



Derivative based global sensitivity measures and their link with global sensitivity indices

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Abstract

A model function $f(x_1, \dots, x_n)$ defined in the unit hypercube H^n with Lebesgue measure $dx = dx_1 \dots dx_n$ is considered. If the function is square integrable, global sensitivity indices provide adequate estimates for the influence of individual factors x_i or groups of such factors. Alternative estimators that require less computer time can also be used. If the function f is differentiable, functionals depending on $\partial f / \partial x_i$ have been suggested as estimators for the influence of x_i . The Morris importance measure modified by Campolongo, Cariboni and Saltelli μ^* is an approximation of the functional $\mu_i = \int_{H^n} |\partial f / \partial x_i| dx$.

In this paper a similar functional is studied

$$v_i = \int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx$$

Evidently, $\mu_i \leq \sqrt{v_i}$, and $v_i \leq C\mu_i$ if $|\partial f / \partial x_i| \leq C$. A link between v_i and the sensitivity index S_i^{tot} is established:

$$S_i^{tot} \leq \frac{v_i}{\pi^2 D}$$

where D is the total variance of $f(x_1, \dots, x_n)$. Thus small v_i imply small S_i^{tot} , and unessential factors x_i (that is x_i corresponding to a very small S_i^{tot}) can be detected analyzing computed values v_1, \dots, v_n . However, ranking influential factors x_i using these values can give false conclusions.

Generalized S_i^{tot} and v_i can be applied in situations where the factors x_1, \dots, x_n are independent random variables. If x_i is a normal random variable with variance σ_i^2 , then $S_i^{tot} \leq v_i \sigma_i^2 / D$.

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1. Introduction

Let $f(x_1, \dots, x_n)$ be a model function defined in the unit hypercube H^n . If the function f is square integrable, global sensitivity indices provide an adequate tool for estimating the effect of individual factors x_i or groups of such factors on f . However, numerical algorithms for computing these indices involve evaluation of f at a large number of random

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or quasi-random points, and if one model evaluation requires more than several minutes of computer time, a direct application of these algorithms (without using multiprocessor schemes) is impractical. Alternative approaches were developed that provide less expensive estimates of the influence of individual factors x_i on f . They can be applied to more complex models. These alternative estimates sometimes disagree with the ones obtained from sensitivity indices.

If the function f is differentiable, the partial derivative $\partial f/\partial x_i$ is used for estimating the local sensitivity of f with respect to x_i at the point x_1, \dots, x_n . Naturally that attempts were made to construct global sensitivity measures as functionals depending on $\partial f/\partial x_i$ [1,3,5]. The Morris importance measure μ is a measure of this type: finite difference approximations to $\partial f/\partial x_i$ are computed at a discrete set of points inside H^n and μ is defined as a weighted mean of this approximate values of $\partial f/\partial x_i$ [3]. Campolongo et al. suggested a modified Morris measure based on absolute values $|\partial f/\partial x_i|$ called μ^* [1]. It was noticed that for some practical problems this measure has similarities with global total sensitivity indices S_i^{tot} in that it gives a ranking of the variables very similar to that based on the S_i^{tot} but no formal proof of the link between μ^* and S_i^{tot} was given.

In this paper we consider partial derivative based global sensitivity measures and establish the link between them and global total sensitivity indices. It is organized as follows: the next section gives a brief description of the Morris method. Section 3 gives an overview of the theory of global sensitivity indices. A link between global sensitivity indices and partial derivatives is established in Section 4. Section 5 introduces derivatives based importance criteria. Section 6 contains examples. A counterexample showing that in some cases derivative based importance estimates suggest false conclusions is presented in Section 7. Section 8 briefly reviews the case when (x_1, \dots, x_n) are independent random variables. Finally, conclusions are presented in the last section. In the Appendix A a limit for μ^* is considered.

2. The Morris method

The sensitivity measures proposed in the original work of Morris [3] are based on what is called an elementary effect. The general scheme of the Morris method is defined as follows. The range of each input variable is divided into p levels. Then the elementary effect of the i th input factor is defined as finite difference

$$EE_i(x^*) = \frac{f(x_1^*, \dots, x_{i-1}^*, x_i^* + \Delta, x_{i+1}^*, \dots, x_n^*) - f(x^*)}{\Delta}, \quad (2.1)$$

where Δ is a predetermined multiple of $1/(p-1)$ and point $x^* \in H^n$ is such that $x_i^* + \Delta \leq 1$. The distribution of elementary effects F_i is obtained by randomly sampling N points from H^n . Two sensitivity measures are evaluated for each factor: $\mu_{(i)}$ an estimate of the mean of the distribution F_i , and $\sigma_{(i)}$ an estimate of the standard deviation of F_i . A high value of $\mu_{(i)}$ indicates an input variable with an important overall influence on the output. A high value of $\sigma_{(i)}$ indicates a factor involved in interaction with other factors or whose effect is nonlinear. The total computational cost for this scheme is $N_F = 2Nn$. Morris suggested a more economical algorithm by using already computed values of functions in calculation of more than one elementary effects. His algorithm involves a calculation of the so-called sampling matrix which is used for generating trajectories of n steps in the input variables space. These trajectories are such that on each step only one component of a starting point $x = (x_1, x_2, \dots, x_n)$ taken from grid-levels is increased by Δ . The computational cost of the Morris method is $N_F = N(n+1)$. The revised version of the $EE_i(x^*)$ measure and a more effective sampling strategy, which allows a better exploration of the space of the uncertain input factors was proposed in [1].

Non-monotonic functions have regions of positive and negative values of $EE_i(x^*)$, hence due to the effect of averaging values of μ can be very small or even zero. For this reason Campolongo et al. [1] considered another sensitivity measure called μ^* , which estimates the mean of the distribution of elementary effect absolute values.

3. Global sensitivity indices

Global sensitivity indices are often classified as variance based. However, they can be defined without assuming that the variable x is random. Consider a function $f(x)$ defined and square integrable in the unit hypercube H^n with the

Lebesgue measure $dx = dx_1 \dots dx_n$. According to [7] the identity

$$f(x) = f_0 + \sum_{s=1}^n \sum_{i_1 < \dots < i_s} f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) \tag{3.1}$$

is called ANOVA-decomposition of $f(x)$ if

$$f_0 = \int_{H^n} f(x) dx \tag{3.2}$$

and for all $p = 1, 2, \dots, s$

$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_p} = 0. \tag{3.3}$$

The interior sum in (3.1) is extended over all different groups of indices i_1, \dots, i_s such that

$$1 \leq i_1 < i_2 < \dots < i_s \leq n. \tag{3.4}$$

Thus (3.1) can be rewritten as

$$f(x) = f_0 + \sum_i f_i(x_i) + \sum_{i < j} f_{i,j}(x_i, x_j) + \dots + f_{1,2,\dots,n}(x_1, x_2, \dots, x_n).$$

It follows from (3.2) and (3.3) that all the terms in (3.1) are orthogonal.

Constants $D_{i_1, \dots, i_s} = \int_{H^n} f_{i_1, \dots, i_s}^2(x_{i_1}, \dots, x_{i_s}) dx$ are called partial variances and the constant

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

is called total variance. Squaring (3.1) and integrating over H^n , we obtain

$$D = \sum_{s=1}^n \sum_{i_1 < \dots < i_s} D_{i_1, \dots, i_s}.$$

Global sensitivity indices are defined as ratios

$$S_{i_1, \dots, i_s} = \frac{D_{i_1, \dots, i_s}}{D}.$$

Obviously

$$\sum_{s=1}^n \sum_{i_1 < \dots < i_s} S_{i_1, \dots, i_s} = 1.$$

One-dimensional index $S_i = D_i/D$ shows the effect of the single factor x_i on the output $f(x)$ but it does not account for the high dimensional terms in (3.1). For estimating the total influence of the factor x_i , total partial variances are introduced:

$$D_i^{tot} = \sum_{(i)} D_{i_1, \dots, i_s},$$

where the sum $\sum_{(i)}$ is extended over all different groups of indices satisfying (3.4) at $1 \leq s \leq n$, where one of the indices is equal i . The corresponding total sensitivity index is

$$S_i^{tot} = \frac{D_i^{tot}}{D}.$$

In general $0 \leq S_i \leq S_i^{tot} \leq 1$.

The output $f(x)$ does not depend on the factor x_i if and only if $S_i^{tot} = 0$. If the value x_i is somehow fixed, the error in $f(x)$ depends on S_i^{tot} (for more details see [9]). Indices S_i^{tot} are often used for ranking variables x_i .

In [7] (Theorem 3) a general formula for D_y^{tot} is given, where y is an arbitrary subset of the variables x_1, \dots, x_n . In the case when $y = (x_i)$, this formula can be rewritten as

$$D_i^{tot} = \frac{1}{2} \int_{H^n} \int_0^1 \left[f(x) - f\left(\overset{\circ}{x}\right) \right]^2 dx dx'_i, \tag{3.5}$$

where

$$\overset{\circ}{x} = (x_1, \dots, x_{i-1}, x'_i, x_{i+1}, \dots, x_n).$$

4. Sensitivity indices and partial derivatives

In this section two theorems that establish links between the index S_i^{tot} and the derivative $\partial f / \partial x_i$ are proved. In the first theorem the limiting values of $|\partial f / \partial x_i|$ and in the second theorem the mean value of $(\partial f / \partial x_i)^2$ are used.

Theorem 1. Assume that $c \leq |\partial f / \partial x_i| \leq C$. Then

$$\frac{c^2}{12D} \leq S_i^{tot} \leq \frac{C^2}{12D}. \tag{4.1}$$

The constant factor 12 in (4.1) cannot be improved.

Proof. Consider the increment of $f(x)$ in (3.5):

$$f(x) - f\left(\overset{\circ}{x}\right) = \frac{\partial f(\hat{x})}{\partial x_i} (x_i - x'_i), \tag{4.2}$$

where \hat{x} is a point between x and $\overset{\circ}{x}$. Substituting (4.2) into (3.5) we obtain

$$D_i^{tot} = \frac{1}{2} \int_{H^n} \int_0^1 \left(\frac{\partial f(\hat{x})}{\partial x_i} \right)^2 (x_i - x'_i)^2 dx dx'_i \tag{4.3}$$

In (4.3) $c^2 \leq (\partial f / \partial x_i)^2 \leq C^2$ while the remaining integral is

$$\int_0^1 \int_0^1 (x'_i - x_i)^2 dx'_i dx_i = \frac{1}{6}.$$

Thus we obtain inequalities that are equivalent to (4.1). Finally consider the function $f = f_0 + c(x_i - 1/2)$. In this case $C = c$, $D = 1/12$, $S_i^{tot} = 1$ and the inequalities (4.1) become equalities. \square

Theorem 2. Assume that $\partial f / \partial x_i \in L_2$. Then

$$S_i^{tot} \leq \frac{1}{\pi^2 D} \int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx. \tag{4.4}$$

Proof. Denote by $u(x)$ the sum of all terms in (3.1) that depend on x_i :

$$u(x) = \sum_{\langle i \rangle} f_{i_1, \dots, i_s} (x_{i_1}, \dots, x_{i_s}).$$

Obviously $D_i^{tot} = \int_{H^n} u^2(x) dx$ and $\frac{\partial f}{\partial x_i} = \frac{\partial u}{\partial x_i}$.

Consider $u(x)$ as a function of x_i only. It follows from (3.3) that the mean $\int_0^1 u(x) dx_i = 0$, therefore an inequality for one-dimensional functions from [6] can be applied:

$$\int_0^1 u^2(x) dx_i \leq \frac{1}{\pi^2} \int_0^1 \left(\frac{\partial u}{\partial x_i} \right)^2 dx_i.$$

Integrating this inequality over all other variables we obtain

$$D_i^{tot} \leq \frac{1}{\pi^2} \int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx.$$

This is equivalent to (4.4).

To complete the proof of Theorem 2, consider an example: $f(x) = \sin \pi(x_i - 1/2)$. In this case $S_i^{tot} = 1$, $D = 1/2$ and $\int_0^1 (\partial f / \partial x_i)^2 dx_i = \pi^2/2$, so the right-hand side in (4.4) is also equal to 1. \square

Remark. From the relation (4.2) we conclude that $D_i^{tot} = \frac{1}{12} [(\partial f / \partial x_i)^2]^*$, where $[]^*$ is a rather sophisticated mean value. If $[]^*$ is replaced by an ordinary mean value we get an approximate relation that yields an approximate formula

$$S_i^{tot} \approx \frac{1}{12D} \int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx.$$

Unfortunately, we have no reliable error estimate for this approximation. We can only expect this approximation to be correct in situations in which the second derivative $\partial^2 f / \partial x_i^2$ is negligible.

5. Derivative based importance criteria

Consider the set of values v_1, \dots, v_n , where

$$v_i = \int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx, \quad 1 \leq i \leq n.$$

One can expect that smaller v_i correspond to less influential variables x_i . This importance criterion is similar to the modified Morris importance measure μ^* , whose limiting values are (see Appendix A)

$$\mu_i = \int_{H^n} \left| \frac{\partial f}{\partial x_i} \right| dx.$$

From a practical point of view the criteria μ_i and v_i are equivalent: they are evaluated by the same numerical algorithm and are linked by relations $v_i \leq C\mu_i$, $\mu_i \leq \sqrt{v_i}$. Therefore the results of Section 4 can be regarded as support for both v_i and μ_i . The only point that can be interpreted as an advantage of v_i is the inequality (4.4):

$$S_i^{tot} \leq \frac{v_i}{\pi^2 D}$$

that provides the estimation of S_i^{tot} without knowing the upper bound C of the partial derivative.

It is been shown in Kucherenko et al. [2] that the computational time required for MC evaluation of derivative based importance criteria is much lower than that for estimation of the Sobol' sensitivity indices. It is also lower than that for the Morris method. The efficiency again is especially dramatic for the Quasi MC integration method based on Sobol' sequences. It is also been shown that the Morris method can produce inaccurate measures for non-monotonic functions such as g -function for which characteristic length of function variation is much smaller than Δ .

6. Functions with separated variables

Consider $f(x) = \prod_{i=1}^n \varphi_i(x_i)$, where $\varphi_i(t) \in L_2$, $\varphi_i'(t) \in L_2$. Denote

$$A_i = \int_0^1 \varphi_i(t) dt, \quad D_i = \int_0^1 \varphi_i^2(t) dt - A_i^2.$$

Then

$$D = \prod_{i=1}^n (D_i + A_i^2) - \prod_{i=1}^n A_i^2,$$

$$D_i^{tot} = \prod_{k \neq i} (D_k + A_k^2) D_i,$$

$$\int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx = \prod_{k \neq i} (D_k + A_k^2) \int_0^1 [\varphi'_i(t)]^2 dt.$$

Thus

$$\frac{\int_{H^n} \left(\frac{\partial f}{\partial x_i} \right)^2 dx}{D_i^{tot}} = \frac{\int_0^1 [\varphi'_i(t)]^2 dt}{D_i}. \tag{6.1}$$

Example 1. Consider the so-called *g*-function that is often used for numerical experiments in sensitivity analysis $f = \prod_{i=1}^n (|4x_i - 2| + a_i)/(1 + a_i)$. Surprisingly, for the *g*-function the ratio (6.1) is constant and does not depend on the parameter a_i . Thus for all important or non-important variables x_i the right-hand side in (4.4) is proportional to the left-hand side. However, the value of this constant 48 is considerably larger than π^2 or 12.

Example 2. If φ_i is strongly nonlinear, the ratio $(\int_0^1 [\varphi'_i(t)]^2 dt)/D_i$ can be very large. Assume that $\varphi_i(t) = t^m$. Then $A_i = 1/(m + 1)$, $D_i = m^2/((2m + 1)(m + 1)^2)$, $\int_0^1 [\varphi'_i(t)]^2 dt = m^2/(2m - 1)$. The ratio $(\int_0^1 [\varphi'_i(t)]^2 dt)/D_i = (m + 1)^2 * (2m + 1)/(2m - 1)$. At $m = 1$ the ratio is 12, but for large m it will be $\approx (m + 1)^2$.

7. Counterexample

Example 3. Consider a function f which has the following ANOVA decomposition:

$$f = \sum_{i=1}^4 c_i \left(x_i - \frac{1}{2} \right) + c_{12} \left(x_1 - \frac{1}{2} \right) \left(x_2 - \frac{1}{2} \right)^5,$$

where $c_i = 1, 1 \leq i \leq 4, c_{12} = 50$. For this function all $S_i = 0.237, 1 \leq i \leq 4, S_{12} = 0.0523$ and $S_1^{tot} = S_2^{tot} = 0.289, S_3^{tot} = S_4^{tot} = 0.237$, so variables 1, 2 and variables 3, 4 have the same importance. However, for derivative based importance criteria variables 1 and 2 have different importance $v_1 = 1.22, v_2 = 3.26$, while variables 3 and 4 still have equal importance $v_3 = v_4 = 1.0$. Moreover, $v_2 > v_1 + v_3 + v_4$.

Comparing left and right-hand side of inequality (4.4) (Table 1), one can see that $v_i/(\pi^2 D)$ is much higher than S_i^{tot} only for variable 2. It is caused by the strong nonlinearity of the term $f_{1,2}(x_1, x_2)$ with respect to x_2 (compare with test function of Example 2).

This example shows that ranking of influential variables based on v_i may result in false conclusions: in our example x_2 seems more important than all the other variables together.

Table 1
 S_i^{tot} and $v_i/(\pi^2 D)$ for the Counterexample.

i	S_i^{tot}	$v_i/(\pi^2 D)$
1	0.289	0.354
2	0.289	0.938
3	0.237	0.288
4	0.237	0.288

8. Random variables

Consider a model function $f(x_1, \dots, x_n)$, where x_1, \dots, x_n are independent random variables with distribution functions $F_1(x_1), \dots, F_n(x_n)$. Thus the point $x = (x_1, \dots, x_n)$ is defined in the Euclidian space R^n and its measure is $dF_1(x_1) \dots dF_n(x_n)$. The theory of global sensitivity indices can be easily generalized and applied in this case (see e.g. [8]). The following assertion is a generalization of Theorem 1.

Theorem 3. Assume that $c \leq |\partial f / \partial x_i| \leq C$ and that the variance of x_i is finite $\sigma_i^2 = \text{var}(x_i) < \infty$. Then $\sigma_i^2 c^2 / D \leq S_i^{\text{tot}} \leq \sigma_i^2 C^2 / D$. The constant factor σ_i^2 cannot be improved.

Proof. One can repeat the proof of Theorem 1 with three changes:

- (1) The starting point is the relation $D_i^{\text{tot}} = \frac{1}{2} \int_{R^n} \int_{-\infty}^{\infty} \left[f(x) - f\left(\overset{\circ}{x}\right) \right]^2 \prod_{k=1}^n dF_k(x_k) dF_i(x'_i)$.
- (2) The “remaining integral” in this case is $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (x'_i - x_i)^2 dF_i(x_i) dF_i(x'_i) = 2\sigma_i^2$.
- (3) Finally consider the function $f(x) = f_0 + c(x_i - E(x_i))$, where $E(x_i)$ is a mean value of x_i . In this case $C = c$, $D = \sigma_i^2$, $S_i^{\text{tot}} = 1$ and the inequalities become equalities. \square

The following results are similar to Theorem 2 but it is not a generalization of Theorem 2.

Theorem 4. Assume that x_i is a normal random variable with parameters $(a_i; \sigma_i)$ and the integral in (8.1) is finite. Then

$$S_i^{\text{tot}} \leq \frac{\sigma_i^2}{D} \int_{R^n} \left(\frac{\partial f}{\partial x_i} \right)^2 \prod_{k=1}^n dF_k(x_k). \tag{8.1}$$

The constant factor σ_i^2 cannot be reduced.

Proof. The logic of the proof is the same as in Theorem 2. However, the inequality from [6] that was used in Theorem 2 must be replaced by a new one:

Inequality. Denote $p(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp[-(t - a)^2 / (2\sigma^2)]$, $-\infty < t < \infty$. If both $u(t)$ and $u'(t)$ are square integrable with weight $p(t)$, and

$$\int_{-\infty}^{\infty} u(t) p(t) dt = 0. \tag{8.2}$$

Then

$$\int_{-\infty}^{\infty} u^2(t) p(t) dt \leq \sigma^2 \int_{-\infty}^{\infty} [u'(t)]^2 p(t) dt. \tag{8.3}$$

The simple example $f(x) = x_i - a_i$ shows that in (8.1) equality is possible: $S_i^{\text{tot}} = 1$, $\partial f / \partial x_i = 1$, $D = \sigma_i^2$. \square

Proof of the inequality. Let $\Phi = \Phi[u]$ be a functional depending on $u(t)$:

$$\Phi = \int_{-\infty}^{\infty} \left[\sigma^2 (u')^2 - u^2 \right] p(t) dt. \tag{8.4}$$

Consider a typical problem in calculus of variations: minimize $\Phi[u]$ while $u(t)$ satisfies (8.2). The extremal function $u^* = t - a$ satisfies the Euler–Lagrange equation and condition (8.2). The minimum value of the functional (8.4) is $\min \Phi[u] = \Phi[t - a] = 0$. Thus $\Phi[u] \geq 0$ and this is equivalent to (8.3). \square

Example 4. We consider the quadratic polynomial Oakley and O’Hagan function defined as follows [4]:

$$f(x) = a_1^T x + a_2^T \cos(x) + a_3^T \sin(x) + x^T Mx.$$

Here x is a vector of fifteen normally distributed variables $N(0, 1)$. For this function the sensitivity indices S_i^{tot} increase monotonically from $S_1^{tot} = 0.059$ up to $S_{15}^{tot} = 0.154$. The estimates on the right-hand side of (8.1) were computed and divided by S_i^{tot} . In full agreement with Theorem 4, all these ratios exceed 1: 1.01; 1.00; 1.00; 1.04; 1.09; 1.18; 1.16; 1.06; 1.26; 1.08; 1.19; 1.20; 1.20; 1.15; 1.14.

9. Conclusions

The main results of the present paper are

- (1) A link between sensitivity indices and measures based on partial derivatives is established.
- (2) It is proved that small values of derivative based measures imply small values of one-dimensional total sensitivity indices. This result supports the recommendation of [1,3,5] that derivative based measures can successfully be used for detecting unessential variables.
- (3) The importance criterion μ^* can be improved by using squared partial derivative rather than its absolute value.
- (4) It is shown that for highly nonlinear functions the ranking of important factors using derivative based importance measures may suggest false conclusions.

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Appendix A. A limit for Morris importance measure

Let $x^{(1)}, \dots, x^{(k)}, \dots$ be a quasi-random sequence of points inside H^n so that for an arbitrary Riemann integrable function $g(x)$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=1}^N g(x^{(k)}) = \int_{H^n} g(x) dx$$

We consider one of the variables, say x_i , and let h be its increment, $0 < h < 1 - x_i$. Denote $\tilde{x} = (x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n)$ and $\Delta f(x) = f(\tilde{x}) - f(x)$.

The following algorithm is a version of the modified Morris measure μ^* . Choose N points $x^{(k)}$, $1 \leq k \leq N$, and N corresponding increments $h^{(k)}$. Compute $2N$ values $f(x^{(k)})$ and $f(\tilde{x}^{(k)})$, $1 \leq k \leq N$. Then

$$\mu^* = \frac{1}{N} \sum_{k=1}^N \frac{|\Delta f(x^{(k)})|}{h^{(k)}}.$$

If $f(x)$ does not depend on x_i , then $\mu^* = 0$.

Theorem A. Assume that $\partial f / \partial x_i$ is Riemann integrable and $\partial^2 f / \partial x_i^2$ is bounded. Then if $N \rightarrow \infty$ and $\max h^{(k)} \rightarrow 0$, then $\mu^* \rightarrow \mu_i$, where

$$\mu_i = \int_{H^n} \left| \frac{\partial f}{\partial x_i} \right| dx.$$

Proof. Given an arbitrary $\varepsilon > 0$, we choose N so large that

$$\left| \frac{1}{N} \sum_{k=1}^N \left| \frac{\partial f(x^{(k)})}{\partial x_i} \right| - \mu_i \right| < \frac{\varepsilon}{2}. \tag{A.1}$$

We choose the increments $h^{(1)}, \dots, h^{(N)}$ so small that $\max h^{(k)} \left| \partial^2 f / \partial x_i^2 \right| \leq \varepsilon$. The function $f(x)$ can be regarded as one-dimensional function of x_i . Its increment has a form

$$\frac{\Delta f(x)}{h} = \frac{\partial f(x)}{\partial x_i} + \frac{1}{2} h \frac{\partial^2 f(\hat{x})}{\partial x_i^2},$$

where \hat{x} is a point between x and \tilde{x} . If $x = x^{(k)}$ and $h = h^{(k)}$, the last term in this expression does not exceed $\varepsilon/2$, therefore we can easily prove that

$$\frac{|\Delta f(x^{(k)})|}{h^{(k)}} = \left| \frac{\partial f(x^{(k)})}{\partial x_i} \right| + r_k,$$

where the remainder $|r_k| \leq \varepsilon/2$. Averaging the last relation over $1 \leq k \leq N$, we obtain

$$\left| \mu^* - \frac{1}{N} \sum_{k=1}^N \left| \frac{\partial f(x^{(k)})}{\partial x_i} \right| \right| < \frac{\varepsilon}{2}. \quad (\text{A.2})$$

From (A.1) and (A.2) it follows that $|\mu^* - \mu_i| < \varepsilon$. \square

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