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The history of Derivative based Global Sensitivity Analysis: from DGSM to Active Subspaces

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Why so many published sensitivity analyses are false?

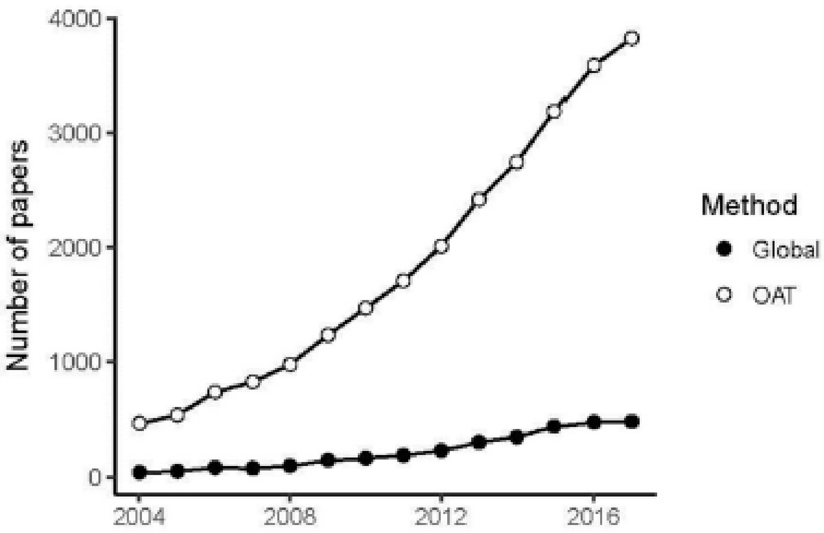


Fig. 7. Results from Ferretti et al., extended to 2016 (present paper).

- Model $y = f(x)$, $x = \{x_1, \dots, x_n\}$, $f(x) \in C(H^n)$
- Local sensitivity (OAT): partial derivative $\partial y / \partial x_i$ at a nominal point x^*
- If f is nonlinear, $\partial y / \partial x_i$ varies across x_i.
- With input interactions, $\partial y / \partial x_i$ depends on other factors.
- Partial derivatives are only reliable for linear models.

Saltelli, A., Aleksankina, K., Becker, W., Fennell, P., Ferretti, F., Holst, N., ... & Wu, Q. (2019). Why so many published sensitivity analyses are false: A systematic review of sensitivity analysis practices. *Environ. modelling & software*, *114*, 29-39.

Derivative-Based ↔ Variance-Based Sensitivity Measures: A Mathematical Bridge

Derivative-Based methods

$$S_i \leq C_i \cdot E\left[\left(\frac{\partial f}{\partial x_i}\right)^2\right]$$

Variance-based methods

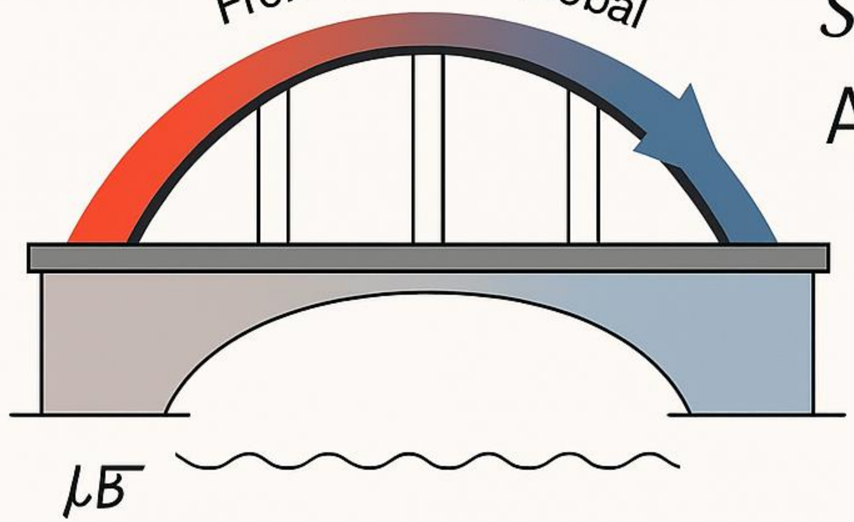
$$\frac{df}{\partial x_i} = \frac{\rho}{\sqrt{f}}$$

Derivative indices

Elementary effects

$\mu \rightarrow e$

Elementary effects

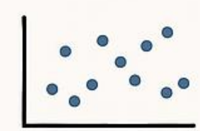


S_i $S_{obol'}$

A

ANOVA

Total effects



Sobol' indices

Derivative-based methods (e.g. DGSM) provide bounds or approximations for variance-based indices (e.g. Sobol').

Outline

1. Local Derivatives & Morris method

2. Derivative based Global Sensitivity Measures (DGSM)
- Upper bounds & Lower bounds
- For groups of variables
- Based on Crossed Derivatives
- For arbitrary input distributions

3. Computing of DGSM

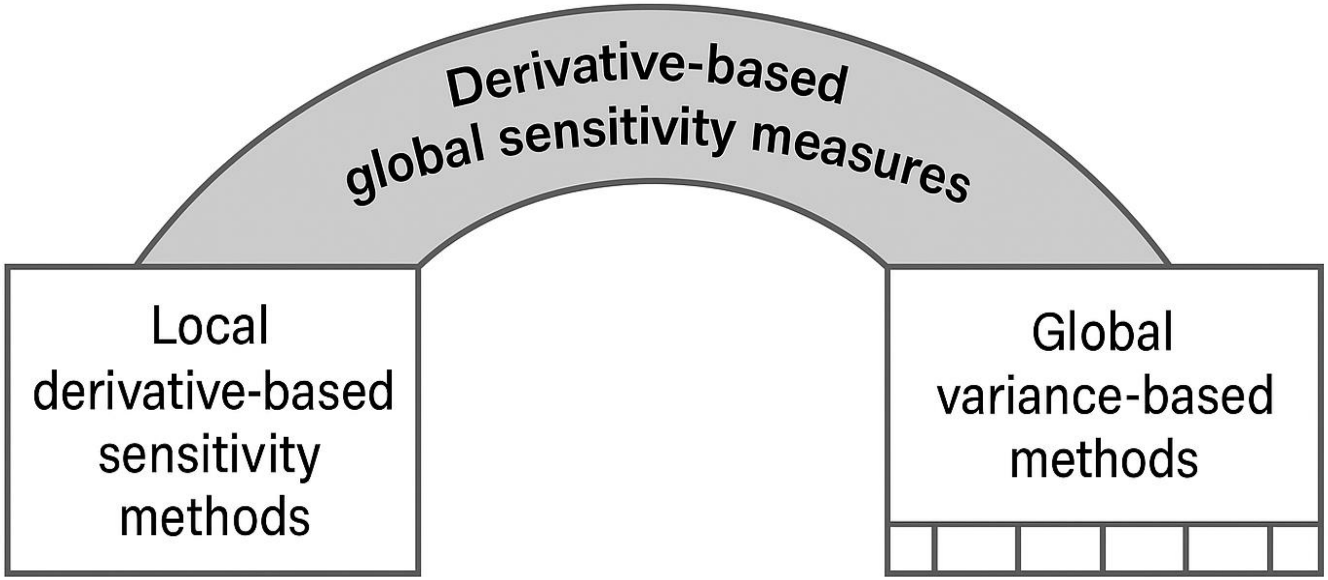
4. Effective dimensions

5. Active Subspaces

6. Derivative-based Shapley value

7. Other applications

The Bridge between local and global measures



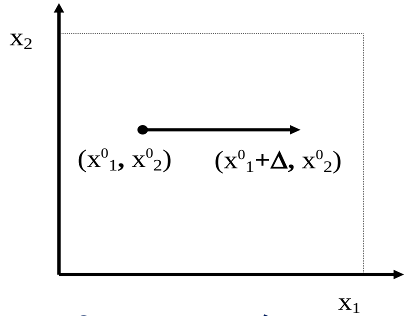
Pros and Cons of Variance-based Sensitivity Indices

Pros: Variance-based sensitivity (Sobol') indices offer a comprehensive approach to the model analysis.

Cons: Generally require a large number of function evaluations to achieve convergence -> become impractical for complex high dimensional problems.

Practical Alternative: Screening methods

Morris screening method



Model $f(x) \in C(H^n)$

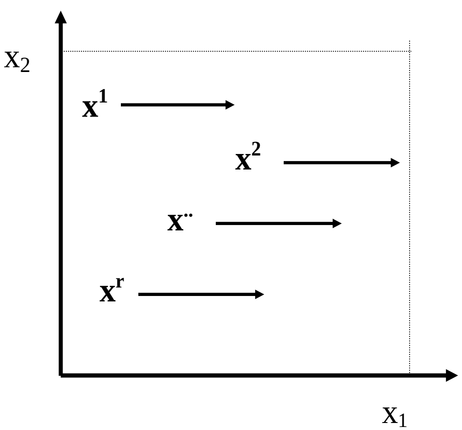
Elementary Effect for the i^{th} factor at $x°$

$$EE_i(x_1^0, \dots, x_k^0) = \frac{f(x_1^0, x_2^0, \dots, x_{i-1}^0, x_i^0 + \Delta, x_{i+1}^0, \dots, x_n^0) - f(x_1^0, \dots, x_n^0)}{\Delta}$$

r elem. effects EE^1_i EE^2_i … EE^r_i are computed at randomly chosen X^1 , … , X^r from the fixed grid (levels)

Average of {EE_i} → $\mu_i = \frac{1}{r}\sum_{j=1}^{r} EE_i^{(j)}$

Standard deviation of {EE_i} → σ_i



To avoid cancelation effect*:

Average of |EE_i| → $\mu_i^* = = \frac{1}{r}\sum_{j=1}^{r} |EE_i^{(j)}|$

Campolongo F, Cariboni J, Saltelli A. Environ Modell Software, 2007;22)

Derivative based Global Sensitivity Measures : DGSM

1. Morris measure in the limit $\Delta \to 0$

$$E_i(x_1^0, \dots, x_n^0) = \lim_{\Delta \to 0} EE_i(x_1^0, \dots x_n^0) = \frac{\partial f}{\partial x_i}$$

2. Bridging the Gap: From Discrete sum to an integral:

L_1-based global sensitivity measures (DGSM) [1]:

$$M_i^* = \int_{H^n} |E_i| dx, \quad \bar{\Sigma}_i^* = \left[\int_{H^n} (|E_i| - \bar{M}_i^*)^2 \, \mathrm{d}x\right]^{1/2}$$

L_2-based DGSM: $$v_i = \int_{H^n} \left(\frac{\partial f}{\partial x_i}\right)^2 dx$$

Alternative global sensitivity measure ($G_i = v_i$) [2]: $\bar{G}_s = \frac{\sum_{i=1}^{s} G_i}{\sum_{i=1}^{n} G_i}$

[1] Kucherenko S., Rodriguez-Fernandez M., Pantelides C., Shah N.. (2009) Monte Carlo evaluation of derivative based global sensitivity measures. Reliab Eng Syst Saf, 94(7).

[2] Sobol' I, Gresham A. On an altenative global sensitivity estimators. In: Proceedings of SAMO, Belgirate, 1995.

Pros and Cons of DGSM

Questions:

Are DGSM less CPU time demanding than variance based?

Do they have a link with Sobol’ sensitivity indices ?

How can they be used ?

Derivative based global sensitivity measures. Upper and Lower bounds

Theorem 1. Assume that $c \le \left|\frac{\partial f}{\partial x_i}\right| \le C$. $D-$ total variance. Then

$$\frac{c^2}{12D} \le S_i^{tot} \le \frac{C^2}{12D}$$

Proof:

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

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

where is $\hat{x}$ a point between x and $\overset{\circ}{x}$

Sobol' I.M., Kucherenko S. (2009) Derivative based Global Sensitivity Measures and their link with global sensitivity indices, Math. and Comp. in Simul., 79(10) 3009-3017

Derivative based global sensitivity measures. Upper bounds

$$f(x) \in C(H^n), \left\{\frac{\partial f(x)}{\partial x_i}\right\} \in L^2(H^n), \forall i = 1, \dots, n$$

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

$$w_i^{(m)} = \int_{H^n} x_i^m \frac{\partial f(x)}{\partial x_i} dx, m > 0$$

$$\varsigma_i = \frac{1}{2}\int_{H^n} x_i(1 - x_i)\left(\frac{\partial f(x)}{\partial x_i}\right)^2 dx$$

Consider the full set of derivative based measures:

$$\Upsilon_i = \left\{v_i, w_i^{(m)}, \varsigma_i\right\}, m > 0$$

Derivative based global sensitivity measures ν_i. Proof components

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

denote the sum of all terms in ANOVA that depend on x_i:

$$u_i(x) = f_i(x_i) + \sum_{j=1, j\neq i}^{n} f_{ij}(x_i, x_j) + \cdots + f_{12\cdots d}(x_1, \cdots, x_n)$$

Obviously $\int_{H^n} u_i(x)dx = 0.$

Denote $z = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$ the vector of all variables but x_i,

then $x \equiv (x_i, z)$ and $f(x) \equiv f(x_i, z)$.

$$f(x) = u_i(x_i, z) + V(z), \qquad \frac{\partial f}{\partial x_i} = \frac{\partial u_i}{\partial x_i}$$

Derivative based global sensitivity measure ν_i. Upper bound UB1

Theorem UB1. $S_i^{tot} \le \frac{\nu_i}{\pi^2 D}$

Proof:

$$D_i^{tot} = \int_{H^n} u_i^2(x)dx\,; \quad \frac{\partial f}{\partial x_i} = \frac{\partial u_i}{\partial x_i}$$

Using $\int_0^1 u_i^2(x)dx_i \le \frac{1}{\pi^2}\int_0^1 \left(\frac{\partial u_i}{\partial x_i}\right)^2 dx_i \rightarrow$

$$UB1 = \frac{\nu_i}{\pi^2 D}$$

Small ν_i corresponds to small S_i^{tot}

Derivative based global sensitivity measure ζ_i. Upper bound UB2

Theorem UB2. $S_i^{tot} \le \frac{\varsigma_i}{D}$

Proof:

$$\varsigma_i = \frac{1}{2}\int_{H^n} x_i(1-x_i)\left(\frac{\partial f(x)}{\partial x_i}\right)^2 dx$$

$$= \frac{1}{2}\int_0^1 x_i(1-x_i)(u_i')^2 dx$$

Using $\int_0^1 u_i^2 dx \le \frac{1}{2}\int_0^1 x(1-x)\left(\frac{\partial u_i}{\partial x_i}\right)^2 dx$

$$UB2 = \frac{\varsigma_i}{D}$$

S. Kucherenko, S. Song (2014) DGSM and their link with Sobol' sensitivity indices. Monte Carlo and Quasi-Monte Carlo Methods 2014, Springer Proc. in Mathematics & Statistics

DGSM. Lower bound LB1

Theorem LB1.

$$\frac{\left(\int_{H^n} [f(1,z)-f(0,z)][f(1,z)+f(0,z)-2f(x)]dx\right)^2}{4v_i D} < S_i^{tot}$$

Proof:

Using Cauchy−Schwarz inequality

$$\left(\int_{H^n} u_i(x)\frac{\partial u_i(x)}{\partial x_i}dx\right)^2 \le \int_{H^n} u_i^2(x)dx \cdot \int_{H^n}\left(\frac{\partial u_i(x)}{\partial x_i}\right)^2 dx \rightarrow \square$$

$$\text{LB1} = \frac{\left(\int_{H^d} [f(1,z)-f(0,z)][f(1,z)+f(0,z)-2f(x)]dx\right)^2}{4v_i D}$$

Derivative based global sensitivity measures. Lower bound LB2

Theorem LB2.

$$\gamma(m) = \frac{(2m+1)\left[\int_{H^n} (f(1,z) - f(x))dx - w_i^{(m+1)}\right]^2}{(m+1)^2 D} < S_i^{tot}$$

Proof: $w_i^{(m)} = \int_{H^n} x_i^m \frac{\partial f(x)}{\partial x_i} dx = \int_{H^n} x_i^m \frac{\partial u_i(x)}{\partial x_i} dx, m > 0$

Using $\left(\int_{H^n} x_i^m u_i(x) dx \right)^2 \leq \int_{H^n} x_i^{2m} dx \cdot \int_{H^n} u_i^2(x) dx \rightarrow \square$

At $m^* = \arg\max(\gamma(m))$, we can get $LB2 = \gamma^*(m^*)$.

$$LB^* = \mathrm{Max}\{LB1, LB2\}$$

DGSM for groups of variables

Consider an arbitrary subset y of $x = (x_1, \dots, x_n)$

$y = (x_{i_1}, \dots, x_{i_s}), 1 \le s < n,$ the decomposition $\rightarrow x = (y, z)$

$$D_y^{tot} = \frac{1}{2} \int [f(y', z) - f(x)]^2 dx dy'$$

Consider the Taylor expansion

$$f(y', z) - f(x) = \sum_{p=1}^{s} \frac{\partial f(x)}{\partial x_{i_p}} (x'_{i_p} - x_{i_p}) + \dots$$

Sobol' I.M., Kucherenko S. (2010) A new derivative based importance criterion for groups of variables and its link with the global sensitivity index S_total. Comp. Physics Comm., 181(7)

DGSM for groups of variables. τ_y

Consider an arbitrary subset y of $x = (x_1, \dots, x_n)$
$y = (x_{i_1}, \dots, x_{i_s}), 1 \le s < n,$ the decomposition $x = (y, z)$

$$\tau_y = \sum_{p=1}^{s} \int \left(\frac{\partial f(x)}{\partial x_{i_p}} \right)^2 \frac{1 - 3x_{i_p} + 3x_{i_p}^2}{6} dx$$

Theorem 1G. A general inequality holds

$$S_y^{tot} \le \frac{24}{\pi^2} \frac{\tau_y}{D}.$$

For $f(x)$ linear with respect to $x_{i_1}, \dots, x_{i_s}$ $S_y^{tot} = \frac{\tau_y}{D}$.

Sobol' I.M., Kucherenko S. (2010) A new derivative based importance criterion for groups of variables and its link with the global sensitivity index S^{tot}. Comp. Physics Comm., 181(7)

Factor fixing

Assume, that $v_i \ll \varepsilon$, then $S_i^{tot} \ll \varepsilon$. How can we use this information ?

Theorem δ*. Consider fixing $x_i = x_i^0$, then the function approximation error

$$\delta(x_i^0) = \frac{\int \left|f(x,y) - f\left(x_{\sim i}, x_i^0, y\right)\right|^2 dxdy}{D}$$

$$E[\delta(x_i^0)] = 2\, S_i^{tot}.$$

If $S_z^{\text{tot}} \ll \varepsilon \rightarrow \delta(z^0) \ll \varepsilon, \quad z$ can be fixed at z^0 :

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

Small values of DGSM always imply small values of S^{tot}.

DGSM can be used for fixing unimportant variables.

**Sobol, I.M., S. Tarantola, D. Gatelli, S.S. Kucherenko, W. Mauntz (2007) Estimating the Approximation Error when fixing Unessential Factors in Global Sensitivity Analysis, Reliab Eng Syst Saf 92(7): 957-960, 2007*

DGSM for functions with random variables

$x = (x_1, \ldots, x_n) \in R^n$, independent r.v. with its measure

$$dF(x) = \prod_{k=1}^{n} dF_k(x_k)$$

$$v_i = \int_{R^n} \left(\frac{\partial f(x)}{\partial x_i}\right)^2 dF(x)$$

$$w_i = \int_{R^n} \frac{\partial f(x)}{\partial x_i} dF(x)$$

Further assume $x_i \sim N(a_i; \sigma_i)$:

Theorem 1N:

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

S. Kucherenko, S. Song (2014) DGSM and their link with Sobol' sensitivity indices. Monte Carlo and Quasi-Monte Carlo Methods 2014, Springer Proc. in Mathematics & Statistics

Test 1: Linear function

$$f(x) = a(z)x_i + b(z), \qquad f(x) \in C(H^n)$$

$$D_i^{tot} = \frac{1}{12}\int_{H^{n-1}} a^2(z)dz$$

Upper bounds :

$$v_i = \int_{H^{n-1}} a^2(z)dz \longrightarrow UB1 = \frac{v_i}{\pi^2 D} \approx 1.22 S_i^{\text{tot}}\, ; UB2 = S_i^{\text{tot}}$$

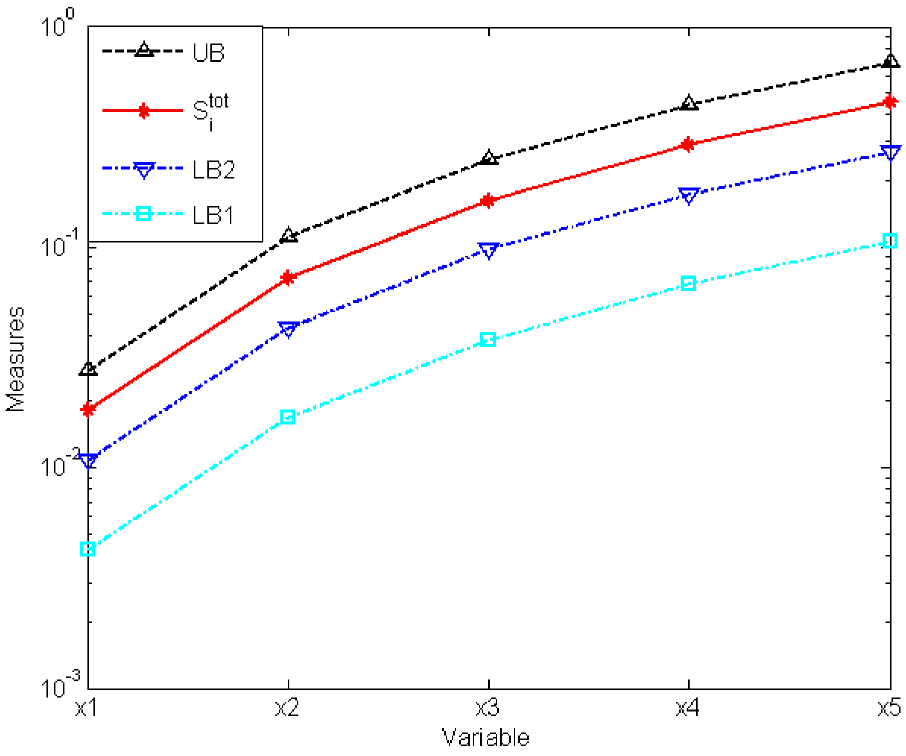
Lower bounds :

$$\left.\begin{array}{c} LB1 = 0 \\ LB2 = \gamma(m) = \dfrac{(2m+1)m^2\left(\int_{H^{d-1}} a(z)dz\right)^2}{4(m+2)^2(m+1)^2 D} \\ \text{at } m^* = 3.745 \end{array}\right\} \longrightarrow LB^* \approx 0.48 S_i^{\text{tot}}$$

Test 2: Ellipsoidal function

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} i x_i^2$$

$$n = 5, \qquad x_i \in [0,1]$$



Tight bounds around S^{tot}

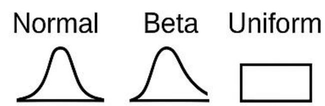
Other Derivative-Based Global Sensitivitiy Measures

Crossed Derivatives ($\ddot{\upsilon}_{ij}$)

$$\frac{\partial^2 f}{\partial x_{cj}}$$

Higher-order interaction screening

DGSM with Arbitrary Distributions



$$D_i \leq C_P E|\left|\frac{\partial f}{\partial x_i}\right|^2$$

Second-Type DGSM (ξ_t)

Euler-Lagrange analysis

DGSM for arbitrary input distributions

- $f(x),\ x = (x_1, \dots, x_n)$ are independent R.V. with CDF $F_1(x_1), \dots, F_p(x_n)$ such that
- Poincaré Inequality:

$$\int f(x)^2 dF(x) \leq C(F) \int \ \| \nabla f(x) \|^2 \, dF(x)$$

is satisfied. Here $C(F)$ is the Poincaré constant.

Theorem*: S_i^{tot} are bounded by DGSM ν_i :

$$D_i^{tot} \leq C(F_i)\nu_i$$

With

$$C(F_i) = 4\left[\sup_{x \in \mathbb{R}} \frac{\min(F_i(x), 1 - F_i(x))}{\rho_i(x)}\right]^2$$

- Analytical $C(F_t)$ for some distributions: normal, exponential, Beta, Gamma, Gumbel*.

**Lamboni et al (2013), Roustant et al. (2014), Roustant et al (2017).*

DGSM Based on Crossed Derivatives

- Crossed-DGSM Definition:

$$\nu_{i,j} = \int \left(\frac{\partial^2 g(x)}{\partial x_i \partial x_j}\right)^2 dF(x)$$

- Superset Importance:

$$\mathrm{D}_{i,j}^{\text{super}} = \sum_{I \supseteq \{i,j\}} D_I$$

- Theorem: For $\forall \ \{i,j\}$:

$$\mathrm{D}_{i,j} \leq \mathrm{D}_{i,j}^{\text{super}} \leq C(F_i)C(F_j)\nu_{i,j}$$

- Application: Enables detection of non-interacting variable pairs. Higher-Order Interactions Screening

Roustant et al. (2014), Muehlenstaedt & Roustant (2012), Liu & Owen (2006).

DGSM of the second type

Song et al. (2019): $\zeta_t = \int_{R^p} A(x_t)\left(\frac{\partial f(x)}{\partial x_t}\right)^2 dF(x)$

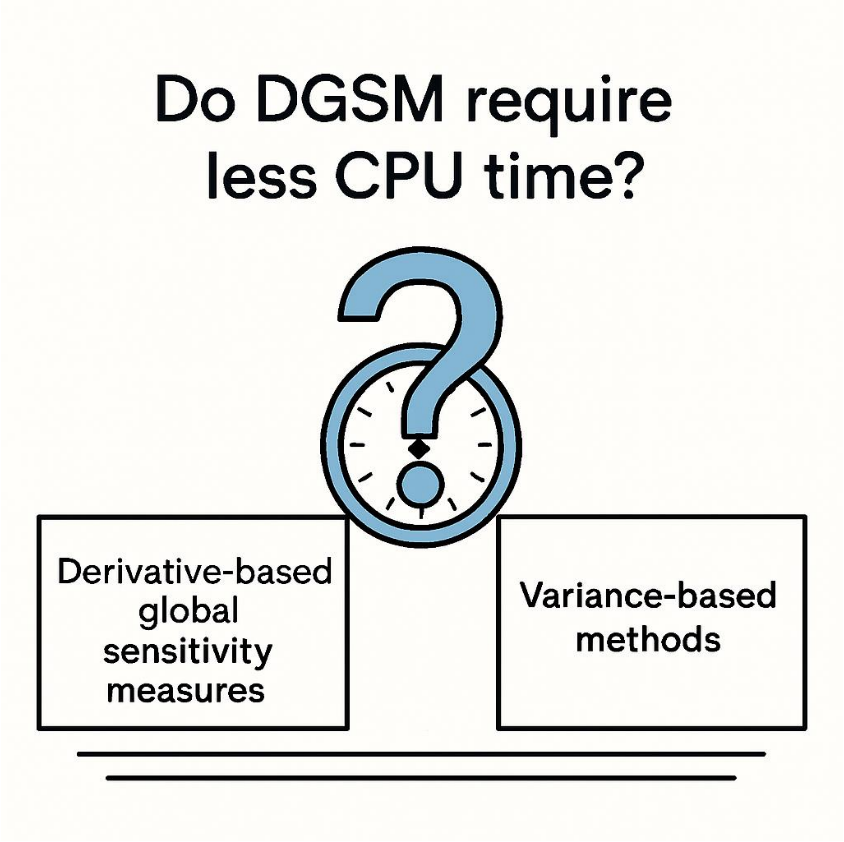
Using the calculus of variations based on the Euler-Lagrange equation:

$$S_t^{tot} \le \frac{\zeta_t}{D}$$

$$A(x_t) = \frac{1}{\rho(x_t)}\left[\int_{RP} (\mu_t - x_t)dF(x) + C\right]$$

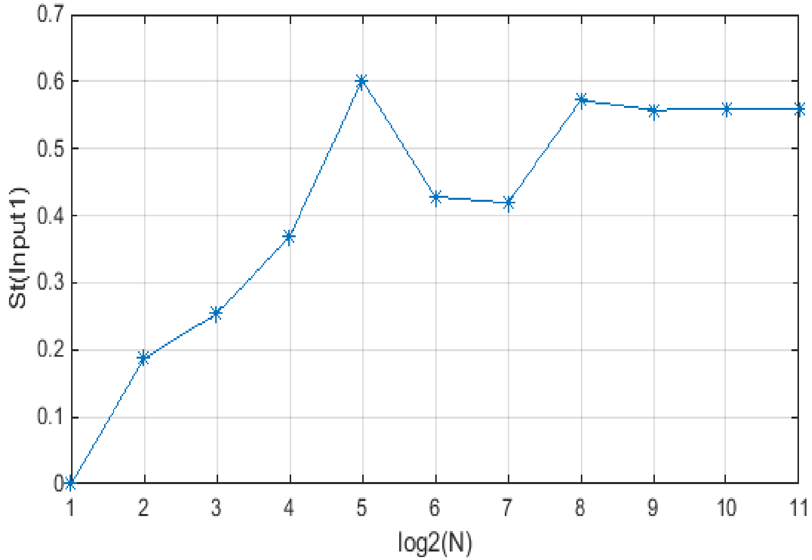
Distribution	PDF	$A(x_t)$
Exponential $E(\lambda)$	$\lambda e^{-\lambda x}, \quad x > 0, \ \lambda > 0$	$\frac{1}{\lambda} x_t$
Beta $B(\alpha,\beta)$	$\frac{x^{\alpha-1}(1-x)^{-1}}{B(\alpha,\beta)}, \quad 0 < x < 1, \ \alpha,\beta > 0$	$\frac{x_t(1-x_t)}{\alpha+\beta}$
Gamma $\Gamma(\alpha,\beta)$	$\frac{1}{\Gamma(\alpha)\beta^{\alpha}} x^{\alpha-1} e^{-\frac{1}{\beta}x}, \quad x > 0, \ \alpha,\beta > 0$	βx_t
Triangular $T(a,c,b)$	$\begin{cases} \frac{2(x-a)}{(b-a)(c-a)}, a < x < c \\ \frac{2(b-x)}{(b-a)(b-c)}, c < x < b \end{cases}$	$\frac{1}{-a}\left[-\frac{1}{3}x_t^3 + \frac{1}{2}(\mu_1 + a)x_t^2 - \mu_1 a x_t + K_1\right], a < x_t$ $\frac{1}{-x_t}\left[\frac{1}{3}x_t^3 - \frac{1}{2}(\mu_2 + b)x_t^2 + \mu_2 b x_t + K_2\right], c < x_t <$
Uniform $U(a,b)$	$\frac{x-a}{b-a}, a < x < b$	$\frac{(x_t-a)(b-x_t)}{2(b-a)}$
Normal $N(\mu,\sigma^2)$	$\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, -\infty < x < +\infty$	σ^2

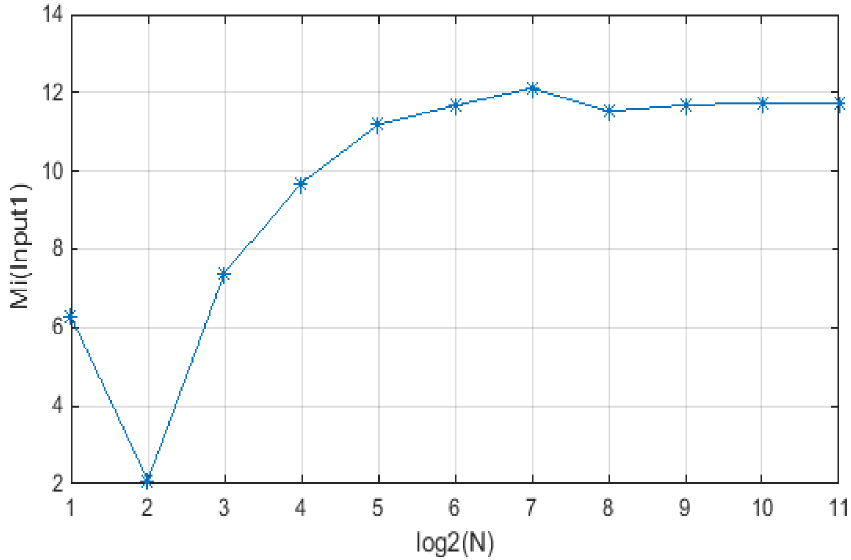
II. Computing of DGSM



Comparison of Convergence: Sobol' sensitivity indices versus DGSM

$$Y = f(X_1, X_2, X_3) = \sin(\pi X_1) + 7\sin(\pi X_2)^2 + 0.1(\pi X_3)^4 \sin(\pi X_1)\,,X_i \in [0,1]$$





Speed up 10 times -> Convergence of DGSM is typically a several times than that for S^{tot}

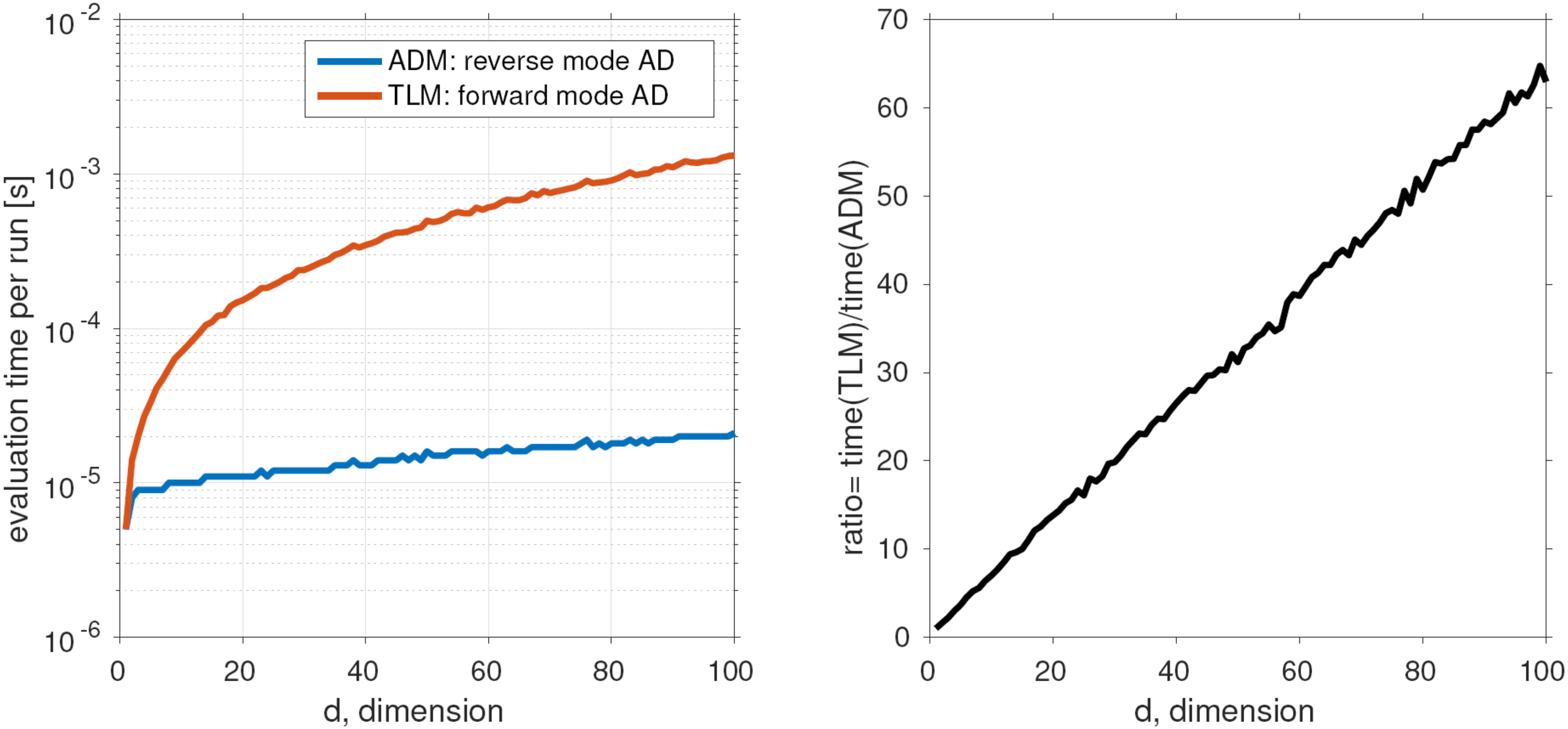
Computational cost: $S^{tot} = N*(n+2) * CPU_F$

DGSM (with numerical diff.) = $N*(n+1) * CPU_F$

DGSM (with algorithmic differentiation) = $5 * CPU_F$

It is independent of the number of inputs *n* !

DGSM with Algorithmic differentiation



Adjoint Algorithmic Differentiation AAD Not to Be Confused With
Symbolic differentiation (computation of derivatives accurately using the code structure)

C. Molkenthin, F. Scherbaum, A. Griewank, H. Leovey, S. Kucherenko, F. Cotton (2017) Derivative-based global sensitivity analysis: Upper bounding of sensitivities in seismic hazard assessment using automatic differentiation, Bulletin of the Seismological Society of America, 107(2), 984.

Computing DGSM using metamodels

1. Polynomial Chaos Expansions (PCE) represents $Y = f(\mathrm{X}), Y \in L^2$ as:

$$Y = \sum_{j=0}^{\infty} a_j \phi_j(\mathrm{X})$$

$\{\phi_j\}$ are orthonormal polynomials (w.r.t. the input distribution of X).

*PCE enables analytical DGSM computation with no extra simulations.

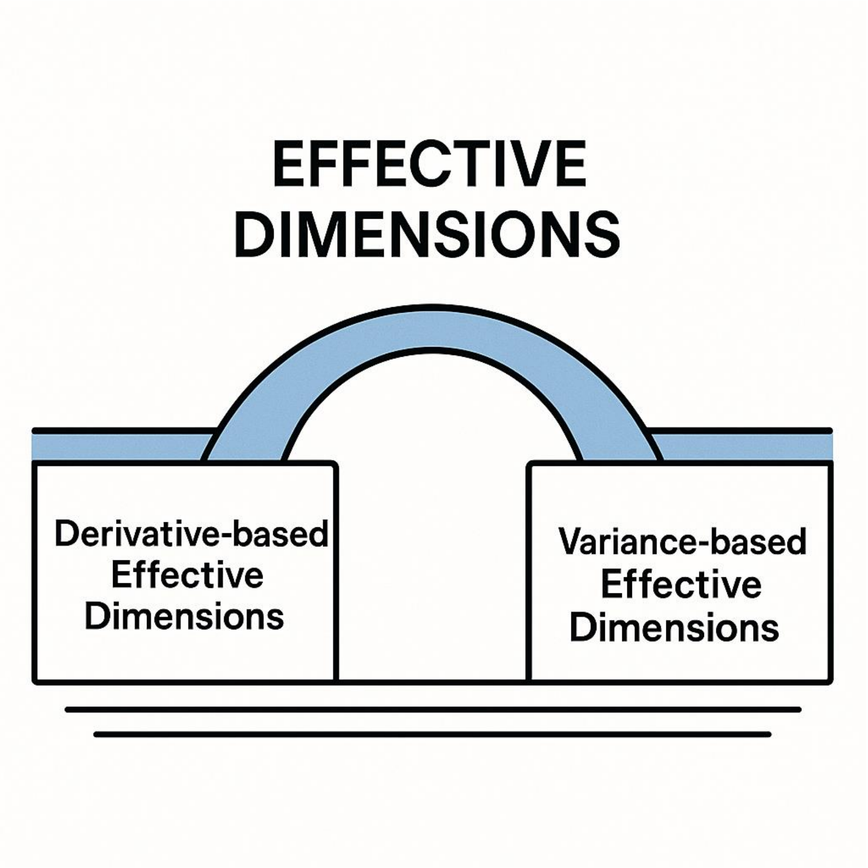
DGSM for PCE based on Hermite, Legendre, Laguerre polynomials are derived explicitly*.

*Sudret, B., Mai, C. V. (2015). Computing derivative-based global sensitivity measures using polynomial chaos expansions. *Reliability Eng. & Syst. Safety*, *134*, 241-250.

2. Computing DGSM using a Gaussian process metamodel:

De Lozzo, M., & Marrel, A. (2016). Estimation of the derivative-based global sensitivity measures using a Gaussian process metamodel. SIAM/ASA Journal on Uncertainty Quantification, 4(1), 708-738

III. Effective dimensions. Classification of functions



Effective dimensions

Let |u| be a cardinality of a set of variables $u, \varepsilon \backsimeq 0.01$

Define Sobol′ indices $S_u = D_u / D$.

The effective dimension of $f(x)$ in the superposition sense is the smallest integer d_S such that $\sum_{0<|u|\leq d_S} S_u \geq 1-\varepsilon$

It means that $f(x)$ is almost a sum of d_S−dimensional functions.

The function $f(x)$ has the effective dimension in the truncation sense d_T if

$$\sum_{u \subseteq \{1,2,\ldots,d_T\}} S_u \geq 1-\varepsilon$$

Example 1 : $f(x) = \sum_{i=1}^{n} x_i \ , \ \ x_i \sim U[0,1] \rightarrow d_S = 1, d_T = n$

Example 2 : $f(x) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{i} \sum_{j>i} f_{ij}(x_i, x_j) \rightarrow d_S = 2, d_T = n$

Classification of functions

Type A. Variables are not equally important

$$\frac{S_y^T}{n_y} >> \frac{S_z^T}{n_z} \leftrightarrow d_T << n$$

Type B,C. Variables are equally important

$$S_i \approx S_j \leftrightarrow d_T \approx n$$

Type B.
Dominant low order terms

$$\sum_{i=1}^{n} S_i \approx 1 \leftrightarrow d_S << n$$

Type C. Dominant higher order terms

$$\sum_{i=1}^{n} S_i << 1 \leftrightarrow d_S \approx n$$

Kucherenko S., Feil B., Shah N., Mauntz W. The identification of model effective dimensions using global sensitivity analysis Reliab. Eng. Syst. Saf. 96 (2011) 440–449

Classification of functions. Efficiencies of MC/QMC/LHS

Function type	Description	Relationship between S_i and S_i^{tot}	d_T	d_S	QMC is more efficient than MC	LHS is more efficient than MC
A	A few dominant variables	$S_y^{tot}/n_y >> S_z^{to} / n_z$	$<< n$	$<< n$	Yes	No
B	No unimportant subsets; only low-order interaction terms are present	$S_i \approx S_j, \forall\ i, j$ $S_i / S_i^{tot} \approx 1, \forall\ \mathrm{i}$	$\approx n$	$<< n$	Yes	Yes
C	No unimportant subsets; high-order interaction terms are present	$S_i \approx S_j, \forall\ i, j$ $S_i / S_i^{tot} << 1, \forall\ i$	$\approx n$	$\approx n$	No	No

S. Kucherenko, D. Albrecht, A. Saltelli, Exploring multi-dimensional spaces: a Comparison of Latin Hypercube and Quasi Monte Carlo Sampling Techniques, 2015 arXiv:1505.02350

Derivative based effective dimension

Recall: $f(x)$ has the effective dimension in the truncation sense d_T if

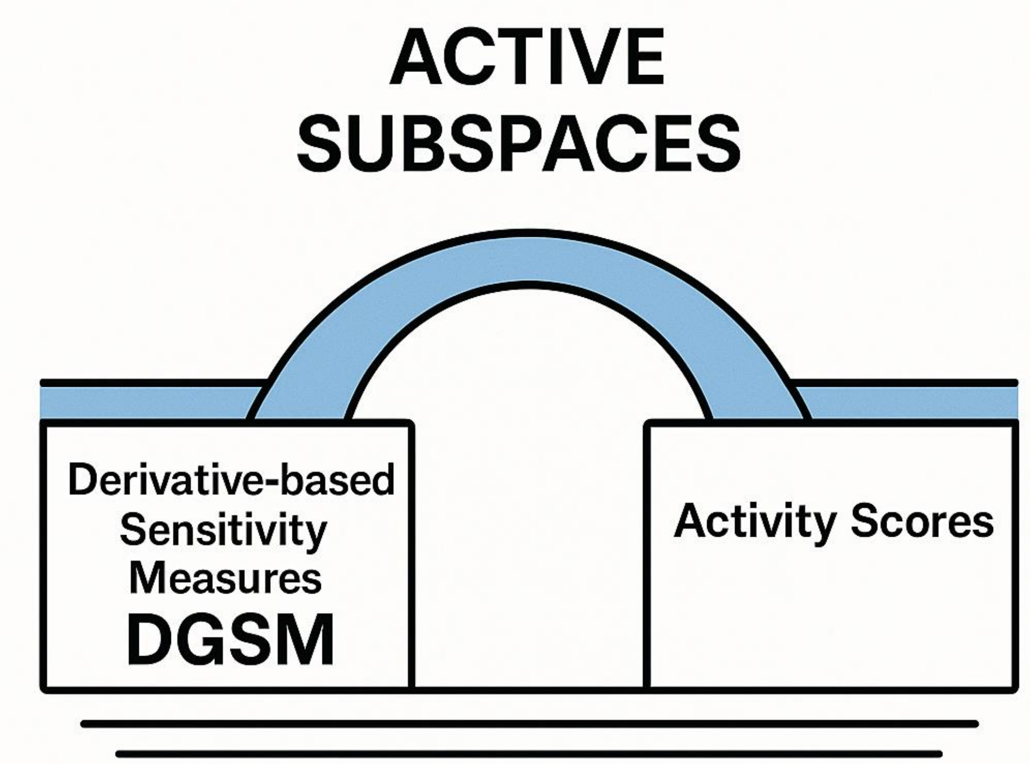
$$\sum_{u \subseteq \{1,2,\ldots,d_T\}} S_u \geq 1 - \varepsilon$$

Theorem*: If there exists an integer m such that

$$\frac{1}{\pi^2 D} \sum_{j=m+1}^{n} v_j \leq \varepsilon,$$

then the effective dimension in the truncation sense $d_T \leq m$; $\varepsilon \backsimeq 0.01$

**Jansen, K., Leovey, H., Ammon, A., Griewank, A., & Müller-Preussker, M. (2014). Quasi-Monte Carlo methods for lattice systems: a first look. Comp. Physics Comm., 185*(3)


ACTIVE
SUBSPACES
Derivative-based
Sensitivity
Measures
DGSM
Activity Scores

Active Subspaces

$f(x) \in \mathrm{C}^1$, R. V. $x \in \mathbb{R}^n$, $x \sim p(x)$, $\left\{\frac{\partial f(x)}{\partial x_i}\right\} \in L^2, \forall i = 1, \dots, n$

Compute matrix $C = \int \nabla f(x) \nabla f(x)^T \rho(x) dx$

Find eigenvalue decomposition: $C = W \Lambda W^T$,

$\Lambda = diag(\lambda_1, \dots \lambda_d)$, $\lambda_1 \geq \cdots \geq \lambda_d$ are eigenvalues,
W - orthogonal matrix of eigenvectors in $\mathbb{R}^n$.

If there is a large gap between $\{\lambda_1, \dots, \lambda_k\}$ and $\{\lambda_{k+1}, \dots, \lambda_n\}$,

find a partition $\Lambda = \begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix}$, $W = [W_1 \ \ W_2]$,

W_1 - eigenvectors of the top k eigenvalues ($k \ll n$), dim (W_1)=*n x k*

Their span is called the “active subspace” (AS) .

Constantine, P.G.: Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies. SIAM (2015)

Active Subspaces. Link with DGSM

$x = WW^T x = W_1 y + W_2 z,$

$y = W_1^T x$, $y \in \mathbb{R}^k$ - active variables,
z $= W_2^T x,$ z $\in \mathbb{R}^{n-k}$ – inactive variables

Approximate $f(x)$: $f(x) = f(W_1 y + W_2 z) \approx g(y),$

$g(y)$ requires low computational efforts when $k \ll n$

Diagonal elements of matrix C: $C_{i,j} = \int \frac{\partial f(x)}{\partial x_i} \frac{\partial f(x)}{\partial x_j} \rho(x) dx,$

are DGSM: $\nu_i = C_{i,i}$

Activity Scores: $a_t = \sum_{j=1}^{k} \lambda_j w_{t,j}^2$, with $a_t(k) \le \nu_t$;

$a_t(k = n) = \nu_t$

rank inputs by contribution to the active subspace.

Constantine, P.G. and Diaz, P. (2017) Global Sensitivity Metrics from Active Subspaces, Reliab. Eng. Syst. Safety, 162:1–13.

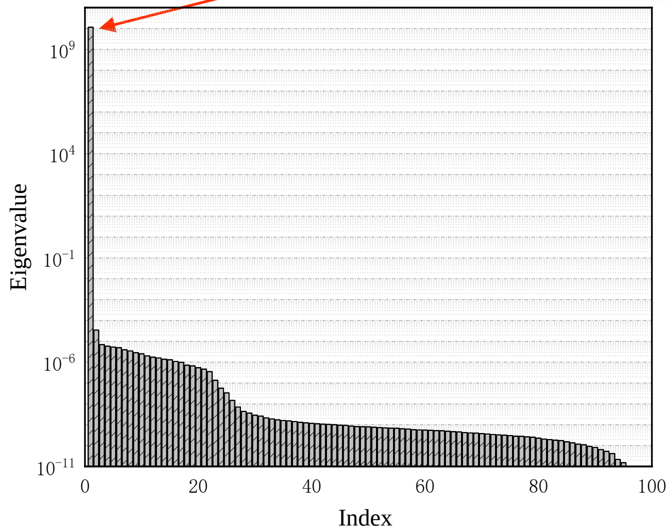
Test case: 100-dimensional quadratic model

- $\{x_i\} \in [0,1]^{100}$ $$f(x) = \left(\sum_{i=1}^{100} c_i x_i\right)^2$$

c_5	c_{15}	c_{25}	c_{35}	c_{45}	c_{55}	c_{65}	c_{75}	c_{85}	c_{95}	The rest
5	15	25	35	45	55	65	75	85	95	1

- Global SA: the importance of the inputs depends on their coefficients: a larger coefficient means higher importance of the corresponding input.
- Global SA: 10 important inputs in total

The first eigenvalue is significantly larger than the rest.

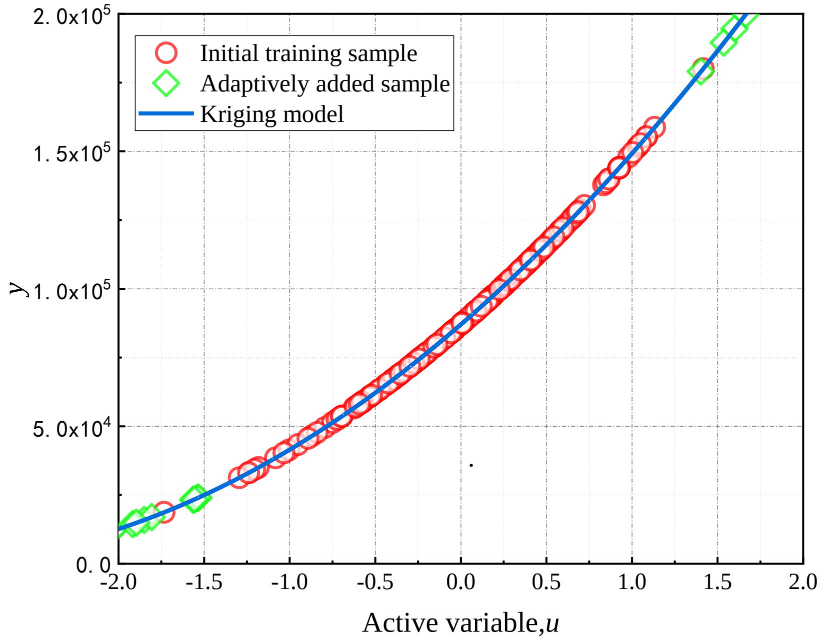


- The gap in the eigenvalues indicates a separation between active and inactive subspaces
- Hence there is 1D active subspace

Zhou, C., Shi, Z., Kucherenko, S., & Zhao, H. (2022). A unified approach for global sensitivity analysis based on active subspace and Kriging. Reliab. Eng. Syst. Saf. 217

100-dimensional quadratic model

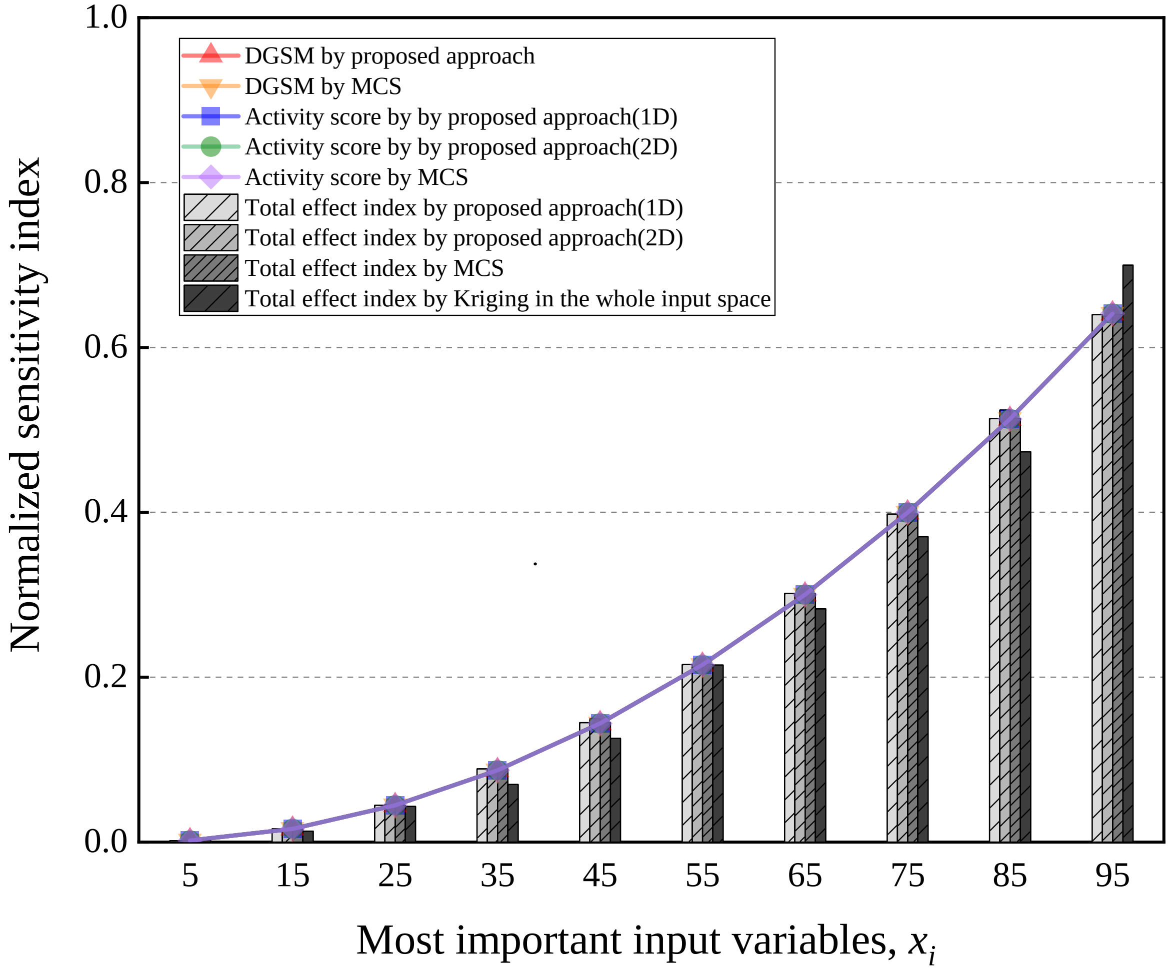
- Scatter plot $\{y_i, f(\boldsymbol{x}_i)\}$ – univariate dependence $\rightarrow$ g(y) :



- A metamodel built in 1D active subspace accurately captures the behavior of the full model

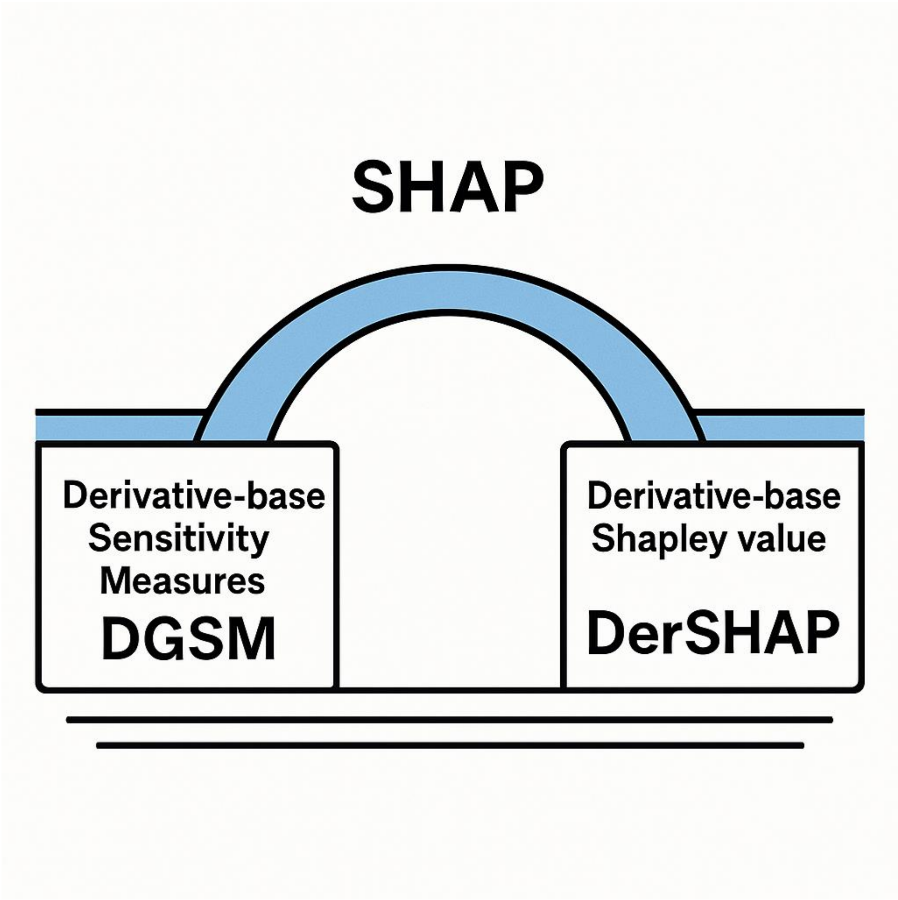
- Global SA: model reduction from d=100 to 10D (fixing non important inputs)
- AS: model reduction from d=100 to 1D (rotation of the domain produced by the eigenvector W_1)

Computation of Sobol SI using 1D metamodel in AS



- Accurate computation of 100 Sobol SI in 100 dim model using only 1D metamodel in AS

VI. Shapley Values



Shapley Values

$N = \{1,2,\ldots,n\}$ be the set of players (features).

$val(u)$ be the payoff (value function) for a subset $u \subseteq N$.

ϕ_i be the Shapley value for player i.

Properties of Shapley Values ϕ_i :

$\boldsymbol{Efficiency}$: $$\sum_{i \in N} \phi_i = val(N)$$

$\boldsymbol{Symmetry}$: If $val(u \cup \{i\}) = val(u \cup \{j\})$ for $\forall u \subseteq N \setminus \{i, j\}$, then $\phi_i = \phi_j$

$\boldsymbol{Dummy\ Player}$: If $val(u \cup \{i\}) = val(u)$ for $\forall u \subseteq N$, then $\phi_i = 0$

$\boldsymbol{Additivity}$: For games v and w, $\phi_i(v + w) = \phi_i(v) + \phi_i(w)$ for $\forall i \in N$

$$\phi_i = \sum_{u \subseteq N \setminus \{i\}} \frac{|u|!\,(|N| - |u| - 1)!}{|N|!} \left(val(u \cup \{i\}) - val(u)\right)$$

Sobol' indices and Shapley value

Owen (2014), Owen & Prieur (2017) used the main effect Sobol' index to define value function as $val(u) = S_u$

then the Shapley value for a player i:

$$\phi_i = \sum_{u \subseteq N \setminus \{i\}} \frac{|u|!\,(|N| - |u| - 1)!}{|N|!} \left(S_{u \cup \{i\}} - S_u\right)$$

Theorem*:

$$\boldsymbol{\phi_i} = \sum_{u \subseteq 1:n, i \in u} \frac{D_u}{|u|}.$$

Then

$$S_i \le \phi_i \le S_i^{tot}$$

Owen, A. B. (2014). SIAM/ASA Journal on Uncertainty Quantification, 2(1), 245-251.

Owen, A. B., & Prieur, C. (2017). SIAM/ASA Journal on Uncertainty Quantification, 5(1), 986-1002.

SHAP (SHapley Additive exPlanations) and Explainable AI (XAI)

In machine learning, SHAP is used to explain the model output.

It treats the model's prediction as the "payoff" and the features as the "players."

Additive Contribution of Features in model's prediction:

$$f(x) = \phi_0 + \sum_{i=1}^{M} \phi_i$$

- ϕ_0 is the baseline prediction (the average prediction over the dataset),
- ϕ_i is the Shapley value for the feature
- M is the total number of features.

Limitations of SHAP

1. **Computational Complexity**:
   requires evaluating all possible subsets of features: 2^M evaluations

2. **Assumption of Feature Independence**:
   assumes that features are independent, which may not hold in real-world datasets.

3. **Handling of Higher-Order Interactions**:
   struggles to capture complex interactions between features, especially in high-dimensional data

4. **Unreliable outcomes**
   may assign excessive importance to improbable instances.

Derivative-based Shapley value (DerSHAP)

- Model $f(x)$, $x = (x_1, \cdots, x_n)$
- Denote the partial derivative of $f(x)$ with respect to x_i as

$$\frac{\partial f(x)}{\partial x_i} = \partial^{(i)} f$$

Define the derivative-based importance of subset u:

$$val(u) = \sum_{i \in u} \sum_{j \in u, j \geq i} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right| =$$

$$\sum_{i \in u} \mathbb{E}\left[\partial^{(i)} f^2\right] + \sum_{i,j \in u, j > i} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

$$= \sum_{i \in u} \alpha_i(d) + \sum_{i,j \in u, j > i} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

Here $\sum_{i \in u} \mathbb{E}\left[\partial^{(i)} f^2\right] = \sum_{i \in u} \alpha_i(n) = \sum_{i \in u} v_i$, α_i is the activity scores.

Duan H, Okten G. Derivative-based Shapley value for global sensitivity analysis and machine learning explainability. Int. J. for Uncertainty Quant. 2025;15(1).

Derivative-based Shapley value: DerSHAP

DGSM–based importance of subset u:

$$val(u) = \sum_{i \in u} \sum_{j \in u, j \geq i} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

$$= \sum_{i \in u} \mathbb{E}\left[\partial^{(i)} f^2\right] + \sum_{i,j \in u, j > i} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

Theorem 1. The Shapley value for the derivative-based importance function:

$$\phi_i = \mathbb{E}\left[\partial^{(i)} f^2\right] + \frac{1}{2} \sum_{j=1, j \neq i}^{n} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

$$= v_i + \frac{1}{2} \sum_{j=1, j \neq i}^{d} \left| \mathbb{E}\left[\partial^{(i)} f \partial^{(j)} f\right] \right|$$

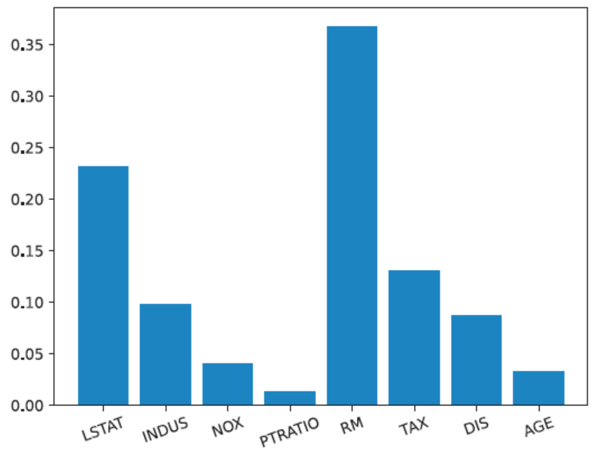
DerSHAP generalizes DGSM by introducing interaction terms between partial derivatives while adopting a Shapley value framework

DerSHAP complexity using MC is $O(nN)$ vrs SHAP - 2^n terms.

DerSHAP can be used with dependent variables

Boston housing data

Target to predict: MEDV (median value of owner-occupied homes in $1000's)
Input features: 8 input features (socioeconomic & property characteristics)



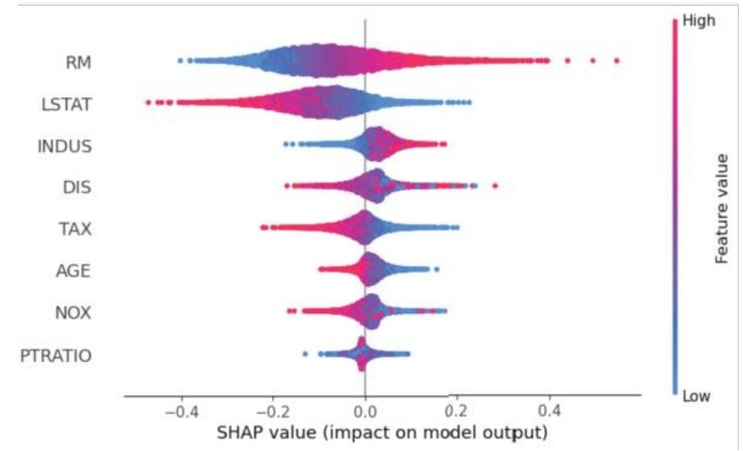


Figure. DerSHAP and KernelSHAP values for independent inputs

DerSHAP works with dependent data; KernelSHAP does not

Computational time comparison

Model	Method	Time
SVR	DerSHAP	6.81 sec.
	KernelSHAP	3.7 hours

Other DGSM extensions

- M. Lamboni, S. Kucherenko (2021) Multivariate sensitivity analysis and derivative-based global sensitivity measures with dependent variables, Reliab Eng Syst Saf 212 107519

- M. Lamboni, S. Kucherenko (2025) Active subspace methods and derivative-based Shapley' effects for functions with non-independent variables, submitted to Math. and Comp. in Simulation.

- SAMO 2025 Presenations:

- Giray Okten, Ruilong Yue, Global activity scores.
- Mayer Patricia, Derivative-based Global Sensitivity Analysis for Energy System Optimization Models via Implicit Differentiation
- Yang Jiannan [et al.], Derivative-based upper bound for entropic total effect sensitivity with high dimensional and dependent inputs
- Lüthen Nora, Gradient-enhanced surrogate modelling and sensitivity analysis with chaos expansions
- ....

DGSM Software

Derivative-based measures in Matlab (Kucherenko and Song, 2014):
https://ec.europa.eu/jrc/en/samo/simlab

GUI driven global sensitivity analysis and metamodeling software SobolGSA (Kucherenko and Zaccheus, 2025).
http://www.imperial.ac.uk/process-systems-engineering/research/free-software/sobolgsa-software/

SALib - an open-source Python library for Sensitivity Analysis (Herman and Usher (2017))
https://github.com/SALib/SALib

Package 'sensitivity' (Iooss et al. (2020)) https://cran.r-project.org/web/packages/sensitivity/

Summary

- DGSM bounds provide good estimates of S^{tot} at much lower computational cost.
- Small DGSM values guarantee small S^{tot}, making DGSM effective for fixing.
- Bounds can be computed via MC/QMC using partial derivatives, or efficiently obtained via adjoint AD. .
- Low computational cost of DGSM makes them attractive for use in Derivative-based Shapley value, active subspaces and other applications

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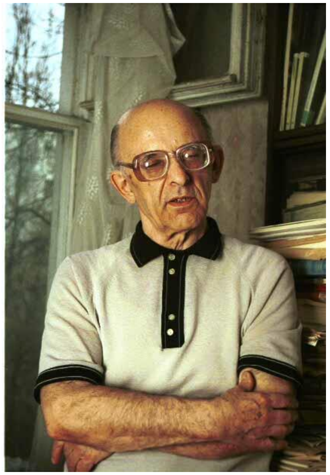
7. *C. Zhou, Z. Shi, S. Kucherenko, S., H. Zhao. A unified approach for global sensitivity analysis based on active subspace and Kriging. Reliab. Eng. Syst. Saf. 217, 2022*
8. M. Lamboni, S. Kucherenko Multivariate sensitivity analysis and derivative-based global sensitivity measures with dependent variables, Reliab. Eng. System Safety 212 (2021) 107519.

Acknowledgments

Prof. Sobol'



S. Song, N. Shah, M. Lamboni, B. Iooss, C. Molkenthin, H. Leovey,

M. Rodriguez-Fernandez, G. Okten