Variance-based methods

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Outline

High-Dimensional Model Representation (HDMR)

ANOVA decomposition

Sobol' Sensitivity Indices (SI)

Improved formulas for Sobol' Main Effect SI

High-Dimensional Model Representation (HDMR)

Consider a model *f(x)*, *x* is a vector of input independent variables, *f(x)* is integrable. Decomposition of *f(x)* is called HDMR:

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{i}\sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,n}(x_1, x_2, \ldots, x_n)$$

For simplisity we assume $\mathbf{x} \in H^n = [0,1]^n$

An example in 3 dimensions:

$$\begin{aligned} f(\mathbf{x}) = {} & f_0 + f_1(x_1) + f_2(x_2) + f_3(x_3) \\ & + f_{12}(x_1, x_2) + f_{13}(x_1, x_3) + f_{23}(x_2, x_3) \\ & + f_{123}(x_1, x_2, x_3) \end{aligned}$$

There are infinite ways to build such an expansion →

High-Dimensional Model Representation (HDMR)

An example in 2 dimensions: $f(x_1, x_2) = 4x_1^2 + 3x_2$

a) $f_0 = 0;$ $f_1(x_1) = 4x_1^2$ $f_2(x_2) = 3x_2$ $f_{12}(x_1, x_2) = 0$

b) $f_0 = 5;$

$$f_1(x_1) = 4x_1^2 - 2x_1$$

$$f_2(x_2) = 3x_2 - \sqrt{x_2}$$

$$f_{12}(x_1, x_2) = 2x_1 + \sqrt{x_2} - 5$$

ANOVA decomposition

$$y = f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i\left(x_i\right) + \sum_{i}\sum_{j>i} f_{ij}\left(x_i, x_j\right) + \ldots + f_{1,2,\ldots,n}\left(x_1, x_2, \ldots, x_n\right)$$

Impose a constraint: each term in the HDMR should be

$$\int f_{i_1 i_2 \ldots i_s}(x_{i_1}, x_{i_2}, \ldots, x_{i_s})dx_j = 0 \quad \forall j = i_1, i_2, \ldots, i_s$$

ANOVA decomposition

THEN the HDMR has the following properties:

1) $$f_0 = \int_{H^n} f(\mathbf{x})\, d\mathbf{x}$$

2) Any pair of terms in the HDMR is orthogonal:

$$\int f_{i_1,\ldots,i_s} f_{j_1,\ldots,j_l}\, d\mathbf{x} = 0 \qquad \text{for } (i_1,\ldots,i_s) \neq (j_1,\ldots,j_l)$$

3) HDMR is unique → ANOVA decomposition (Sobol' 1993)

ANOVA decomposition and Sobol' Sensitivity Indices

$$Y = f(X)$$
$$X = (X_1, X_2, ..., X_n) \in H^n$$
$$0 \le X_i \le 1$$

$f(x)$ is L2 integrable

ANOVA decomposition is unique:

$$Y = f(X) = f_0 + \sum_{i=1}^{n} f_i(X_i) + \sum_i \sum_{j>i} f_{ij}\left(X_i, X_j\right) + ... + f_{1,2,...,k}\left(X_1, X_2, ..., X_n\right),$$

$$\int_0^1 f_{i_1 \ldots i_s}(X_{i_1}, ,..., X_{i_s}) dX_{i_p} = 0, \ \forall p, \ 1 \le p \le s, \rightarrow \int_0^1 f_{i_1 \ldots i_s} f_{i_1 \ldots i_l} dX_{i_p} dX_{i_l} = 0, \ \forall i_p \ne i_l$$

Let's square each side and integrate over dx :

$$\int_{H^n} (f(X) - f_0)^2 dx = \int_{H^n} \Big(\sum_{i=1}^{n} f_i(X_i) + \sum_i \sum_{j>i} f_{ij}\left(X_i, X_j\right) + ... + f_{1,2,...,k}\left(X_1, X_2, ..., X_n\right)\Big)^2 dx$$

Total variance:

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

ANOVA decomposition and Sobol' Sensitivity Indices

Due to the orthogonality of the terms:

$$\int_0^1 f_{i_1 \ldots i_s} f_{i_1 \ldots i_l} dX_{i_p} dX_{i_l} = 0, \quad \forall i_p \neq i_l$$

we obtain variance decomposition :

$$D = \sum_i D_i + \sum_{i,j} D_{ij} + \ldots + D_{1,2,\ldots,n}$$

Partial variances:

$$D_{ij} = \iint f_{ij}^2(x_i, x_j) dx_i dx_j - \left[\iint f_{ij}(x_i, x_j) dx_i dx_j \right]^2 = \iint f_{ij}^2(x_i, x_j) dx_i dx_j$$

Sobol' SI:

$$1 = \sum_{i=1}^{n} S_i + \sum_{i<j} S_{ij} + \sum_{i<j<l} S_{ijl} + \ldots + S_{1,2,\ldots,n}$$

Sobol' Sensitivity Indices (SI)

- *Definition:* $$\boxed{S_{i_1 \ldots i_s} = D_{i_1 \ldots i_s} / D}$$

$$D_{i_1 \ldots i_s} = \int_0^1 f_{i_1 \ldots i_s}^2 \left(x_{i_1}, \ldots, x_{is} \right) dx_{i_1}, \ldots, x_{is}$$ *- partial variances*

$$D = \int_0^1 \left(f\left(x\right) - f_0 \right)^2 dx$$ *- total variance*

- *Sensitivity indices for subsets of variables:* $x = \left(y, z \right)$

$$D_y = \sum_{s=1}^{m} \sum_{\left(i_1 \langle \ldots \langle i_s \right) \in K} D_{i_1, \ldots, i_s}$$

The total variance (Homma&Saltelli 96) : $D_y^{tot} = D_y + D_{yz} = D - D_z$

Corresponding Sobol' sensitivity indices (SI):

$$S_y = D_y / D, \qquad S_y^{tot} = D_y^{tot} / D.$$

How to use Sobol' Sensitivity Indices?

$$\boxed{0 \le S_y \le S_y^{tot} \le 1}$$

- $S_y^{tot} - S_y$ *accounts for all interactions between y and z, x=(y,z).*
- *The important indices in practice are* S_i *and* S_i^{tot}

  $S_i^{tot} = 0 \rightarrow f(x)$ does not depend on x_i ;

  $S_i = 1 \rightarrow f(x)$ depends only on x_i ;

  $S_i = S_i^{tot}$ *corresponds to the absence of interactions between* x_i and other variables

  If $\sum_{s=1}^{n} S_i = 1$, then function has an additive structure: $f(x) = f_0 + \sum_i f_i(x_i)$

- *Fixing unessential variables*

  If $S_z^{tot} << 1 \rightarrow f(x)$ does not depend on z so it can be fixed

  $f(x) \approx f(y, z_0) \rightarrow$ complexity reduction, from k to $k - k_z$ variables

ANOVA decomposition. Finding component functions

$$f(x) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + \ldots + f_{1,2,\ldots,n}(x_1, x_2, \ldots, x_n),$$

$$\int_0^1 f_{i_1 \cdots i_s}(x_{i_1}, , \ldots, x_{i_s}) dx_{i_k} = 0, \ \forall k, \ 1 \le k \le s$$

$$\int_0^1 f_v(x_v) f_u(x_u) dx = 0, \ \forall v \ne u.$$

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

$$f_i(x_i) = \int_{H^n} f(x) \prod_{j \ne i}^{n} dx_j - f_0,$$

$$f_{ij}(x_i, x_j) = \int_{H^n} f(x) \prod_{k \ne i, j}^{n} dx_k - f_i(x_i) - f_j(x_j) - f_0, \ldots$$

2^n integral evaluations

ANOVA decomposition. Test case

$$f(x_1, x_2) = f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2),$$

$$f(x_1, x_2) = x_1 x_2 \in H^2 \to f_0 = \frac{1}{4},$$

$$f_1(x_1) = \int_{H^n} f(x)\,dx_2 - f_0 = \frac{1}{2}x_1 - \frac{1}{4},$$

$$f_2(x_2) = \int_{H^n} f(x)\,dx_1 - f_0 = \frac{1}{2}x_2 - \frac{1}{4},$$

$$f_{12}(x_1, x_2) = x_1 x_2 - \frac{1}{2}x_1 - \frac{1}{2}x_2 + \frac{1}{4}.$$

$$S_1 = \frac{\int_{H^2} f_1^2(x_1)\,dx_1}{D} = \frac{3}{7},$$

$$S_2 = S_1 = \frac{3}{7},\ S_{12} = \frac{1}{7}.$$

$$S_1^{tot} = S_1 + S_{12} = \frac{4}{7},\ S_2^{tot} = S_2 + S_{12} = \frac{4}{7}$$

Evaluation of Sobol' Sensitivity Indices

Straightforward use of ANOVA decomposition requires

2^n integral evaluations – not practical !

There are efficient formulas for evaluation of Sobol' SI (Sobol' 2001):

$$S_y = \frac{1}{D}\left[\int_0^1 f(y,z')^2\, dydzdz' - f_0^2\right]$$

$$S_y^{tot} = \frac{1}{2D}\int_0^1 [f(y,z) - f(y',z)]^2\, dydzdz'$$

$$D = \int_0^1 f^2(y,z)\, dydz - f_0^2$$

Evaluation is reduced to high-dimensional integration by MC/QMC methods.

Definition of Sobol' SI for subsets

Consider two sets of variables : x=(y,z)

ANOVA decomposition:

$$f(y,z) = f_0 + g_1(y) + g_2(z) + g_{12}(y,z) \qquad (1)$$

$$\int g_1(y)dy = \int g_2(z)dz = \int g_{12}(y,z)dy = \int g_{12}(y,z)dz = 0 \qquad (2)$$

We square and integrate (1) and because of (2)

$$D = D_y + D_z + D_{yz}$$

Define

$$D_y^{tot} = D_y + D_{yz}$$

$$D_z^{tot} = D_z + D_{yz}$$

$$S_y = \frac{D_y}{D}, S_y^{tot} = \frac{D_y^{tot}}{D}$$

Formulas for the main effect Sobol' SI

$$S_y = \frac{1}{D}[\int_0^1 f(y,z')^2 dydz' - f_0^2] =$$

$$= \frac{1}{D}[\int_0^1 f(y,z) f(y,z') dydzdz' - f_0^2].$$

That is

$$D_y = [\int_0^1 f(y,z) f(y,z') dydzdz' - f_0^2]$$

We need to prove that

$$\int_0^1 f(y,z) f(y,z') dydzdz' = f_0^2 + D_y :$$

Recall that $D_y = \int g_1(y)^2 dy$

Derivation of formulas for the main effect Sobol' SI

$$D_y = [\int_0^1 f(y,z) f(y,z')dydzdz' - f_0^2]$$

$$\int_0^1 f(y,z) f(y,z')dydzdz' = \int dy \int f(y,z)dz \int f(y,z')dz'$$

$$= \int dy \left[\int f(y,z)dz \right]^2 = \int dy \left[\int (f_0 + g_1(y) + \cancel{g_2(z)} + \cancel{g_{12}(y,z)})dz \right]^2$$

$$= \int dy \left[\int (f_0 + g_1(y))dz \right]^2 = \int dy [f_0 + g_1(y)]^2$$

$$= f_0^2 + 2 f_0 \int \cancel{g_1(y)dy} + \int g_1(y)^2 dy = f_0^2 + D_y$$

Similarly

$$D_z = [\int_0^1 f(y,z) f(y',z)dydy'dz - f_0^2]$$

Derivation of formula for the total effect Sobol' SI

Jansen's formula (1994), Sobol (2001):

$$S_y^{tot} = \frac{1}{2D}\int_0^1 [f(y,z) - f(y',z)]^2 dydzdy',$$

$$D_y^{tot} = \frac{1}{2}\int_0^1 [f(y,z) - f(y',z)]^2 dydzdy'$$

$$= \frac{1}{2}\int_0^1 [f(y,z)]^2 dydz + \frac{1}{2}\int_0^1 [f(y',z)]^2 dy'dz - \int_0^1 f(y,z)f(y',z)dydy'dz$$

$$= \int_0^1 [f(y,z)]^2 dydz - (D_z + f_0^2) = D - D_z = (D_y + D_z + D_{yz}) - D_z = D_y + D_{yz}$$

Recall

$$D_z = [\int_0^1 f(y,z)f(y',z)dydy'dz - f_0^2],$$

$$\int_0^1 [f(y,z)]^2 dydz - f_0^2 = D$$

Evaluation of Sobol' Main Effect SI with small values

Original Sobol' formula:

$$\underline{x} = (y, z), \quad x' = (y', z')$$

using values $f(y, z), \quad f(y, z'), \quad f(y', z)$

$$S_y = \frac{1}{D} \int_0^1 f(y, z) f(y, z') \, dydzdz' - f_0^2$$

for small indices $S_y << 1$

$$\int_0^1 f(y, z) f(y, z') \, dydzdz' \approx f_0^2$$

$\rightarrow$ loss of accuracy

Improved formula for Sobol' Main Effect SI

Notice that $f_0^2 = \int_0^1 f(y,z)dydz \int_0^1 f(y',z')\ dy'dz'$

using values $f(y,z),\ \ f(y',z),\ \ f(y',z')$

$$S_y = \frac{1}{D}\int_0^1 f(y,z)f(y',z)\ dydy'dz - \ f_0^2 \rightarrow$$

$$S_y = \frac{1}{D}[\int_0^1 f(y',z')[f(y',z) - f(y,z)]\ dydy'dzdz'$$

--gives much more accurate results (Kucherenko, Mauntz, 2002)

Additional advantage (Saltelli 2002):

Requires $N(n+2)$ model evalution rather than

$N(2n+1)$ for original Sobol' formulas.

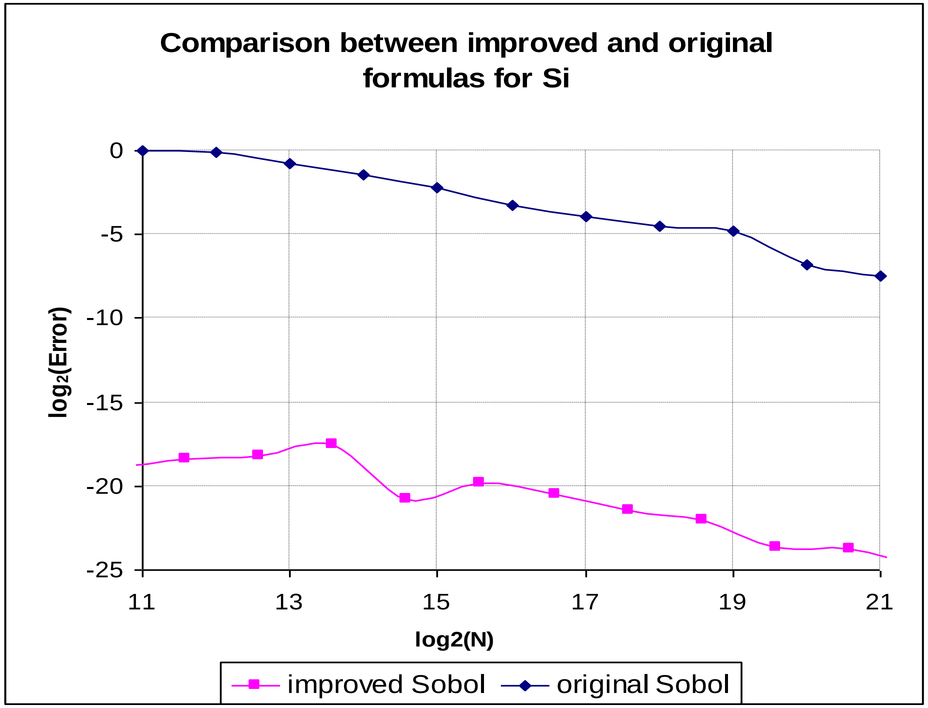
Further improvements: Sobol' and Mishetskaya 2007, A. Owen 2012

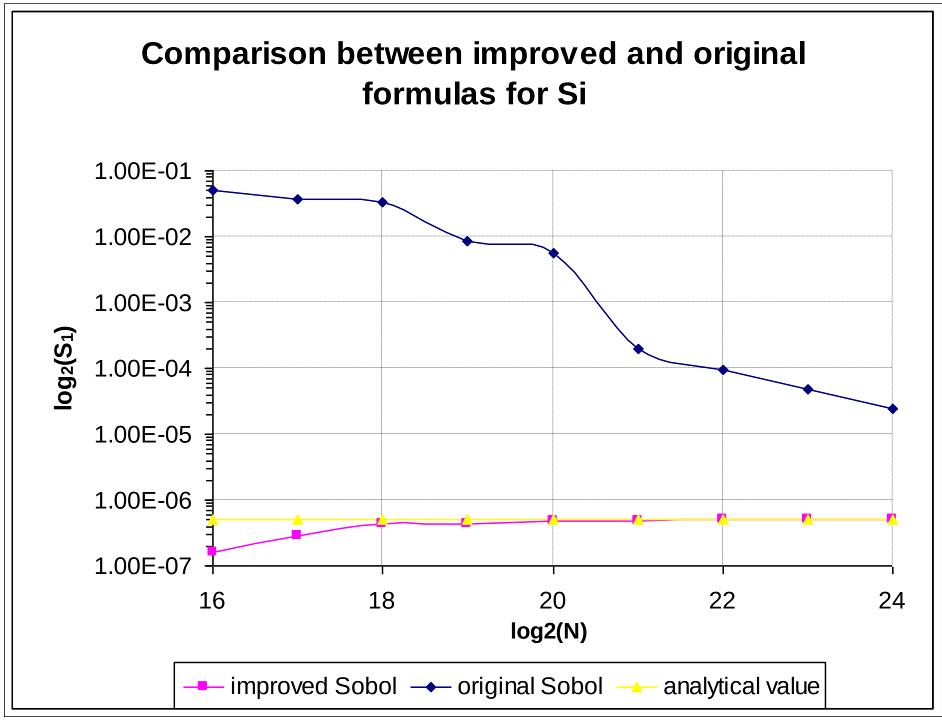
Saltelli 2002 - computation of second order indices at no extra costs.

Improved formula for Sobol' Main Effect SI

$$Test: f(x) = \sum_{i=1}^{n} i x_i\,,\quad S_i = S^T = \frac{6}{n(n+1)(2n+1)}$$

$$n = 180,\quad S_1 = 5.1\,10^{-7}$$





Improved formula have much higher convergence rate than the original Sobol' formula.

Evaluation of Sobol' Sensitivity Indices. Monte Carlo estimates

Main effect SI:

$$S_y = \frac{\frac{1}{N}\sum_{j=1}^{N} f\left(x_j^{'}\right)\left(f\left(y_j^{'}, z_j\right) - f\left(x_j\right)\right)}{D}$$

Total order effect SI:

$$S_y^T = \frac{\frac{1}{N}\sum_{j=1}^{N}\left(f\left(x_j\right) - f\left(y_j^{'}, z_j\right)\right)^2}{2D}$$

Each MC trial reqires three function values for $f(x), f(x'), f(y^{'}, z)$

The total number of function evaluations for a set $(S_i, S_i^T),\ i = 1, \ldots, n$

is equal to $N_F = N(n+2)$.

How to sample ?

Evaluation of Sobol' Sensitivity Indices. MC and QMC Sampling

To sample x and x' (they are vector points in H^n):

A. For Monte Carlo sample 2n random numbers

$$\xi_j = (\gamma_1^j, \gamma_2^j, ..., \gamma_n^j), \xi_j^{'} = (\gamma_{n+1}^j, \gamma_{n+2}^j, ..., \gamma_{2n}^j), \; j = 1, 2, ..., N$$

B. For Quasi Monte Carlo sample one

2n-dimensional quasi random number

$Q_j = (q_1^j, q_2^j, ..., q_{2n}^j)$ and split it into two points

$$\xi_j = (q_1^j, q_2^j, ..., q_n^j), \xi_j^{'} = (q_{n+1}^j, q_{n+2}^j, ..., q_{2n}^j), \; j = 1, 2, ..., N$$

How to use Sobol' sequence generators. MATLAB version

Specification (www.broda.co.uk) :

Successive calls to the function

SobolSeq(i,n)

generates an n- dimensional vector containing the Cartesian coordinates of the i-th point of the Sobol' sequence in the n- dimensional unit cube $[0,1]^n$.

Input parameters:

i - index of a point (i=[0,2**31-1]),

n - dimension of the Sobol' sequence;

Syntax:

r = SobolSeq(i,n)

How to use Sobol' sequence generators

To sample n independent inputs $x = (x_1, x_n, ..., x_n)$ in H^n

A. Monte Carlo: sample n random numbers $(\gamma_1^j, \gamma_2^j, ..., \gamma_n^j) = \xi_j, \ j = 1, 2, ..., N$

B. Quasi Monte Carlo: sample one n-dimensional quasi random vector

$\xi_j = (q_1^j, q_2^j, ..., q_n^j);$

to sample another vector - increase index $j \to j+1$.

Sets $\{q_k^j\}, \{q_p^j\}, j = 1, 2, ..., N, k \neq p$ (different dimensions) are independent;

Vectors $\xi_j = (q_1^j, q_2^j, ..., q_n^j), \xi_{j+1} = (q_1^{j+1}, q_2^{j+1}, ..., q_n^{j+1}),.. \ \ j = 1, 2, ..., N$ are dependent

INDEX	x1	X2	X3
1	0.5	0.5	0.5
2	0.25	0.75	0.25
3	0.75	0.25	0.75
4	0.125	0.625	0.875
5	0.625	0.125	0.375
6	0.375	0.375	0.625
7	0.875	0.875	0.125
8	0.0625	0.9375	0.6875

Different formulas for the main effect index

	D_y	Monte Carlo estimator
Sobol'	$\int f(x) f(y,z') dx dz' - f_0^2$	$\frac{1}{N}\sum_{k=1}^{N} f(y,z) f(y,z') - \left[\frac{1}{N}\sum_{k=1}^{N} f(y,z)\right]^2$
Kucherenko 2002	$\int f(x)[f(y,z') - f(x')] dx dx'$	$\frac{1}{N}\sum_{k=1}^{N} f(y,z)[f(y,z') - f(y',z')]$
Owen 2012	$\int [f(x) - f(y'',z)][f(y,z') - f(x')] dx dx' dx''$	$\frac{1}{N}\sum_{k=1}^{N} [f(y,z) - f(y'',z)][f(y,z') - f(y',z')]$
Sobol-Myshetzskay (Oracle) 2007	$\int [f(x) - \mu][f(y,z') - f(x')] dx dx' dx''$	$\frac{1}{N}\sum_{k=1}^{N} [f(y,z) - \mu][f(y,z') - f(y',z')]$

Comparison of computational costs

Method	Sobol'	S-K	Owen	Oracle
Number of function evaluations N_{CPU}	$N(2n+1)$	$N(n+2)$	$N(2n+2)$	$N(n+2)$

The root mean square error (RMSE) is determined using K independent runs

$$\boxed{\varepsilon_i\,(N) = \left[\frac{1}{K}\sum_{k=1}^{K}(S_i^{(n),k} - S_i^{(a)})^2\right]^{1/2}}$$

For QMC, the convergence rate is $\varepsilon_{QMC} = \dfrac{O(\ln N)^d}{N}$

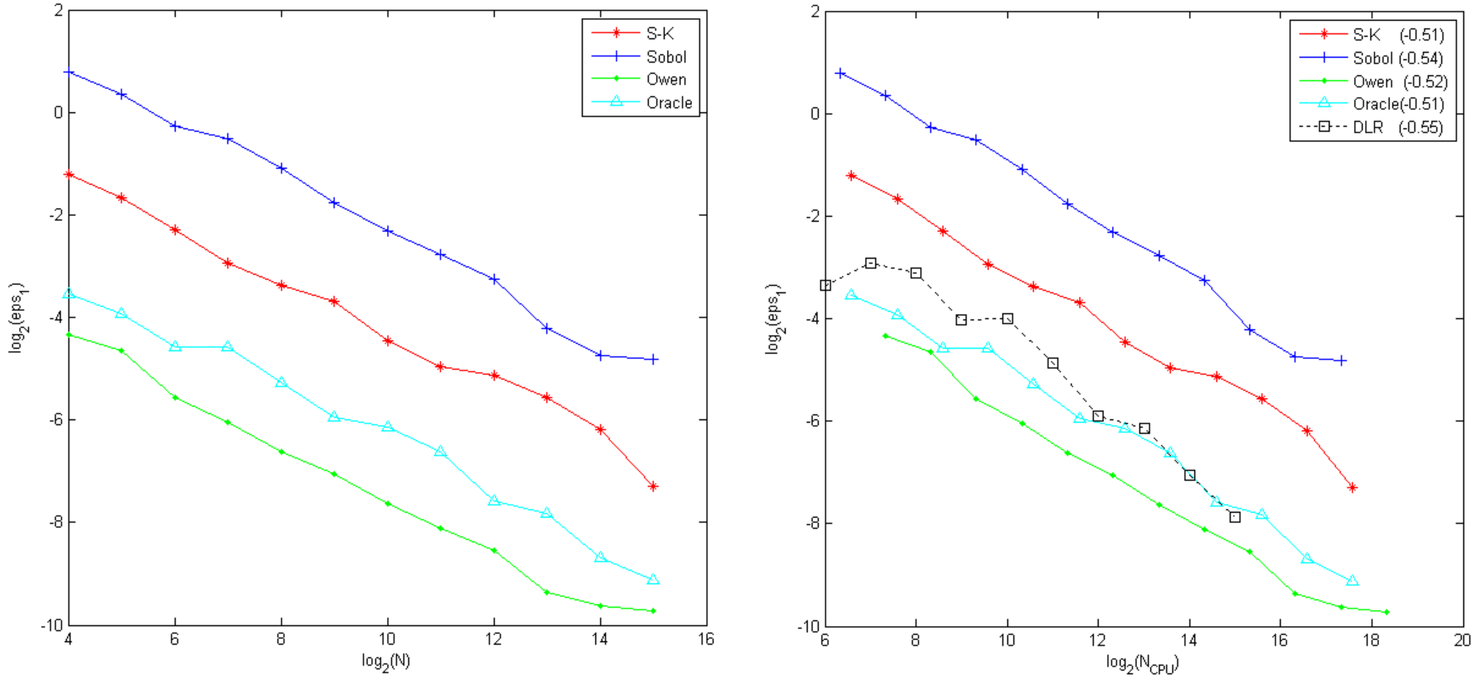
In practice, RMSE is approximated by $\boxed{cN^{-\alpha},\ 0<\alpha<1}$

Convergence significantly improves when using QMC (Sobol' sequences) sampling.

Comparison of different formulas

$$f(x) = a_1 x_1 + a_2 x_2 + \ldots + a_n x_n, \quad x_i \sim N(\mu_i, \sigma_i^2)$$

$$n = 4, \quad \mu = (1, 3, 5, 7), \quad \sigma = (1, 1.5, 2, 2.5), \quad a_i = 1, \ i = 1,2,3,4$$



Log2(RMSE) versus Lof2(N) for i=1, S1= 0.0741

Improved formulas have much higher convergence rate than the original Sobol' formula. Owen and Oracle - outperforming other methods

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