with best regards
from the author.

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Sensitivity Estimates for Nonlinear Mathematical Models

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The theorem that an integrable function can be decomposed into summands of different dimensions is proved. The Monte Carlo algorithm is proposed for estimating the sensitivity of a function with respect to arbitrary groups of variables.

INTRODUCTION

Let us suppose that a mathematical model is described by a function $f(x)$, where $x = (x_1, \ldots, x_n)$, and is defined in a unit n-dimensional cube

$$K^n = \{x | 0 \le x_i \le 1;\ i = 1, \ldots, n\},$$

and we have a program which allows us to calculate the value of $f(x)$ at any given point x. We want to estimate the sensitivity of $f(x)$ with respect to different variables or their groups.

Although [1] and [2] are devoted to estimates of sensitivity, the approach suggested in [3] is more complete. In [3], the expansion of the function $f(x)$ into summands of different dimension, which was constructed in [4], is used.

Here the expansion theorem from [4] is generalized, the Monte Carlo and quasi-Monte-Carlo algorithms for estimating sensitivity are considered, and the problem of freezing unessential variables is touched on.

EXPANSION INTO SUMMANDS OF DIFFERENT DIMENSIONS

Consider a group of indices $i_1, \ldots, i_s$, where $1 \le i_1 < \ldots < i_s \le n$ and $s = 1, \ldots, n$. We introduce a notation for a sum over all the different groups of indices

$$\widehat{\sum} T_{i_1,\ldots,i_s} = \sum_{i=1}^{n} T_i + \sum \sum_{1 \le i < j \le n} T_{ij} + \ldots T_{1,2,\ldots,n}.$$

This sum has $2^n - 1$ summands.

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Definition. A representation of a function $f(x_1, \ldots, x_n)$ as the sum

$$f = f_0 + \widehat{\sum} f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) \tag{1}$$

is referred to as an expansion into summands of different dimensions, if f_0 is constant and the integrals of the summands $f_{i_1 \ldots i_s}$ with respect to any of their "own" variables are zero, *i.e.*,

$$\int_0^1 f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s})\, dx_{i_k} = 0, \qquad 1 \le k \le s. \tag{2}$$

It follows from this definition that

$$f_0 = \int_{K^n} f(x)\, dx, \tag{3}$$

and all the summands on the right-hand side of (1) are orthogonal, *i.e.*, if $(i_1, \ldots, i_s) \not\equiv (j_1, \ldots, j_l)$, then

$$\int_{K^n} f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l}\, dx = 0, \tag{4}$$

since at least one of the indices $i_1, \ldots, i_s, j_1, \ldots, j_l$ is not repeated and the integral with respect to that variable vanishes because of (2).

In [4], the representation ~~of~~ (1) ~~in [4]~~ was constructed by expanding $f(x)$ into multiple Fourier-Haar series. But we can prove a more general statement:

Theorem 1. *There exists a unique expansion of (1) for any function $f(x)$ integrable in K^n.*

Proof. For brevity, we will represent the product of all except certain of the dx_i as a quotient, *e.g.* dx/dx_j is the product of all the dx_i, except dx_j. We now prove that all the summands in (1) are uniquely expressed in terms of different integrals of the function f.

Obviously, ~~the function~~ f_0 is defined by (3). Consider the function

$$g_i(x_i) = \int_0^1 \cdots \int_0^1 f(x)\, dx / dx_i.$$

By integrating (1) with respect to all the variables, except x_i, we obtain

$$g_i(x_i) = f_0 + f_i(x_i). \tag{5}$$

All the summands f_i with one index are defined from this.

Now let $i < j$. Let us consider the function

$$g_{ij}(x_i, x_j) = \int_0^1 \cdots \int_0^1 f(x)\, dx / dx_i\, dx_j.$$

Integrating (1) with respect to all the variables, except x_i and x_j, yields

$$g_{ij}(x_i, x_j) = f_0 + f_i(x_i) + f_j(x_j) + f_{ij}(x_i, x_j). \tag{6}$$

All the summands f_{ij} with two indices are defined from this.

Continuing this process, we introduce the functions with s indices, *i.e.*,

$$g_{i_1,\dots,i_s}(x_{i_1},\dots,x_{i_s}) = \int_0^1 \cdots \int_0^1 f(x)\,dx/\,dx_{i_1}\cdots dx_{i_s} \tag{7}$$

and express all $f_{i_1\dots i_s}$ for $s = 3, 4, \dots, n-1$ in terms of them. The last summand $f_{1,2\dots n}$ is defined immediately from (1).

Given this definition of summands in (1), the property in (2) can be verified immediately. In fact, after integrating the function in (7) with respect to some of its "own" variables we again obtain a function of the same type.

First, by integrating (5) with respect to x_i, we get

$$\int_0^1 f_i(x_i)\,dx_i = 0.$$

Then, by integrating (6) with respect to x_j, we get

$$g_i(x_i) = f_0 + f_i(x_i) + \int_0^1 f_{ij}(x_i, x_j)\,dx_j.$$

We find from this and (5) that the last integral is zero, and so on. □

THE SENSITIVITY ESTIMATE

If $f(x) \in L_2$, then using the Schwarz inequality and (7) it is easy to prove that $g_{i_1\dots i_s} \in L_2$. But then all $f_{i_1\dots i_s} \in L_2$. Hence,

$$D = \int_{K^n} f^2(x)\,dx - f_0^2$$

and

$$D_{i_1,\dots,i_s} = \int_0^1 \cdots \int_0^1 f^2_{i_1,\dots,i_s}\,dx_{i_1}\cdots dx_{i_s}$$

are finite. By squaring (1) and integrating it over K^n [taking into account (4)], we get

$$D = \widehat{\sum} D_{i_1,\dots,i_s}. \tag{8}$$

It is natural to call these values variances because if we treat the point x to be random and uniformly distributed in K^n, then $f(x)$ and $f_{i_1\dots i_s}(x_{i_1},\dots,x_{i_s})$ are random, and D and

$D_{i_1\ldots i_s}$ are their variances. Obviously, these variances characterize how the corresponding functions vary. Thus, we can use the following numbers to estimate sensitivity

$$S_{i_1,\ldots,i_s} = D_{i_1,\ldots,i_s}/D. \tag{9}$$

It follows from (8) and (9) that

$$\widehat{\sum} S_{i_1,\ldots,i_s} = 1. \tag{10}$$

Only quantities with one index, the sum of which is less than or equal to unity, were considered in [1] and [2]. Equation (10) was obtained in [3]. It is easy to see that $f_{i_1\ldots i_s} \equiv 0$ if and only if $S_{i_1\ldots i_s} = 0$. The function $f(x)$ is independent of x_i if and only if all the $S_{i_1\ldots i_s}$ containing the index i are zero. The function $f(x)$ represents the sum of the one-dimensional summands

$$f(x) = f_0 + f_1(x_1) + \ldots + f_n(x_n)$$

if and only if all the $S_{i_1\ldots i_s}$ at $s \geq 2$ are zero.

Note the obvious generalization of (1). Suppose that the variables $x_1, \ldots, x_n$ are divided into m groups $y_1, \ldots, y_m$; $m < n$, which do not intersect in pairs. Then $f(x) \equiv f(y_1, \ldots, y_m)$. Combining the summands in (1) dependent on the variables of each group, we get the following expansion instead of (1)

$$f(x) = f_0 + \widehat{\sum} f_{k_1,\ldots,k_s}(y_{k_1}, \ldots, y_{k_s}), \tag{11}$$

where the indices in $\hat{\Sigma}$ are $1 \leq k_1 < \ldots < k_s \leq m$; $s = 1, \ldots, m$. The property defined by (2) remains, but by integration with respect to y_k we mean integration with respect to all the x_i in y_k.

ANALYTICAL EXAMPLES

1. A linear function $f(x)$. The representation (1) has the form

$$f = f_0 + \sum_{i=1}^{n} c_i(x_i - 1/2).$$

The terms with one index are $S_i = c_i^2/(c_1^2 + \ldots + c_n^2)$ and all the multiple index terms $S_{i_1\ldots i_s}$ are zero.

2. The products of the binomials used in [5] (two of these functions are also encountered in [6]):

   (a) The function

$$f = (2x_1 + 1)\ldots(2x_n + 1)/2^n.$$

Using the representation of (1) we have

$$f = 1 + \widehat{\sum}(2x_{i_1} - 1)\ldots(2x_{i_s} - 1)/2^s$$

and the variances are

$$D_{i_1,\ldots,i_s} = 12^{-s}, \qquad D = (13/12)^n - 1.$$

(b) The function

$$f = (3x_1^2 + 1)\dots(3x_n^2 + 1)/2^n.$$

Using the representation (1) we have

$$f = 1 + \widehat{\sum}(3x_{i_1}^2 - 1)\dots(3x_{i_s}^2 - 1)/2^s$$

and the variances are

$$D_{i_1,\dots,i_s} = 5^{-s}, \qquad D = (6/5)^n - 1.$$

(c) The function

$$f = (2x_1 + 1)(2x_2 + 2)\dots(2x_n + n)/(n+1)!\,.$$

Using the representation (1) we have

$$f = 1 + \widehat{\sum}(2x_{i_1} - 1)\dots(2x_{i_s} - 1)/(i_1 + 1)\dots(i_s + 1)$$

and the variances are

$$D_{i_1,\dots,i_s} = 3^{-s}[(i_1 + 1)\dots(i_s + 1)]^{-2}, \qquad D = \prod_{i=1}^{n}\left[1 + \frac{1}{3(i+1)^2}\right] - 1.$$

It was noted in [5] that from the viewpoint of numerical integration, functions (a) and (b) become bad as n increases, whereas function (c) remains good. It can easily be verified that as $n \to \infty$ the sum $S_1 + \dots + S_n$ tends to zero for functions (a) and (b), while for function (c) the sum tends to the finite limit

$$\lim_{n\to\infty}\sum_{i=1}^{n} S_i = \frac{(1/3)[(\pi^2/6) - 1]}{(3\sqrt{3}/4\pi)\sinh(\pi\sqrt{3}) - 1} = 0.917.$$

CALCULATION ALGORITHMS

Calculation of the individual summands in (1) can be shown to be unnecessary when calculating the quantities in (9). If we agree to an increase in the multiplicity of the calculated integrals, then we can get by with only the values of the function $f(x)$.

Let us consider the more common case in which we want an estimate of how a model depends on one group of variables. Hence, we consider that the variables $x_1, \dots, x_n$ can be divided into two groups, denoted y and z. Let the dimension of y be s and the dimension of z be $n - s$. Instead of (11), we get the expansion

$$f(x) = f_0 + f_1(y) + f_2(z) + f_{1\,2}(y, z),$$

where

$$f_1(y) = \int_0^1 \dots \int_0^1 f(x)\,dz - f_0, \qquad f_2(z) = \int_0^1 \dots \int_0^1 f(x)\,dy - f_0,$$

$$f_{12}(y, z) = f(x) - f_0 - f_1(y) - f_2(z).$$

The corresponding variances are

$$D_1 = \int_0^1 \cdots \int_0^1 f_1^2(y)\,dy, \qquad D_2 = \int_0^1 \cdots \int_0^1 f_2^2(z)\,dz,$$

$$D = \int_{K^n} f^2(x)\,dx - f_0^2, \qquad D_{1\,2} = D - D_1 - D_2.$$

We develop an expression for D_1 that doesn't include $f_1(y)$

$$D_1 = \int_0^1 \cdots \int_0^1 \left[\int_0^1 \cdots \int_0^1 f(x)\,dz\right]^2 dy - f_0^2$$

$$= \int_0^1 \cdots \int_0^1 f(y,z)f(y,v)\,dz\,dv\,dy - f_0^2. \qquad S + (M-S) + (M-S)$$

The multiplicity of the last integral is $2n - s$.

Similarly, we obtain

$$D_2 = \int_0^1 \cdots \int_0^1 f(y,z)f(u,z)\,dy\,du\,dz - f_0^2,$$

and the multiplicity of this integral is $n + s$.

All the necessary integrals can be calculated using the Monte Carlo method: as $N \to \infty$, we have

$$f_0 \approx \frac{1}{N}\sum_{j=1}^{N} f(y_j, z_j),$$

$$D + f_0^2 \approx \frac{1}{N}\sum_{j=1}^{N} f^2(y_j, z_j),$$

$$D_1 + f_0^2 \approx \frac{1}{N}\sum_{j=1}^{N} f(y_j, z_j)f(y_j, v_j),$$

$$D_2 + f_0^2 \approx \frac{1}{N}\sum_{j=1}^{N} f(y_j, z_j)f(u_j, z_j).$$

Here j is the ordinal number of a test and N is the number of tests. In each test we have to calculate three values of the function f : $f(y_j,\ z_j)$, $f(y_j,\ v_j)$, and $f(u_j,\ z_j)$. The random points y_j and u_j are uniformly distributed in K^s, the points z_j and v_j in K^{n-s}. Since D_1 and D_2 are calculated independently, we can use the same random numbers for the realization of u_j and v_j. Therefore, the constructive dimension [7] of the algorithm is $t = \max(n + s,\ 2n - s)$.

If $t \leq 51$, we can accelerate the convergence by using quasirandom points $Q_1, Q_2, \ldots$ which are chosen specifically [6]. Then, in order to realize the jth test we should calculate

the t-dimensional point Q_j and, using its Cartesian coordinates $q_{j,1}, \ldots, q_{j,t}$, we need to find the arguments of the function f, *i.e.*,

$$y_j = (q_{j,1}, \ldots, q_{j,s}), \qquad z_j = (q_{j,s+1}, \ldots, q_{j,n}),$$
$$u_j = (q_{j,n+1}, \ldots, q_{j,n+s}), \qquad v_j = (q_{j,n+1}, \ldots, q_{j,2n-s}).$$

Remark. If the number f_0 is great, then it is natural to assume that when finding D, D_1, and D_2, we can loose accuracy. This can be avoided by replacing the function $f(x)$ with the function $f(x) - c_0$, where c_0 is a number close to f_0.

FREEZING UNESSENTIAL VARIABLES

If above $S_2 + S_{1\,2} \ll 1$, then it is natural to assume that the function $f(y, z)$ is only weakly dependent on variables from group z; so we can use the function $f(y, z_0)$, where z_0 is a fixed point from K^{n-s}, instead of $f(y, z)$.

Let us consider the difference

$$f(y, z) - f(y, z_0) = f_2(z) + f_{1\,2}(y, z) - f_2(z_0) - f_{1\,2}(y, z_0). \tag{12}$$

We take the value

$$\delta(z_0) = \frac{1}{D} \int_{K^n} [f(y, z) - f(y, z_0)]^2 \, dx$$

as a measure of the error of using $f(y, z_0)$ in place of $f(y, z)$. We introduce an auxiliary function

$$\varphi(z) = f_2^2(z) + \int_0^1 \cdots \int_0^1 f_{1\,2}^2(y, z) \, dy,$$

whose integral is

$$\int_0^1 \cdots \int_0^1 \varphi(z) \, dz = D_2 + D_{12}.$$

Squaring (12) and integrating it with respect to all the variables yields

$$\delta(z_0) = S_2 + S_{12} + \varphi(z_0)/D. \tag{13}$$

It follows that $\delta(z_0) \geq S_2 + S_{12}$ for any choice of z_0.

Theorem 2. *If the random point z_0 is uniformly distributed in K^{n-s} then we get the following with a probability exceeding $1 - \varepsilon$:*

$$\delta(z_0) < (1 + \varepsilon^{-1})(S_2 + S_{12}).$$

Proof. Since the random variable $\varphi(z_0)$ is nonnegative and $\mathrm{M}\varphi(z_0) = D_2 + D_{12}$, by virtue of the first Chebyshev inequality, we have the following for an arbitrary $h > 0$

$$\mathrm{P}\{\varphi(z_0) \geq h\} \leq h^{-1}(D_2 + D_{1\,2}).$$

After choosing $h = (D_2 + D_{1\,2})/\varepsilon$, we can write the probability of the opposite event:

$$\mathrm{P}\{\varphi(z_0) < (D_2 + D_{12})/\varepsilon\} \geq 1 - \varepsilon.$$

Because of (13), this is equivalent to the statement of the theorem.□

Example. The above quasi-Monte-Carlo algorithm was successfully employed by Yu. L. Baranov (Institute of Machine-Building of USSR Acad. Sci.) to estimate the effect the parameters of a car suspension has on the distance between eigenvalues. In this example $n = 35$ and $s = 23$. The calculated value $S_1 = 0.98$ confirmed the assumption of designers that the chosen group of variables were dominant.

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