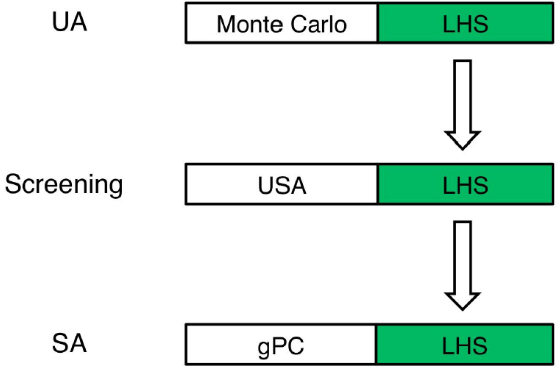
- Black-box function, which can be nonlinear and non-additive.
- High dimensions, where a few of the input parameters are significant. Variable selection is challenging.
- No experimental error.

Framework

- UA:
  Monte Carlo simulation with Latin Hypercube Samples (LHS);
- Variable selection:
  a new hierarchical approach on generalized Polynomial Chaos expansions (gPC, Xiu and Karniadakis, 2002);
- SA:
  Sobol' indices in gPC can be computed analytically (Sudret, 2008).

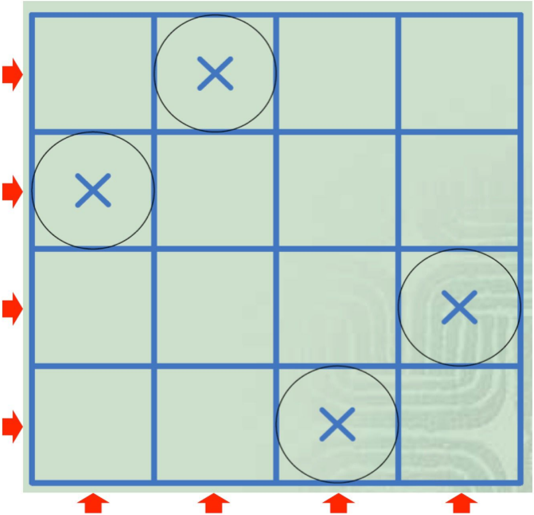
Since the approach connects UA and SA using one design, we call it *Uncertainty-Sensitivity-Analysis* (or abbreviated as USA).

Framework: the USA



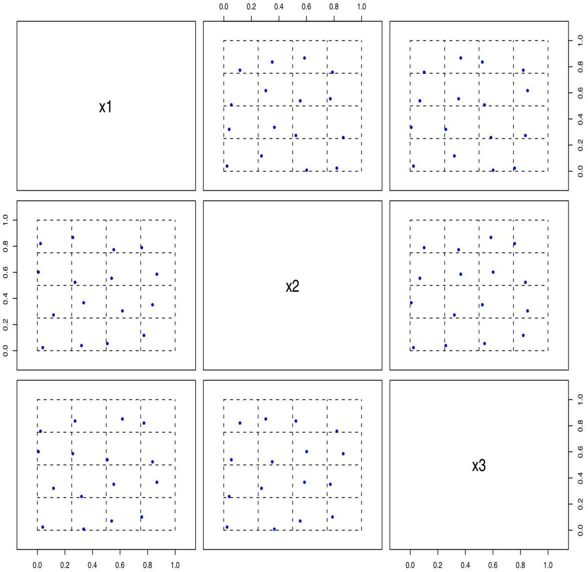
- The computational time in the simulation is drastically reduced.
- Work efficiently for high dimensions.

Latin Hypercube Sampling/Designs



$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \\ 3 & 1 \\ 4 & 2 \end{bmatrix}$$

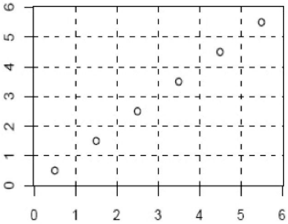
2-D Projection of a 16-run LHD

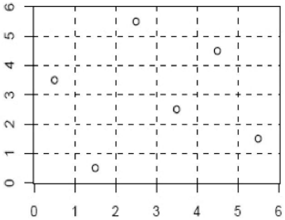


Latin Hypercube Designs: Properties

- Easy to construct:
  - randomly permute integers $\{1, \ldots, n\}$ for each factor.
- Each input factor has n different levels.
- Guarantee one-dimensional uniformity.
- Can be poor in terms of space-filling.

$$\begin{bmatrix} 1 & 1 \\ 2 & 2 \\ 3 & 3 \\ 4 & 4 \\ 5 & 5 \\ 6 & 6 \end{bmatrix}$$





$$\begin{bmatrix} 1 & 4 \\ 2 & 1 \\ 3 & 6 \\ 4 & 3 \\ 5 & 5 \\ 6 & 2 \end{bmatrix}$$

Latin Hypercube Designs: Space-filling

- Maximin and minimax LHDs (Johnson et al., 1990);
- Orthogonal Array-based LHDs (Owen, 1992, and Tang, 1993);
- LHDs using correlation criteria (Tang, 1998);
- Orthogonal-maximin LHDs (Joseph and Hung, 2008);
- Multi-layer designs (Ba and Joseph, 2011).

gPC: Basis

An orthogonal polynomial basis $\phi_\alpha(x)$ (α corresponds to the order) satisfies

$$\int \phi_\alpha(x)\phi_\beta(x)p(x)dx = \gamma\delta_{\alpha\beta},$$

where $p(x)$ is the density function of x, γ is a normalizing constant, and $\delta_{\alpha\beta} = 1$ if $\alpha = \beta$ and 0 otherwise.
For $\boldsymbol{x} = (x_1, \ldots, x_p)^T$, define the p-dimensional basis

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \phi_{\alpha_1}(x_1) \cdots \phi_{\alpha_p}(x_p),$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)^T$. The order of $\Psi_{\boldsymbol{\alpha}}$ is $|\boldsymbol{\alpha}| = \sum_{j=1}^{p} \alpha_j$.

gPC: Basis Table

The correspondence of the polynomials and their underlying random variables is listed below.

Random Variables	Polynomials
Gaussian	Hermite
Uniform	Legendre
Beta	Jacobi
Gamma	Laguerre
Binomial	Krawtchouk
Hypergeometric	Hahn
Negative Binomial	Meixner
Poisson	Charlier

gPC: Model

The gPC is given by

$$g(\boldsymbol{x}) = \sum_{k=0}^{\infty} \beta_k \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}), \tag{1}$$

where β_k are unknown coefficients.

$g(\boldsymbol{x})$ in (1) with a proper choice of β_k converges in quadratic mean to $f(\boldsymbol{x})$ (Soize and Ghanem, 2004).

For practical computation, consider the truncated form of the gPC

$$g_P(\boldsymbol{x}) = \sum_{k=0}^{P} \beta_k \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}).$$

gPC: Inference

To estimate the unknown coefficients β_k:

- Intrusive methods: Galerkin minimization (Ghanem and Spanos, 2003);
- Non-intrusive methods: *regression method* (Sudret, 2008), projection method (Crestaux *et al.*, 2009).

Regression method

Minimize the following sum of squares of residuals:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left\{ f(\boldsymbol{x}_i) - \sum_{k=0}^{P} \beta_k \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_i) \right\}^2 .$$

The solution is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{\Psi}^T \boldsymbol{\Psi})^{-1} \boldsymbol{\Psi}^T \boldsymbol{y},$$

where $\boldsymbol{\Psi}$ denotes the $n \times P$ matrix with (i, k)th entry $\Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_i)$, and $\boldsymbol{y} = (f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n))^T$.

gPC: Variable Selection

Variable selection techniques in linear regression can be applied to the gPC after some modifications:

- Stepwise regression (Blatman and Sudret, 2011);
- LARS (Blatman and Sudret, 2011);
- Bayesian variable selection (Tan, 2014).

However, they work only for a small number of input parameters. Consider the gPC with order L. The number of candidate bases $P = (p + L)!/p!L!$ increases rapidly.

Existing Variable Selection Methods

Variable selection methods with two levels of accuracy for linear models are needed. A quick method with low accuracy is used for ultrahigh dimensions.

Sure Independence Screening (SIS, Fan and Lv, 2008) for selecting bases

Denote $\Psi_{\boldsymbol{\alpha}_k}(X) = (\Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_1), \ldots, \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_n))^T$.

1. Compute the correlation $\omega_k = \text{corr}(\Psi_{\boldsymbol{\alpha}_k}(X), \boldsymbol{y}),$ for $k = 1, \ldots, P$.
2. Choose first $[\gamma n]$ bases with the largest correlations,

where $\gamma n = n - 1$ or $n/\log(n)$.

Alternatives:

- Forward selection (Wang, 2009);
- Correlation pursuit (Zhong et al., 2012).

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Existing Variable Selection Methods (Cont'd)

A more elaborate method with high accuracy is used for moderate dimensions.

Lasso (Tibshirani, 1996) for selecting bases

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \left\{ f(\boldsymbol{x}_i) - \sum_{k=0}^{P} \beta_k \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_i) \right\}^2 + \lambda \sum_{k=0}^{P} |\beta_k|,$$

where λ is a tuning parameter that controls the number of selected bases.

Alternatives:

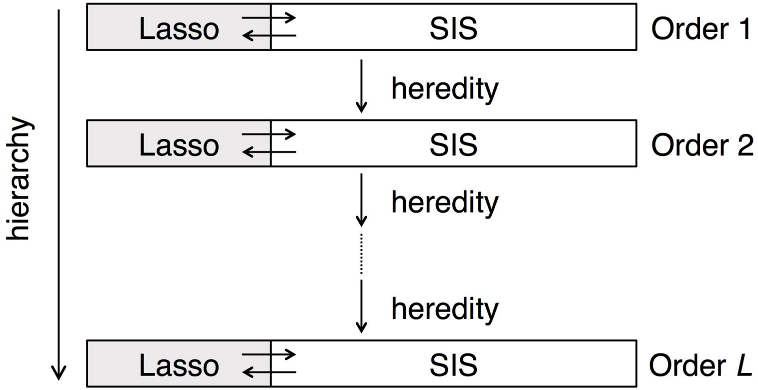
- Smoothly Clipped Absolute Deviation (SCAD, Fan and Li, 2001);
- Adaptive Lasso (Zou, 2006).

Two Principles

Two principles (Wu and Hamada, 2009), originated in design of experiments, are commonly considered in variable selection.

- The effect hierarchy principle:
  Lower order effects are more likely to be important than higher order effects.
- The effect heredity principle:
  An interaction can be active only if one or all of its parent effects are also active.

Basic Idea


hierarchy
Lasso
SIS
Order 1
heredity
Lasso
SIS
Order 2
heredity
heredity
Lasso
SIS
Order L

Within the Layer

Iteratively select bases within the layer

Let $\mathcal{M}^{(l)} = \{\boldsymbol{\alpha}_k : k = i_{k_1}, \ldots, i_{k_l};\ \text{and } |\boldsymbol{\alpha}_k| \le l\}$ be the set of selected bases in the lth layer, and $\mathcal{C}^{(l)}$ a candidate set for the lth layer. In the lth layer, based on $\mathcal{M}^{(l-1)}$ and $\mathcal{C}^{(l)}$:

1. Set $\boldsymbol{r}_0 = \boldsymbol{y}$ and $\mathcal{S}_0^{(l)} = \varnothing$.
2. At iteration m, set the residual $\boldsymbol{r}_{m-1}$, which is a vector with ith entry $f(\boldsymbol{x}_i) - \sum_{\boldsymbol{\alpha}_k \in \mathcal{S}_{m-1}^{(l)}} \hat{\beta}_k \Psi_{\boldsymbol{\alpha}_k}(\boldsymbol{x}_i)$, to be the response.
3. Apply the SIS on $\mathcal{C}^{(l)} \setminus \mathcal{S}_{m-1}^{(l)}$ to select a subset of bases $\mathcal{A}_m^{(l)}$.
4. Apply the lasso on $\mathcal{S}_{m-1}^{(l)} \cup \mathcal{A}_m^{(l)}$ to obtain the set of selected bases $\mathcal{S}_m^{(l)}$.
5. Stop if converge; go to step 2 otherwise. Denote the last $\mathcal{S}_m^{(l)}$ by $\mathcal{S}^{(l)}$.

Between Adjacent Layers

How to generate $\mathcal{C}^{(l)}$?

Note that it is very likely that some of the parent effects of significant interactions are not significant in lower layers.

At the beginning of each layer, $\mathcal{C}^{(l)}$ is generated by expanding $\mathcal{M}^{(l-1)}$ (*weak* heredity):

$$\mathcal{C}^{(l)} = \{\boldsymbol{\alpha}_k : \exists\ \boldsymbol{\alpha}' \in \mathcal{M}^{(l-1)}, \boldsymbol{\alpha}'' \in \mathcal{C} \text{ s.t. } \boldsymbol{\alpha}' + \boldsymbol{\alpha}'' = \boldsymbol{\alpha}_k; \text{ and } |\boldsymbol{\alpha}_k| \leq l\}. \tag{2}$$

Explanation: $\boldsymbol{\alpha}_k$ has a *single* parent $\boldsymbol{\alpha}'$ from $\mathcal{M}^{(l-1)}$. For example, consider three candidate bases $\mathcal{C} = \{\Psi_{(1,0,0)}, \Psi_{(0,1,0)}, \Psi_{(0,0,1)}\}$ and $\mathcal{M}^{(l-1)} = \{\Psi_{(0,1,0)}\}$. From (2), it follows

$$\mathcal{C}^{(l)} = \{\Psi_{(1,1,0)}, \Psi_{(0,2,0)}, \Psi_{(0,1,1)}\}.$$

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Between Adjacent Layers (Cont'd)

How to generate $\mathcal{M}^{(l)}$?

At the end of each layer, expand $\mathcal{S}^{(l)}$ (*strong* heredity) to:

$$\mathcal{D}^{(l)} = \{\boldsymbol{\alpha}_k : \exists\, \boldsymbol{\alpha}', \boldsymbol{\alpha}'' \in \mathcal{S}^{(l)} \text{ s.t. } \boldsymbol{\alpha}' + \boldsymbol{\alpha}'' = \boldsymbol{\alpha}_k;\ \text{and } |\boldsymbol{\alpha}_k| \leq l\}. \quad (3)$$

Explanation: $\boldsymbol{\alpha}_k$ has *both* parents $\boldsymbol{\alpha}', \boldsymbol{\alpha}''$ from $\mathcal{S}^{(l)}$. For example, consider $\mathcal{S}^{(l)} = \{\Psi_{(1,0,0)}, \Psi_{(0,1,0)}, \Psi_{(0,0,1)}\}$. From (3), it follows

$$\mathcal{D}^{(l)} = \{\Psi_{(2,0,0)}, \Psi_{(1,1,0)}, \Psi_{(1,0,1)}, \Psi_{(0,2,0)}, \Psi_{(0,1,1)}, \Psi_{(0,0,2)}\}.$$

Then use the lasso on $\mathcal{D}^{(l)}$ with the response $\boldsymbol{y}$. The set of the final selected bases is denoted by $\mathcal{M}^{(l)}$.
By doing so, the interactions between significant bases, which are likely to be significant, can be re-examined.

Pseudo-code

Set $\mathcal{M}^{(0)} = \varnothing$
for $l = 1, 2, \ldots, L$
    Expand $\mathcal{M}^{(l-1)}$ by (2) to obtain $\mathcal{C}^{(l)}$
    Set $\boldsymbol{r}_0 = \boldsymbol{y}$ and $\mathcal{S}_0^{(l)} = \varnothing$
    for $m = 1, 2, \ldots$
        Set $\boldsymbol{r}_{m-1}$ to be the response
        Apply the SIS on $\mathcal{C}^{(l)} \setminus \mathcal{S}_{m-1}^{(l)}$ to obtain $\mathcal{A}_m^{(l)}$
        Apply the lasso on $\mathcal{S}_{m-1}^{(l)} \cup \mathcal{A}_m^{(l)}$ to obtain $\mathcal{S}_m^{(l)}$
    endfor if converge; denote the last $\mathcal{S}_m^{(l)}$ by $\mathcal{S}^{(l)}$
    Expand $\mathcal{S}^{(l)}$ by (3) to obtain $\mathcal{D}^{(l)}$
    Set $\boldsymbol{y}$ to be the response
    Apply the lasso on $\mathcal{D}^{(l)}$ to obtain $\mathcal{M}^{(l)}$
endfor

Morris Function

$$
\begin{aligned}
y \quad = \quad & \beta_0 + \textstyle\sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{ij} w_i w_j + \\
& \textstyle\sum_{i<j<l}^{20} \beta_{ijl} w_i w_j w_l + \sum_{i<j<l<s}^{20} \beta_{ijls} w_i w_j w_l w_s,
\end{aligned}
$$

where

$$
w_i = \begin{cases} 2(1.1X_i/(X_i + 0.1) - 0.5) & \text{for } i = 3, 5, 7, \\ 2(X_i - 0.5) & \text{otherwise,} \end{cases}
$$

and $X_i \sim U(0, 1)$. The β_i are assigned as

$$
\begin{aligned}
&\beta_i = 20 && \text{for } i = 1, \ldots, 10, \\
&\beta_{ij} = -15 && \text{for } i, j = 1, \ldots, 6, \\
&\beta_{ijl} = -10 && \text{for } i, j, l = 1, \ldots, 5, \\
&\beta_{ijls} = 5 && \text{for } i, j, l, s = 1, \ldots, 4.
\end{aligned}
$$

The remaining coefficients are zero. The true model has 20 X_i input parameters, out of which the first ten are significant. 980 dummy parameters are added. So we have $p = 1000$ parameters in total.

Layer	Stage	Bases
1	Weak heredity	N/A; $\mathcal{C}^{(1)} = 1000$ bases
1	First: SIS	$\mathcal{A}_1^{(1)} = 81$ bases
1	First: Lasso	$\mathcal{S}_1^{(1)} = 19$ bases: $3, 5, 7, 8, 9, 10,$ $93, 203, 284, 286, 362, 434, 510, 511, 623, 815, 896, 940, 941$
1	Last: SIS, Lasso	$\mathcal{S}^{(1)} = 17$ bases: $3, 5, 7, 8, 9, 10,$ $93, 203, 284, 286, 362, 434, 510, 511, 556, 896, 966$
1	Strong heredity	N/A; $\mathcal{M}^{(1)} = \mathcal{S}^{(1)}$
2	Weak heredity	$\mathcal{C}^{(2)} = 16711$ bases
2	First: SIS	$\mathcal{A}_1^{(2)} = 81$ bases
2	First: Lasso	$\mathcal{S}_1^{(2)} = 23$ bases: $5, 7, 8, 9, 10, 286, 1\&3, 1\&5, 2\&5, 3\&4, 3\&6, 4\&6$ $161\&284, 163\&556, 167\&896, 198\&284, 198\&544, 238\&284,$ $284\&858, 284\&885, 510\&592, 510\&966, 673\&792$
2	Last: SIS, Lasso	$\mathcal{S}^{(2)} = 19$ bases: $5, 7, 8, 9, 10, 286, 1\&3, 1\&5, 2\&5, 3\&4, 3\&6,$ $93\&108, 161\&284, 163\&556, 167\&896,$ $198\&284, 238\&284, 510\&592, 510\&869$
2	Strong heredity	$\mathcal{M}^{(2)} = 16$ bases: $7, 8, 9, 10, 1\&2, 1\&3, 1\&5, 1\&6,$ $2\&4, 2\&5, 2\&6, 3\&4, 3\&6, 4\&6, 7\&7, 163\&556$
3	Weak heredity	$\mathcal{C}^{(3)} = 15744$ bases
3	First: SIS	$\mathcal{A}_1^{(3)} = 81$ bases
3	First: Lasso	$\mathcal{S}_1^{(3)} = 21$ bases: $7, 8, 9, 10,$ $1\&2, 1\&3, 1\&4, 1\&5, 1\&6, 2\&4, 2\&5, 2\&6, 3\&4,$ $3\&6, 4\&5, 4\&6, 5\&6, 7\&7, 3\&4\&421, 5\&574, 7\&32$
3	Last: SIS, Lasso	$\mathcal{S}^{(3)} = 16$ bases: $7, 8, 9, 10,$ $1\&2, 1\&3, 1\&4, 1\&5, 1\&6, 2\&4, 2\&5, 2\&6, 3\&4, 3\&6, 4\&6, 7\&7$
3	Strong heredity	$\mathcal{M}^{(3)} = 20$ bases: $7, 8, 9, 10,$ $1\&2, 1\&3, 1\&4, 1\&5, 1\&6, 2\&4, 2\&5, 2\&6, 3\&4,$ $3\&6, 4\&6, 7\&7, 3\&4\&5, 3\&5\&5, 7\&7\&7, 10\&10\&10$

Morris Function: Results

Table shows the average values of the numbers of true positives and false positives with 20 replications. Standard deviations are given in parentheses.

n	True Positives	False Positives
300	7.11(1.66)	9.58(4.05)
500	9.26(0.87)	2.95(2.83)
1000	10(0)	1.36(0.56)

Building Energy Simulation

Background

- The building sector accounts for 40% of the total energy consumption in U.S.
- Retrofit existing buildings to reduce energy consumption and greenhouse gas emissions.
- Uncertainties in the input parameters come from a variety of sources.

Building Energy Simulation: Data

Large Offices in Prototype Buildings

- Energy Plus simulator.
- 2307 input parameters (pre-retrofit, post-retrofit, and common) regarding building physical properties, system settings, usages, and weather.
- Outputs were the energy consumed in the buildings (cooling and electricity).
- 1200 runs.

Building Energy Simulation: Input Parameters

Pre-Retrofit Only 1313 parameters	Post-Retrofit Only 978 parameters	Common 16 parameters
Construction-Pre	Construction-Post	Urban Heat Island
Window-Pre	Window-Post	Local Wind Speed
Infiltration-Pre	Infiltration-Post	Diffuse Solar Irradiation
Ventilation-Pre	Ventilation-Post	Ground Reflectance
HVAC & Lighting System-Pre	HVAC & Lighting System-Post	Convective Heat Transfer
Electric Equipment-Pre	Electric Equipment-Post	Occupant Density

Building Energy Simulation: Results

- In cooling and electricity, the USA selected the gPC which explained 90% and 92% variation of the data, respectively. In contrast, the linear regression model can only explain 78% and 71%, respectively.
- The linear model can be viewed as the gPC with order one. The significant improvement is due to the use of higher-order gPC, which was selected in higher layers of the USA.

Building Energy Simulation: Sensitivity Indices

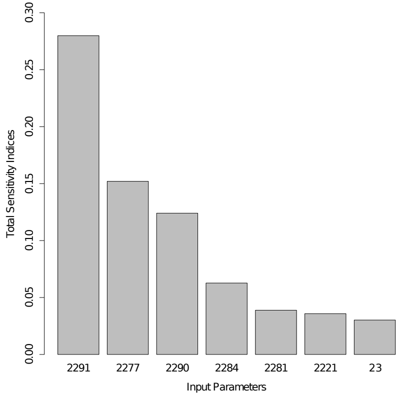

Figure : Cooling: 39 out of 2307

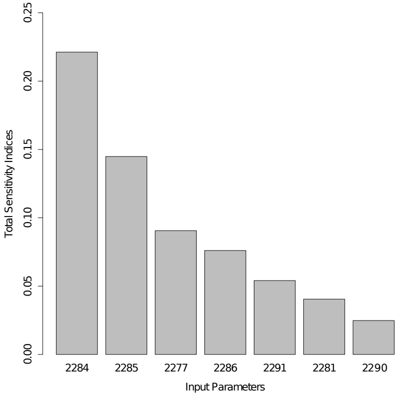

Figure : Electricity: 31 out of 2307

Summary

We have proposed a framework dubbed the USA. The USA unifies UA and SA with the use of one design, and significantly reduce the number of simulations required.

In the USA, a new hierarchical variable selection approach is applied for computational models with many input parameters.

- By incorporating the effect hierarchy principle and the effect heredity principle, the number of candidate bases in each layer is reduced to an acceptable level for variable selection.
- By applying the SIS and the lasso alternately, the USA strikes a balance between computation and performance.

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