Introduction to Sensitivity Analysis

Thomas Santner

Department of Statistics
The Ohio State University
Columbus, Ohio

January 14, 2013

Outline

Overview

Elementary Effects and Their Estimation

Global Sensitivity Analysis

Local Sensitivity Analysis

This talk will describe the Two Basic Forms of Sensitivity Analysis

- **Local Sensitivity Analysis** assesses change in $y(\mathbf{x})$ at each input $(x_1, \ldots, x_d)$

Example Let $y(x_1, x_2) = x_1 + x_2$ with domain $(x_1, x_2) \in (0, 1) \times (0, 2)$. Then

$$\frac{\partial y(x_1^0, x_2^0)}{\partial x_1} = 1 = \frac{\partial y(x_1^0, x_2^0)}{\partial x_2}. \tag{1}$$

Local Sensitivity Analysis concludes that $y(x_1, x_2)$ is equally sensitive to x_1 and x_2 (*starting from any input*, small changes in x_1 or x_2 parallel to the axes produce the same change in $y(x_1, x_2)$).

Global Sensitivity Analysis

- **Global Sensitivity Analysis** Assess change in **range** of $y(\mathbf{x})$ as each input x_i varies over its possible values

Example For fixed x_1^0, the change in $y(x_1^0, \cdot)$ as x_2 ranges over $(0, 2)$, is

$$2 = \max_{x_2} y(x_1^0, x_2) - \min_{x_2} y(x_1^0, x_2) = y(x_1^0, 2) - y(x_1^0, 0)$$

which is *twice* as large as the change of

$$1 = \max_{x_1} y(\cdot, x_2^0) - \min_{x_1} y(x_1^0, x_2)$$

in $y(\cdot, x_2^0)$ for any fixed x_2^0. Global SA concludes that $y(x_1, x_2)$ is **twice** as sensitive to x_2 as x_1.

Standing Assumption

• We assume throughout that $y(\mathbf{x})$ has domain which is hyperrectangle, say $\prod_{i=1}^{d}[a_i, b_i]$;

• For examples of global SA, but not local SA, we assume that the input domain is $[0,1]^d$ because given $y^\star(\cdot)$ with domain $\prod_{i=1}^{d}[a_i, b_i]$, one can apply the methods below to

$$y(x_1, \ldots, x_d) = y^\star(a_1 + x_1(b_1 - a_1), \ldots, a_d + x_d(b_d - a_d)\cdot).$$

and the notation required to describe global SA methods are simplest to state for the case $[0,1]^d$.

Outline

Elementary Effects

The **Elementary Effects** (EEs) of a function $y(\mathbf{x}) = y(x_1, \ldots, x_d)$ having d inputs are measures of the sensitivity of $y(\mathbf{x})$ to each of the inputs x_j. EEs are based on the slopes of secant lines parallel to each of the input axes. Given $j \in \{1, \ldots, d\}$, the j^{th} EE of $y(\mathbf{x})$ at distance δ is

$$d_j(\mathbf{x}) = \frac{y(x_1, \ldots, x_{j-1}, x_j + \delta, x_{j+1}, \ldots, x_d) - y(\mathbf{x})}{\delta}\,. \qquad (2)$$

The ratio $d_j(\mathbf{x})$ is the slope of the secant line connecting $\mathbf{x}$ and $\mathbf{x} + \delta \mathbf{e}_j$ where $\mathbf{e}_j = (0, 0, \ldots, 1, 0, \ldots, 0)$ is the j^{th} unit vector.

• For "small" δ, $d_j(\mathbf{x})$ is a numerical approximation to $\frac{\partial y(\mathbf{x}^o)}{\partial x_j}$ and is thus a local SA tool.

• In most applications, EEs are evaluated for "large" δ (and a widely sampled set of inputs $\mathbf{x}$) and are thus not a local SA tool.

Elementary Effects

Example Suppose

$$y(\mathbf{x}) = 1.0 + 1.5x_2 + 1.5x_3 + .6x_4 + 1.7x_4^2 + .7x_5 + .8x_6 + .5(x_5 \times x_6),$$

where $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5, x_6)$ $0 \leq x_{1,}, x_2, x_4, x_5, x_6 \leq 1$, $0 \leq x_3 \leq 5$.

- $y(\mathbf{x})$ is functionally independent of (constant in) x_1,
- is linear in x_2 and x_3 (and x_3 has the wider range)
- is non-linear in x_4,
- contains an interaction in x_5 and x_6

Elementary Effects

Algebra gives

1. $d_1(\mathbf{x}) \equiv 0$: The EE of the totally inactive variable x_1 is zero because $y(\mathbf{x})$ is independent of x_1.
2. $d_2(\mathbf{x}) \equiv 1.5 \equiv d_3(\mathbf{x})$: The EEs of the linear terms x_2 and x_3 are the same non-zero constant and thus act like a **local** SA measure. (true in general for additive linear terms.)
3. $d_4(\mathbf{x}) = +0.6 + 1.7\delta + 3.4x_4$: The EE of the quadratic term x_4 depends on *both* the starting x_4 and δ; hence for *fixed* δ $d_4(\mathbf{x})$ will vary only with x_4
4. $d_5(\mathbf{x}) = +0.7 + 0.5x_6$, and
5. $d_6(\mathbf{x}) = +0.8 + 0.5x_5$: The EEs of the interacting x_5 and x_6 depends on other variables.

Morris Design for Sampling EEs for Expensive Simulators

• For expensive-to-compute codes with (hyper-rectangular) input regions $[0,1]^d$, Morris (1991) proposed a one-at-a-time (OAT) design for evaluating $y(\mathbf{x})$ in order to estimate the EEs for every input based on $r \times (d+1)$ function evaluations

Example Suppose $y(\mathbf{x}) = y(x_1, x_2, x_3, x_4)$ $(d = 4)$ inputs where $\mathbf{x} \in \mathcal{X} = [0,1]^4$. Suppose $\delta = 0.2$; starting with initial input $(0.4, 0.6, 0.6, 0.0)$, suppose that $y(\mathbf{x})$ is evaluated at the rows of the design

$$\begin{bmatrix} 0.4 & 0.6 & 0.6 & 0.0 \\ 0.4 & 0.4 & 0.6 & 0.0 \\ 0.2 & 0.4 & 0.6 & 0.0 \\ 0.2 & 0.4 & 0.6 & 0.2 \\ 0.2 & 0.4 & 0.4 & 0.2 \end{bmatrix}.$$

Then $d_2(0.4, 0.6, 0.6, 0.0)$ for $\delta = -0.2$ and $d_1(0.4, 0.4, 0.6, 0.0)$ for $\delta = -0.2$,

Morris Design for Sampling EEs for Expensive Simulators

- The Morris design consists of r blocks, each $(d+1) \times d$, that are based on
  - a fixed **griding** of the input region (usually fixed for all blocks)
  - a fixed $\delta > 0$ which is a **multiple** of the grid spacing (usually fixed for all blocks)
  - a **random** permutation π of $1, \ldots, d$
  - a vector $\mathbf{s} = (s_1, \ldots, s_d)$ of **randomly** selected directions with each $s_j \in \{-, +1\}$, $j \in \{1, \ldots, d\}$

Example Suppose that $[0, 1]^4$ is the input space and a grid is selected that divides each input into 10 equal parts. Suppose $\delta = 0.2 = 2 \times \frac{1}{20}$ is selected, the EEs are to be constructed in the order $\boldsymbol{\pi} = (2, 1, 4, 3)$, and in the directions $\mathbf{s} = (-1, -1, +1, -1)$, then starting at $\mathbf{x} = (0.4, 0.6, 0.6, 0.0)$ produces the design on the previous page

Morris Design for Sampling EEs for Expensive Simulators

• Given $(\delta, \boldsymbol{\pi}, \mathbf{s})$, Morris selects selects r starting points $\mathbf{x} \in [0, 1]^d$ randomly from among those points in the grid that satisfy

- $\mathbf{x} + s_{\pi(1)} \times \delta \mathbf{e}_{\pi(1)} \in [0, 1]^d$
- $\mathbf{x} + s_{\pi(1)} \delta \mathbf{e}_{\pi(1)} + s_{\pi(2)} \delta \mathbf{e}_{\pi(2)} \in [0, 1]^d$
- etc.

• **Summary** The OAT design shifts each input coordinate $\pm\delta$ in a random order, until all inputs have been altered (called a *complete tour* starting at $\mathbf{x}$).

• A complete tour is conducted from each starting point $\mathbf{x}$. A total of $r \times (d + 1)$ function evaluations are required to produced r values of each elementary effect.

Morris Design for Sampling EEs for Expensive Simulators

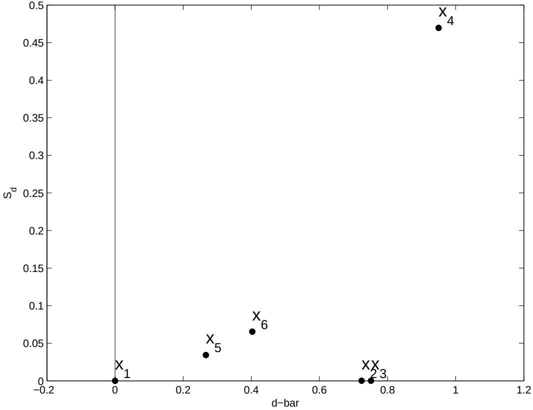
• Suppose each $d_j(\mathbf{x})$, $j = 1, ..., d$, has been computed at r inputs, say $\mathbf{x}^j_1, \ldots \mathbf{x}^j_r$, each for *fixed* δ.

• Let $\overline{d_j}$ denote the sample mean of $d_j(\mathbf{x}^j_1), \ldots, d_j(\mathbf{x}^j_r)$ and S_j their sample standard deviation.

• Plot $(\overline{d_j}, S_j)$, $j = 1, ..., d$.

Example (cont) Based on $r = 5$ values for each EE, the $d = 6$ input function examined above has $(\overline{d_j}, S_j)$ plot

Morris Design for Sampling EEs for Expensive Simulators



which clearly shows the character of x_1, x_2, and x_3 and that x_4, x_5, and x_6 have EEs that depend on the values of other variables.

Outline

Overview

Elementary Effects and Their Estimation

Global Sensitivity Analysis

The functional ANOVA decomposition

- Given $y(\mathbf{x})$, $\mathbf{x} \in [0,1]^d$, define the *overall mean* of $y(\cdot)$ to be

$$y_0 \equiv \int_0^1 \cdots \int_0^1 y(x_1, \ldots, x_d) \prod_{i=1}^{d} dx_i .$$

- The overall mean can be interpreted as the expectation $y_0 = E\left[y(\mathbf{X})\right]$ where $\mathbf{X} = (X_1, \ldots, X_d)$ has i.i.d. $U(0,1)$ component distributions.

- for any $i \in \{1, \ldots, d\}$, the i^{th} **main effect function** is defined to be the average $y(\mathbf{x})$, when x_i is **fixed** , i.e.,

$$u_i(x_i) = \int_0^1 \cdot \int_0^1 y(x_1, \ldots, x_d) \prod_{\ell \neq i} dx_\ell = E\left[y(\mathbf{X}) | X_i = x_i\right];$$

The functional ANOVA decomposition

- Fix any nonempty subset Q of $\{1, \ldots d\}$ and $Q \setminus \{1, \ldots d\}$ are non-empty (so that the integral below are averages over at least one variable). Let $\mathbf{x}_Q$ denote the vector of components x_i with $i \in Q$ in some linear order. Define the joint effect function of $y(\mathbf{x})$ with respect to x_Q to be

$$u_Q(\mathbf{x}_Q) = \int_0^1 \cdots \int_0^1 y(x_1, \ldots, x_d) \prod_{i \notin Q} dx_i = E\left[y(\mathbf{X}) | \mathbf{X}_Q = \mathbf{x}_Q\right] .$$

- For completeness, set

$$u_{12\ldots d}(x_1, \ldots, x_d) \equiv y(x_1, \ldots, x_d).$$

The functional ANOVA decomposition

- $u_Q(\mathbf{x}_Q)$ is the average change in $y(\mathbf{x})$; $u_Q(\mathbf{x}_Q)$ values are on the same scale and in the same range as $y(\mathbf{x})$.
- The standard global SA consists of two tools
  1. Plots of estimated main effect ($u_Q(\mathbf{x}_Q)$ with $Q = \{j\}$) or joint effect ($u_Q(\mathbf{x}_Q)$ with $Q = \{j_1, j_2\}$) functions versus $\mathbf{x}_Q$
  2. Numerical approximations of the variability of $u_Q(\mathbf{X}_Q)$ assuming that the components of $\mathbf{X}_Q$ are i.i.d. $U(0, 1)$

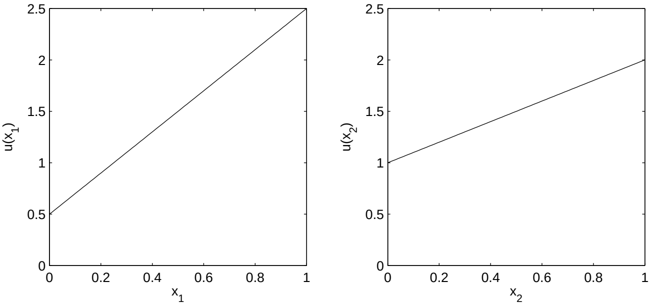
Example

Suppose $y(x_1, x_2) = 2x_1 + x_2$, $(x_1, x_2) \in [0, 1]^2$.

$$
\begin{aligned}
y_0 &= \int_0^1 \int_0^1 (2x_1 + x_2) dx_2 dx_1 = 1.5 \\
u_1(x_1) &= \int_0^1 (2x_1 + x_2) dx_2 = 2x_1 + 0.5 \\
u_2(x_2) &= \int_0^1 (2x_1 + x_2) dx_1 = 1.0 + x_2 \\
u_{12}(x_1, x_2) &= y(x_1, x_2) = 2x_1 + x_2 \ .
\end{aligned}
$$

Example

- The main effect functions for x_1 and x_2 are



- **Aside** It is simple to calculate that

$$\int_0^1 u_1(x_1)\,dx_1 = \int_0^1 u_2(x_2)\,dx_2 = \int_0^1 u_{12}(x_1,x_2)\,dx_1\,dx_2 = 1.5 = y_0\ .$$

(and this is true in general)

Example

• The $u_Q(x_Q)$ terms include all influences of x_Q, not just linear ones.

Example Let $y(x_1, x_2) = x_1 + 2x_1^2 + x_1 x_2$, $\mathbf{x} \in [0.1]^2$ then

- $u_1(x_1) = x_1 + 2x_1^2 + x_1/2$
- $u_2(x_2) = \frac{7}{6} + x_2/2$
- $u_{12}(x_1, x_2) = y(x_1, x_2)$

A Pathological Example

Suppose $y(x_1, x_2, x_3) = (x_1 + 1)\cos(\pi x_2) + 0x_3$ which is independent of x_3 but depends on the interaction of x_1 and $\cos(\pi x_2)$ has overall mean $y_0 = 0$. So

- $u_1(x_1) = \int_0^1 \int_0^1 y(x_1, x_2, x_3) dx_2 dx_3 = 0,\ x_1 \in [0, 1]$ **which is non-intuitive since $y(\mathbf{x})$ depends on x_1**
- $u_2(x_2) = \int_0^1 \int_0^1 y(x_1, x_2, x_3) dx_1 dx_3 = \frac{3}{2}\cos(\pi x_2)$
- $u_3(x_3) = \int_0^1 \int_0^1 y(x_1, x_2, x_3) dx_1 dx_2 = 0$
- $u_{12}(x_1, x_2) = \int_0^1 y(x_1, x_2, x_3) dx_3 = y(x_1, x_2, 0.5)$
- $u_{13}(x_1, x_3) = 0$

A Pathological Example (cont)

- $u_{23}(x_2, x_3) = \frac{3}{2}\cos(\pi x_2)$
- $u_{123}(x_1, x_2, x_3) = 0$

• **Centering** $u_Q(\mathbf{x}_Q)$: The function $u_Q(\mathbf{X}_Q) - y_0$ is one way to create centered $u_Q(\mathbf{X}_Q)$ terms because $E\{u_Q(\mathbf{X}_Q)\} = y_0$.

The functional ANOVA decomposition

- BUT the use of an ANOVA-like centering provides a stronger form of centering and terms with better statistical properties.
- ANOVA-centering of effect functions:
  - For any $i \in \{1, \ldots, d\}$ define

$$y_i(x_i) = u_i(x_i) - \; y_0 \tag{3}$$

  - For (i, j), $1 \le i < j \le d$, define

$$y_{ij}(x_i, x_j) = u_{ij}(x_i, x_j) \; - \; y_i(x_i) \; - \; y_j(x_j) - \; y_0 \tag{4}$$

  to be the centered interaction effect function of x_i and x_j.

The functional ANOVA decomposition

- Suppose that Q is a *non-empty* subset of $\{1, \ldots d\}$,

$$y_Q(\mathbf{x}_Q) = u_Q(\mathbf{x}_Q) - \sum_{E} y_E(\mathbf{x}_E) - y_0 \tag{5}$$

where the sum over all non-empty proper subsets E of Q ($E \subset Q$ is proper provided $E \neq Q$), i.e., if $y(\mathbf{x})$ has three (or more) arguments,

$$\begin{aligned} y_{123}(x_1, x_2, x_3) &= u_{123}(x_1, x_2, x_3) - y_{12}(x_1, x_2) - y_{13}(x_1, x_3) \\ &\quad - y_{23}(x_2, x_3) - y_1(x_1) - y_2(x_2) - y_3(x_3) - y_0 \end{aligned}$$

The functional ANOVA decomposition

Special Case Setting $Q = \{1, \ldots, d\}$

$$
\begin{aligned}
y_{1,2,\ldots,d}(x_1, x_2, \ldots, x_d) &= u_{1,2,\ldots,d}(x_1, x_2, \ldots, x_d) - \sum_{E} y_E(x_E) - y_0 \\
&= y(x_1, x_2, \ldots, x_d) - \sum_{E} y_E(x_E) - y_0
\end{aligned}
$$

- **Application** The **Sobol´ decomposition** of $y(\mathbf{x})$

$$
y(\mathbf{x}) = y_0 + \sum_{i=1}^{d} y_i(x_i) + \sum_{1 \leq i < j \leq d} y_{ij}(x_i, x_j) + \cdots + y_{1,2,\ldots,d}(x_1, \ldots, x_d)
$$

Two Properties of ANOVA-centered Components

• The ANOVA-centered functions have **mean zero** wrt **any single** component, i.e., for any $Q = \{j_1, \ldots, j_s\} \subseteq \{1, \ldots, d\}$ and any $j_k \in Q$

$$\int_0^1 y_Q(\mathbf{x}_Q) dx_{j_k} = 0$$

and are **pairwise orthogonal** , i.e., for any $(k_1, \ldots, k_s) \neq (j_1, \ldots, j_t)$,

$$E\left[y_{k_1,\ldots,k_s}(X_{k_1}, \ldots, X_{k_s}) y_{j_1,\ldots,j_t}(X_{j_1}, \ldots, X_{j_t})\right] = \int y_{k_1,\ldots,k_s}(x_{k_1}, \ldots, x_{k_s}) y_{j_1,\ldots,j_t}(x_{j_1}, \ldots, x_{j_t})\, d\mathbf{x}_Q = 0. \quad (6)$$

where $Q = \{k_1, \ldots, k_s\} \cup \{j_1, \ldots, j_t\}$.

The functional ANOVA decomposition

- Define the *total variance* of $y(\mathbf{x})$ to be

$$v = E\left\{(y(\mathbf{X}) - y_0)^2\right\}$$

- For any subset $Q \subset \{1, \ldots, d\}$, the variance of $y_Q(\mathbf{X}_Q)$ is

$$v_Q = Var(y_Q(\mathbf{X}_Q)) = E\left\{y_Q^2(\mathbf{X}_Q)\right\}$$

because $y_Q(\mathbf{X}_Q)$ has mean zero

The functional ANOVA decomposition

- Thus

$$\begin{aligned} v &= E\left[(y(\mathbf{X}) - y_0)^2\right] \\ &= E\left[\left(\sum_{i=1}^{d} y_i(X_i) + \sum_{i<j} y_{ij}(X_i, X_j) + \ldots + y_{1,2,\ldots,d}(X_1, \ldots, X_d)\right)^2\right] \\ &= \sum_{i=1}^{d} E\left[y_i^2(X_i)\right] + \sum_{i<j} E\left[y_{ij}^2(X_i, X_j)\right] + \cdots \\ &\quad + E\left[y_{1,2,\ldots,d}^2(X_1, \ldots, X_d)\right] + 0 \\ &= \sum_{i=1}^{d} v_i + \sum_{i<j} v_{ij} + \cdots + v_{1,2,\ldots,d} \end{aligned}$$

where all cross product terms are zero by the pairwise orthogonality

The functional ANOVA decomposition

- For any subset $Q \subset \{1, \ldots, d\}$, define the sensitivity index (SI) of $y(\mathbf{x})$ with respect the set of inputs x_i, $i \in Q$, to be

$$S_Q = \frac{v_Q}{v}.$$

- By construction,

$$\sum_{i=1}^{d} S_i + \sum_{1 \le i < j \le d} S_{ij} + \cdots + S_{1,2,\ldots,d} = 1.$$

- S_i, corresponding to $Q = \{i\}$, is called the **first-order or main effect sensitivity index** of input x_i; S_i measures the proportion of the variation v that is due to input x_i.
- S_{ij} is called the **second-order sensitivity index** ; S_{ij} measures the proportion of v that is due to the joint effects of x_i and x_j.

The total sensitivity index

• The **total sensitivity index** (TSI) of $y(\mathbf{x})$ with respect to a given input x_i, denoted T_i, is meant to include the effect of x_i on $y(\mathbf{x})$ and all interactions of x_i with all other inputs. The TSI of $y(\mathbf{x})$ wrt x_i is defined to be

$$T_i = S_i + \sum_{j \neq i} S_{ij} + \cdots + S_{1,2,\ldots,d} \ . \tag{7}$$

Example When $d = 3$,

$$T_1 = S_1 + S_{12} + S_{13} + S_{123}. \tag{8}$$

• By construction, $T_i \geq S_i$, $i = 1, \ldots, d$ *and* the difference $T_i - S_i$ measures the influence of x_i due to its interactions with other variables.

Example (cont) For $y(x_1, x_2) = 2x_1 + x_2$, we calculate that

$$\begin{aligned} v &= Var(y(X_1, X_2)) = Var(2X_1 + X_2) = 4/12 + 1/12 = 5/12 \\ v_1 &= Var(y_1(X_1)) = Var(-1 + 2X_1) = 4/12 \\ v_2 &= Var(y_2(X_2)) = Var(-0.5 + X_2) = 1/12 \\ v_{12} &= Var(y_{12}(X_1, X_2)) = Var(0) = 0 \end{aligned}$$

$\longrightarrow v = v_1 + v_2 + v_{12}$ and

$$S_1 = \frac{4/12}{5/12} = 0.8, \; S_2 = \frac{1/12}{5/12} = 0.2, \text{ and } S_{12} = 0.0.$$

- $T_1 = S_1$ and $T_2 = S_2$
- Interpretation: x_1 is more important than x_2; there is no interaction between x_1 and x_2.
- Deviation from our intuition: based on the functional relationship, the reader might have assessed that x_1 was **twice** as important x_2.

Functional ANOVA decomposition

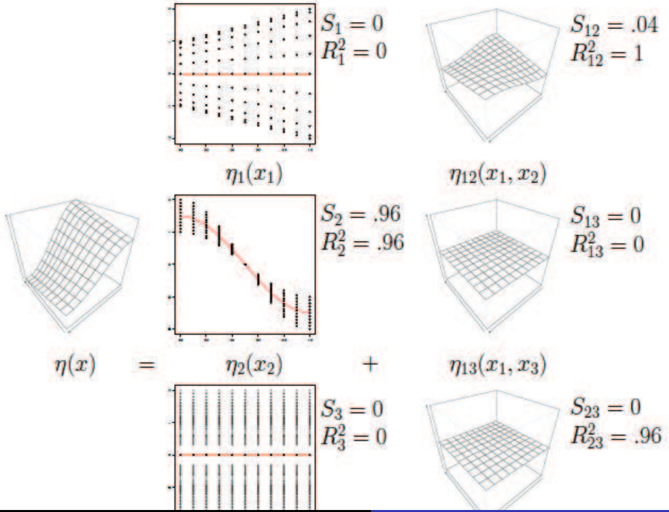
A Pathological Example $y(x_1, x_2, x_3) = (x_1 + 1)\cos(\pi x_2) + 0x_3$.
Because $y_0 = 0$,

$$v = \text{Var}((X_1{+}1)\cos(\pi X_2)) = E\left\{(X_1 + 1)^2 \cos^2(\pi X_2))\right\} = \frac{7}{3}\times\frac{1}{2} = \frac{7}{6}$$

- $y_1(x_1) = 0$, $y_3(x_3) = 0$, $y_{13}(x_1, x_3) = 0$, $y_{23}(x_2, x_3) = 0$, and $y_{123}(x_1, x_2, x_3) = 0$
- So $v_1 = v_3 = v_{13} = v_{23} = v_{123} = 0$
- $y_2(x_2) = \frac{3}{2}\cos(\pi x_2)$ so $v_2 = E\left\{\frac{9}{4}\cos^2(\pi X_2)\right\} = \frac{9}{8}$ and $s_2 = \frac{9/8}{7/6} = 0.96$
- $y_{12}(x_1, x_2) = (x_1 - 0.5)\cos(\pi x_2)$ so $v_{12} = E\left\{(X_1 - 0.5)^2 \cos^2(\pi X_2))\right\} = \frac{1}{24}$ and $s_{12} = 0.04$

Example-Functional ANOVA decomposition

Sobol' decomposition of $\eta(x_1, x_2, x_3) = (x_1 + 1)\cos(\pi x_2) + 0x_3$



Inference for Effect Plots and SIs

- **Method 1** Quadrature-based Estimation of Effect Plots

$$\widehat{u}_Q(\mathbf{x}_Q) = \int_{[0,1]^{d-|Q|}} \widehat{y}(x_1, \ldots, x_d) \prod_{i \notin Q} dx_i = \frac{1}{n} \sum_{\ell=1}^{n} \widehat{y}(\mathbf{x}_Q, \mathbf{x}_{-Q,\ell}) w_\ell$$

where $\widehat{y}(\mathbf{x}_Q, \mathbf{x}_{-Q,\ell})$ is a REML or other EBLUP of $y(\mathbf{x}_Q, \mathbf{x}_{-Q,\ell})$; the weights $\{w_\ell\}$ and points $\{\mathbf{x}_{-Q,\ell}\}$ depend on the selected quadrature method.

Inference for Effect Plots and SIs

- For the EBLUP based on the GP model

$$Y(\mathbf{x}) = \beta_0 + Z(\mathbf{x})$$

where β_0 is unknown and $Z(\mathbf{x})$ is a stationary GP on $[0,1]^d$ having zero mean, variance σ_Z^2, and has **separable** correlation function

$$\prod_{\ell=1}^{d} R(h_\ell | \ \psi_\ell)$$

the integral $\widehat{u}_Q(\mathbf{x}_Q) = \int_{[0,1]^{d-|Q|}} \widehat{y}(x_1, \ldots, x_d) \prod_{i \notin Q} dx_i$ can be computed analytically.

Inference for Effect Plots and SIs

- **Method 2** Process-based Estimators of Sensitivity Indices

For $Y(\mathbf{x}) \sim GP(\beta_0, \sigma^2_Y, R(\cdot))$, the integral

$$U_Q(\mathbf{x}_Q) \equiv \int_0^1 \cdots \int_0^1 Y(x_1, \ldots, x_d) \prod_{i \notin Q} dx_i = E\left[Y(\mathbf{X}) | \mathbf{X}_Q = \mathbf{x}_Q\right],$$

is (under mild conditions) a process for which

$$\left[\left(U_Q(\mathbf{x}_Q), Y(\mathbf{x}_1), \ldots, Y(\mathbf{x}_n)\right) | \xi\right] = \left[\left(U_Q(\mathbf{x}_Q), Y^n\right) | \xi\right]$$

has the joint multivariate normal distribution

$$N_{1+n}\left[\begin{pmatrix} \beta_0 \\ \mathbf{1}_n \beta_0 \end{pmatrix}, \begin{pmatrix} \sigma^2_u & \mathbf{\Sigma}_{nu} \\ \mathbf{\Sigma}_{nu} & \mathbf{\Sigma}_{nn} \end{pmatrix}\right]$$

Estimating Global Sensitivity Indices

• The posterior mean of $U_Q(\mathbf{x}_Q)$ given training data and parameters is

$$\widehat{u}_Q = E_P \left\{ U_Q(\mathbf{x}_Q) \right| \mathbf{Y}^n = \mathbf{y}^n, \boldsymbol{\xi} \} = \beta_0 + \boldsymbol{\Sigma}_{nu} \boldsymbol{\Sigma}_{nn}^{-1} (\mathbf{Y}^n - \mathbf{1}_n \beta_0)$$

is an estimator of $u_Q(\mathbf{x}_Q)$. In practice, $\widehat{u}_Q$ is evaluated for plug-in $\boldsymbol{\xi}$ parameters or $\widehat{u}_Q$ is averaged for a sample from $[\boldsymbol{\xi} | \mathbf{Y}^n = \mathbf{y}^n]$ under a Bayesian model.

• The posterior mean of the **variance** of $U_i(X_i)$ given training data and parameters,

$$\widehat{v}_i = E_P \left\{ Var \left[U_i(X_i) \right] \right| \mathbf{Y}^n = \mathbf{y}^n, \boldsymbol{\xi} \},$$

can be used to estimate

$$v_i = Var\left(u_i(X_i)\right) = Var\left(u_i(X_i) - y_0\right) = Var\left(y_i(X_i)\right)$$

and hence the ME S_i

Estimating Global Sensitivity Indices

- A similar estimator can be used to estimate the **total effect** sensitivity
- In practice, v_i is estimated by plugging estimated $\boldsymbol{\xi}$ parameters into $\widehat{v}_i$ *or* by averaging $\widehat{v}_i$ for a sample of $\boldsymbol{\xi}$ draws from $[\boldsymbol{\xi}|\mathbf{Y}^n = \mathbf{y}^n]$ under a Bayesian model.

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.
- EEs are used to partially determine the linear and low impact inputs.

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.
- EEs are used to partially determine the linear and low impact inputs.
- OAT designs are used to efficiently estimate EEs

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.
- EEs are used to partially determine the linear and low impact inputs.
- OAT designs are used to efficiently estimate EEs
- Main Effect and Joint Effect plots describe the average $y(\mathbf{x})$ over non-fixed inputs

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.
- EEs are used to partially determine the linear and low impact inputs.
- OAT designs are used to efficiently estimate EEs
- Main Effect and Joint Effect plots describe the average $y(\mathbf{x})$ over non-fixed inputs
- ME indices, S_i measure the variability of $u_i(x_i)$ (or $y_i(x_i)$) over x_i

Summary

- Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.
- EEs are used to partially determine the linear and low impact inputs.
- OAT designs are used to efficiently estimate EEs
- Main Effect and Joint Effect plots describe the average $y(\mathbf{x})$ over non-fixed inputs
- ME indices, S_i measure the variability of $u_i(x_i)$ (or $y_i(x_i)$) over x_i
- The Campalongo et al paper gives an improvement to the Morris method for selecting starting points $\mathbf{x}$ at which to eveluate EEs

Summary

• Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.

• EEs are used to partially determine the linear and low impact inputs.

• OAT designs are used to efficiently estimate EEs

• Main Effect and Joint Effect plots describe the average $y(\mathbf{x})$ over non-fixed inputs

• ME indices, S_i measure the variability of $u_i(x_i)$ (or $y_i(x_i)$) over x_i

• The Campalongo et al paper gives an improvement to the Morris method for selecting starting points $\mathbf{x}$ at which to eveluate EEs

• The functional ANOVA decomposition of real-valued $y(\mathbf{x})$ can be used to form other types of SIs such as total effect SIs

Summary

• Sensitivity Analysis is a set of tools used to analyze the local and global sensitivity of a function $y(\mathbf{x})$ to individual inputs x_i.

• EEs are used to partially determine the linear and low impact inputs.

• OAT designs are used to efficiently estimate EEs

• Main Effect and Joint Effect plots describe the average $y(\mathbf{x})$ over non-fixed inputs

• ME indices, S_i measure the variability of $u_i(x_i)$ (or $y_i(x_i)$) over x_i

• The Campalongo et al paper gives an improvement to the Morris method for selecting starting points $\mathbf{x}$ at which to eveluate EEs

• The functional ANOVA decomposition of real-valued $y(\mathbf{x})$ can be used to form other types of SIs such as total effect SIs

• How to form SIs for functional, as opposed to real-valued, output??

Experiments

gpmsa program

http://www.stat.lanl.gov/source/orgs/ccs/ccs6/gpmsa/gpmsa.l