Comparison of Active Subspaces and Global Sensitivity Measures for Problems with Rotations and Dependent Variables

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Outline

Motivation: Sensitivity analysis of parameters, or their combinations regardless of their space orientation

Active subspaces

Link between Active subspaces, Derivative based global sensitivity measures (DGSM) and Sobol' sensitivity indices

Models with rotations and correlated variables

Motivation

Sensitivity analysis (SA) should be able to quantify uncertainty of parameters, or their combinations regardless of their space orientation for example for directions not aligned with the axes of the parameter space

Active subspaces (AS) identifies important directions in the parameter space which allows

1) dimension reduction
2) to perform SA invariant of space rotations

Active Subspaces

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

Compute matrix $C = E\left[\nabla f \nabla f^T\right]$ and its eigenvalue decomposition: $C = W \Lambda W^T$,

$\Lambda = diag(\lambda_1, \dots \lambda_n), \lambda_1 \geq \cdots \geq \lambda_n$ are eigenvalues,

W - orthogonal matrix of eigenvectors forming the basis of $\mathbb{R}^{\mathrm{n}}$.

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 ($k \ll n$),

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

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

$f(x) = f(W_1 y + W_2 z) \approx g(y)$, where $y = W_1^T x$, $y \in \mathbb{R}^k$ - active variables,
z $\in \mathbb{R}^{n-k}$– inactive variables

Ref.: *P.G. Constantine, Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies, SIAM, Philadelphia, 2015*

Derivative based global sensitivity measures (DGSM) and and their link with Active subspaces

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

$$\nu_i = \int_{H^n} \left(\frac{\partial f(\boldsymbol{x})}{\partial x_i}\right)^2 d\,\boldsymbol{x}$$

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

Link with Active subspaces

$$\nu_i = C_{ii}$$

Ref.: *Sobol' I.M., Kucherenko S. A new derivative based importance criterion for groups of variables and its link with the global sensitivity index. Comp. Physics Comm., 181, 1212-1217, 2010*)

Active Subspaces for Problems with Rotations

Consider model in transformed coordinates: $x' = \hat{R}x$,
rotation matrix $\hat{R}$ is orthogonal.

Consider the link between sensitivity measures of $f(x')$ with respect to x' coordinates and $f_R = f\left(\hat{R}x\right)$ with respect to x coordinates.

Example 1. Ishigami function

$$f(x') = sin\, x'_1 + a\, sin^2\, x'_2 + bx_3'^4\, sin\, x'_1\,,\; x'_i \in [-\pi, -\pi],\;\; i=1, 2, 3$$

Example 2. Ishigami function with rotation on θ

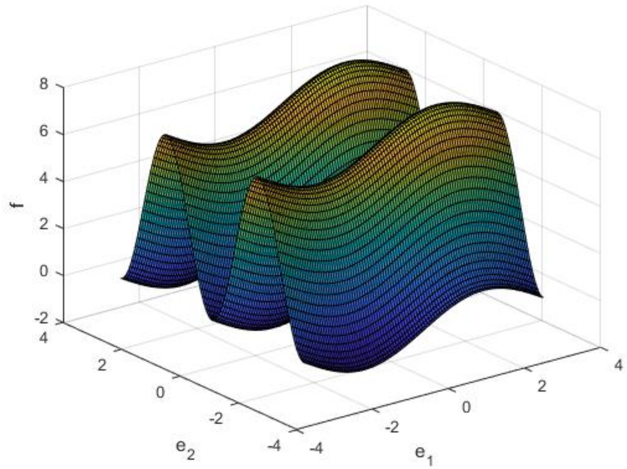
$$\hat{\boldsymbol{R}} = \begin{bmatrix} cos(\theta) & -sin(\theta) & 0 \\ sin(\theta) & cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

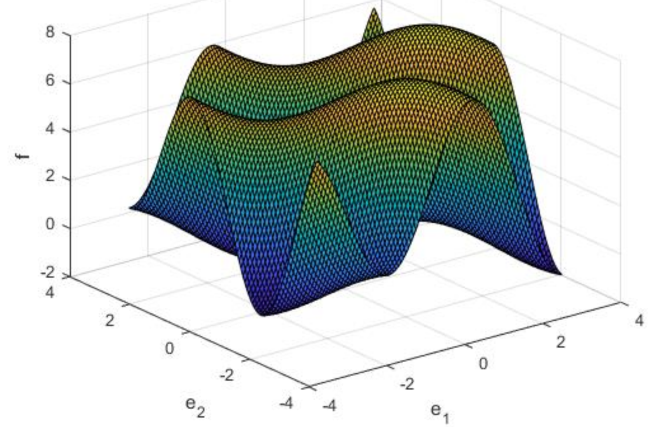
$$f_R(x) = sin(\,cos(\,\theta)x_1 - sin(\,\theta)x_2) + a\, sin^2(\,cos(\,\theta)x_1 + sin(\,\theta)x_2)$$
$$+bx_3^4\, sin(\,cos(\,\theta)x_1 - sin(\,\theta)x_2)$$

Ishigami function

without rotation

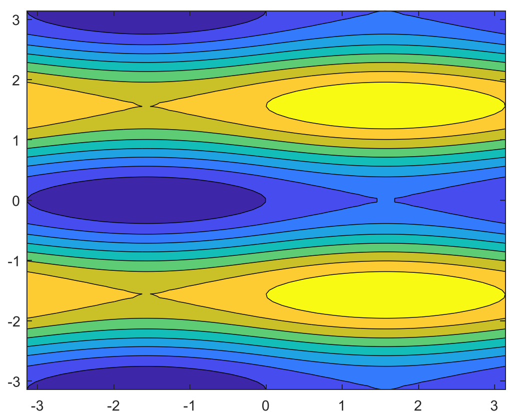
rotation on $\theta = \pi/4$

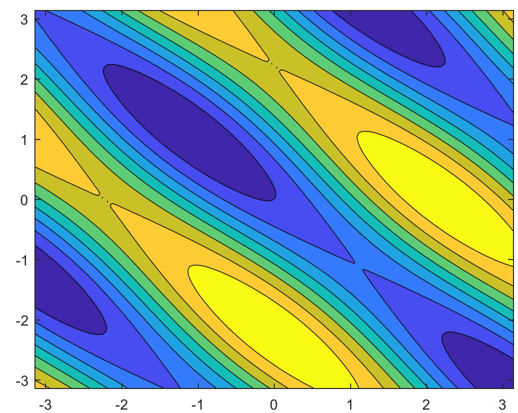




$f\left(x'_1, x'_2, x'_3 = 0.0\right)$

$f_R(x_1, x_2, x_3 = 0.0)$





Contour lines

Link between DGSM for problems with rotations

Note that $\frac{\partial f_R}{\partial x_i} = \sum_{j=1}^{n} \frac{\partial f}{\partial x'_j} \frac{\partial x'_j}{\partial x_i}$.

$\frac{\partial x'_j}{\partial x_i} = r_{ji}, r_{ji}$ - elements of $\hat{R}$

$$\nu_i^R = \int_{H^n} \left[\sum_{j=1}^{n} r_{ji} \frac{\partial f}{\partial x'_j} \right]^2 dx = \sum_{j=1}^{n} r_{ji} \nu_i + \sum_{j=1}^{n} \sum_{k \neq j,}^{n} r_{ji}\, r_{ki} \int_{H^n} \left[\frac{\partial f}{\partial x'_j} \frac{\partial f}{\partial x'_k} \right] dx$$

Example. $f(x'_1, x'_2, x'_3)$ with corresponding ν_1, ν_2, ν_3 .

$$\hat{R} = \begin{bmatrix} cos(\theta) & -sin(\theta) & 0 \\ sin(\theta) & cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\nu_1^R = cos(\theta)^2 \nu_1 + sin(\theta)^2 \nu_2 + sin(\theta)\, cos(\theta) \int_{H^n} \left[\frac{\partial f}{\partial x'_1} \frac{\partial f}{\partial x'_2} \right] dx$$

$$\nu_2^R = sin(\theta)^2 \nu_1 + cos(\theta)^2 \nu_2 - sin(\theta)\, cos(\theta) \int_{H^n} \left[\frac{\partial f}{\partial x'_1} \frac{\partial f}{\partial x'_2} \right] dx$$

$$\nu_3^R = \nu_3$$

Active Subspaces for Problems with Rotations

Note that $\nabla_x f_R(\hat{R}x) = \hat{R}^T \nabla_{x'} f(x')$

$C_R = \int \nabla_x f_R \nabla_x f_R{}^T \, dx = \hat{R}^T C \, \hat{R}$, $C = W \Lambda W^T$ - a matrix of $f(x')$

The results of AS are exactly the same as in the case with no rotation:

C_R and C have the same eigenvalues, $W_R = \hat{R}^T W$.

Active directions $\hat{R}^T W_1$,

A low-dimensional approximation of $f_R \approx g(\hat{R}^T W_1 x)$.

DGSM and Sobol SI. Ishigami function without rotation

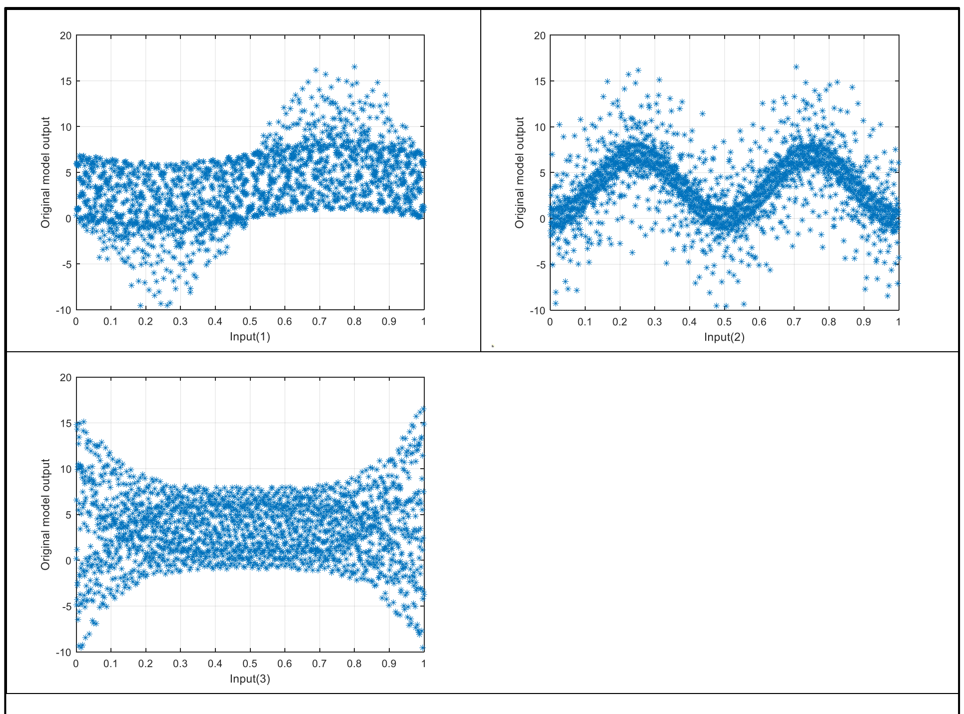
Sobol' SI: $D = \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18} + \frac{1}{2}$,

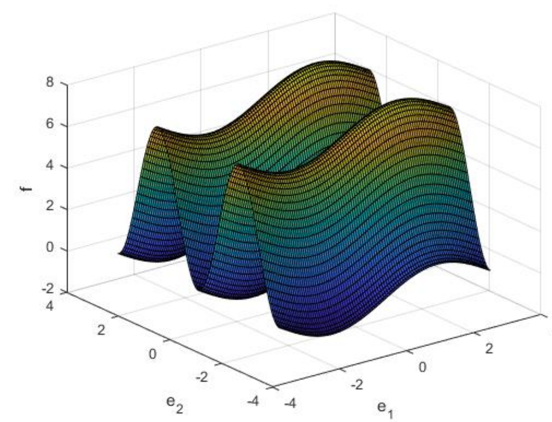
$S_1^{tot} = \frac{1}{D}\left[\frac{1}{2} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18}\right], S_2^{tot} = \frac{a^2}{8D}, S_3^{tot} = \frac{b^2\pi^8}{225D}$.

DGSM: $\nu_1 = 2\pi^2 + \frac{4b\pi^6}{5} + \frac{2b^2\pi^{10}}{9}, \nu_2 = 2a^2\pi^2, \nu_3 = \frac{32b^2\pi^8}{7}$.

Variable	S_i^{tot}	ν_i
1	0.55	304.75
2	0.44	967.22
3	0.24	433.76

Results for *a*=7, *b*=0.1.



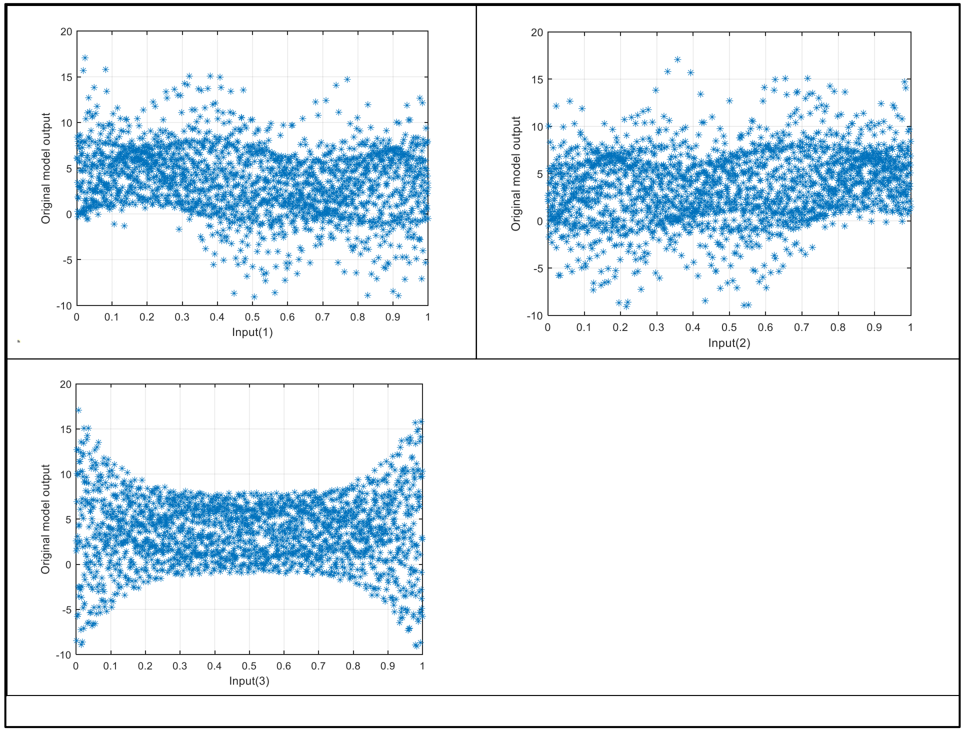


DGSM and Sobol SI. Ishigami function (*a*=7, *b*=0.1) with rotation

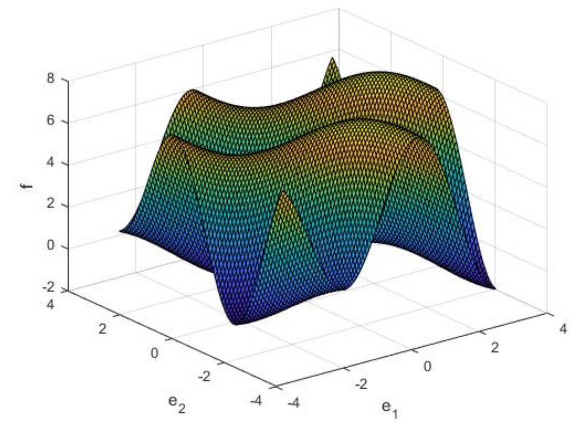
Rotation: $\theta = \pi/4$,

$\nu_i^R = \nu_1 + \nu_2,\ i = 1{,}2\ ;\ \nu_3^R = \nu_3$

Variable	S_i^{tot}	ν_i
1	0.75	635
2	0.73	635
3	0.24	411



Scatter plots



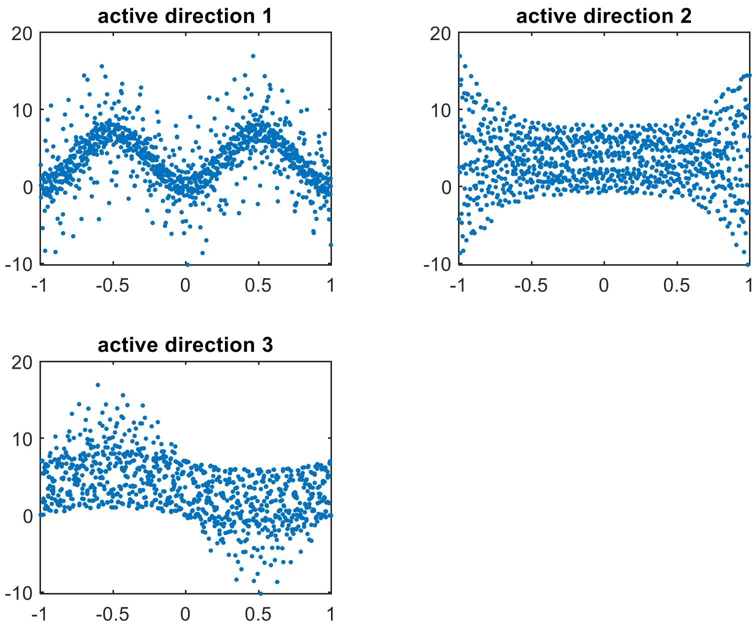
Results are inconclusive

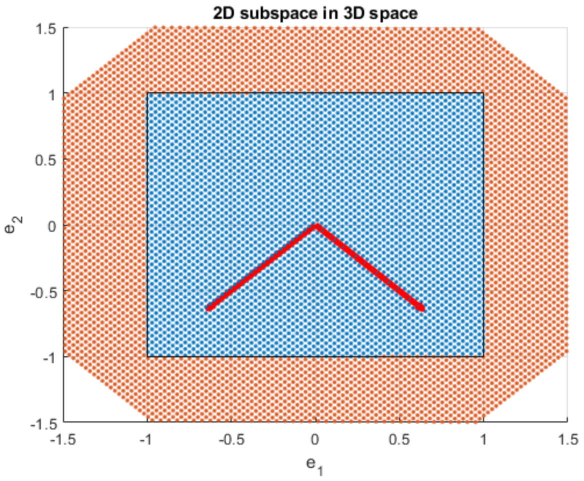
Active Subspaces. Ishigami function (a=7, b=0.1) with rotation

Rotation: $\theta = \pi/4$.

Λ = [240.4; 103.4; 78.8],

$$W = \begin{bmatrix} -\sqrt{2}/2 & 0.0 & -\sqrt{2}/2 \\ -\sqrt{2}/2 & 0.0 & \sqrt{2}/2 \\ 0.0 & 1.0 & 0.0 \end{bmatrix}$$





The scatter plots in the active dimensional space are the same as in the case of no rotation

Active directions

DGSM and Sobol SI. Ishigami function (*a*=1, *b*=0.01) with rotation

rotation: $\theta = \pi/4$

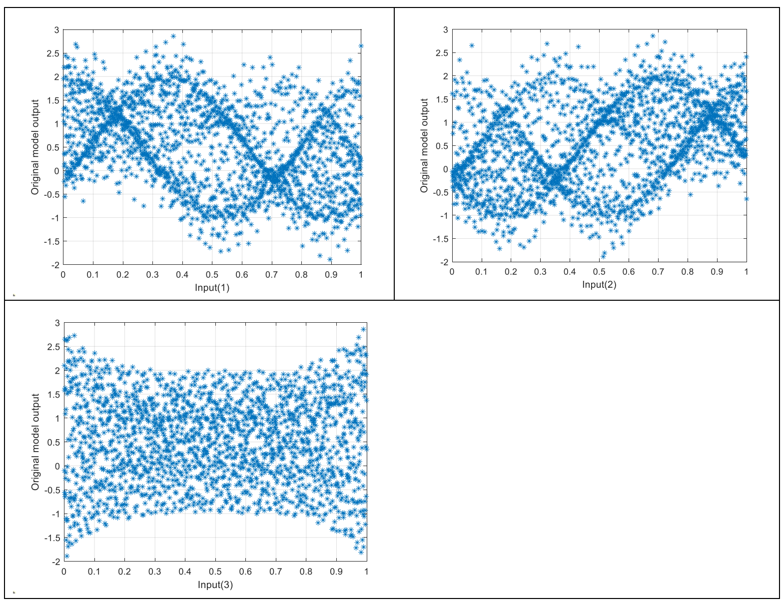
Variable	S_i	S_i^{tot}	ν_i
1	0.15	0.81	26
2	0.13	0.79	26
3	0.0	0.04	4.1

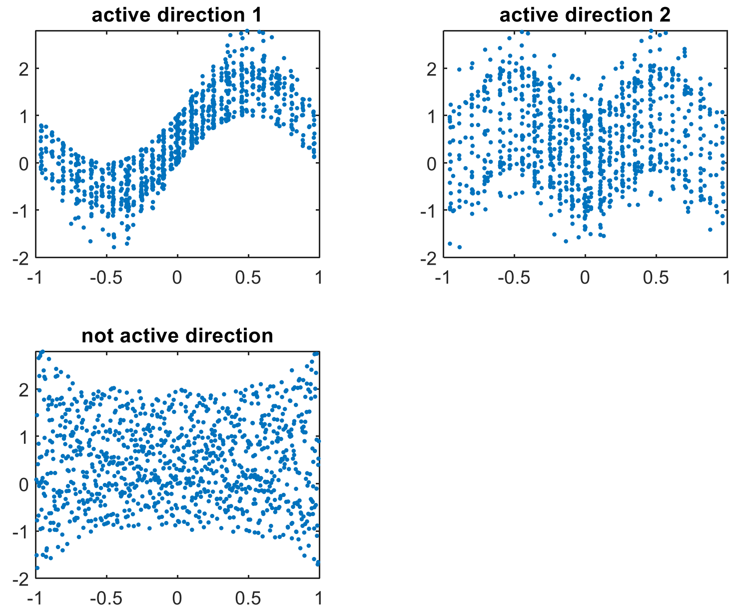
without rotation

Variable	S_i	S_i^{tot}	ν_i
1	0.82	0.86	29.5
2	0.14	0.14	19.7
3	0.0	0.04	4.33

dominant first two inputs – same ranking

different ranking for all inputs





Scatter plots don't reveal any patterns

Scatter plots in the active dimensional space are the same as in the case of no rotation

Active Subspaces. Ishigami function (a=1, b=0.01)

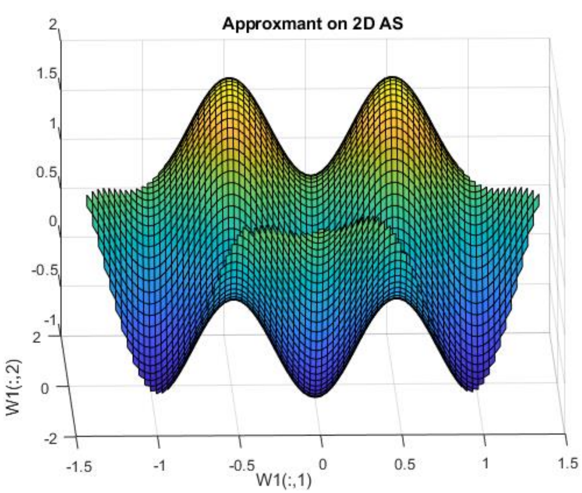
rotation: $\theta = \pi/4$

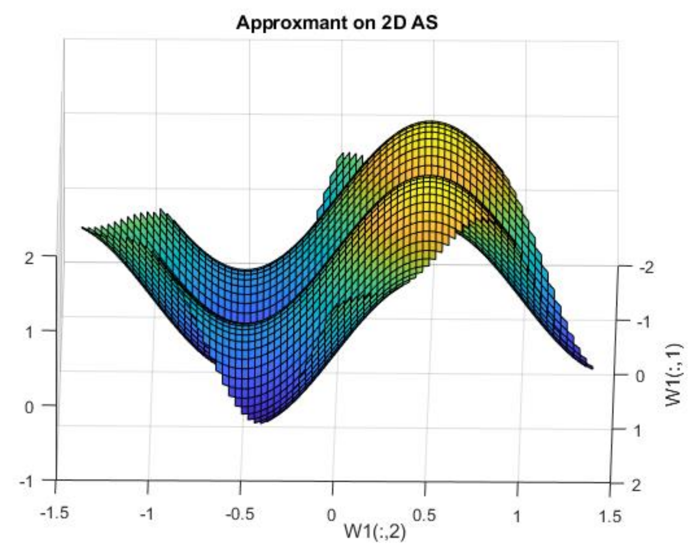
Λ = [7.6; 4.9; 1.04],

$$W = \begin{bmatrix} -\sqrt{2}/2 & -\sqrt{2}/2 & 0.0 \\ \sqrt{2}/2 & -\sqrt{2}/2 & 0.0 \\ 0.0 & 0.0 & 1.0 \end{bmatrix}$$

$\lambda_1, \lambda_2 \gg \lambda_3$ – 2D active subspace is defined by

Λ_1= [7.6; 4.9], $W_1 = \begin{bmatrix} \sqrt{2}/2 & -\sqrt{2}/2 \\ -\sqrt{2}/2 & -\sqrt{2}/2 \\ 0.0 & 0.0 \end{bmatrix}$ - dimension reduction from 3D to 2D





2D plots in the active dimensional space are the same as in the case of no rotation

Models with correlated inputs

Proposition. Let $\mathcal{N}_n(\mu, \Sigma)$ be the n-multivariate Gaussian distribution, $\mathcal{L}$ be the Cholesky factor of Σ

If $x = (x_j, x_{\sim j}) \sim \mathcal{N}_n(\mu, \Sigma)$, then there exists $d-1$ independent random variables $\mathrm{Z} \sim \mathcal{N}_{n-1}(0, I)$ and a function $r_j\colon R^n \rightarrow R^{n-1}$ such that x_j is independent of Z and

$$x_{\sim j} \stackrel{n}{=} r_j\left(x_j, Z\right) = \left[\mathcal{L}\begin{bmatrix}\frac{1}{\sigma_j}[x_j - E(x_j)] \\ Z\end{bmatrix} + \mu\right]_{\sim 1},$$

where σ_j is the standard deviation of x_j and $[.]_{\sim 1}$ means that the first element of the vector is excluded.

Ref: *M. Lamboni, S. Kucherenko Multivariate sensitivity analysis and derivative-based global sensitivity measures with dependent variables, RESS, 212 (2021) 107519*

Linear model with correlated inputs. Active Subspaces

$$f(x) = x_1 + x_2\,,$$

$$x \sim \mathcal{N}\left(0, \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}\right).$$

Using representation $f(X_1, r_1(x_1, Z_2)), f(x_2, r_2(x_2, Z_1))$

We find $\frac{\partial f}{\partial x_1} = \left(1 + \frac{\rho\sigma_2}{\sigma_1}\right), \frac{\partial f}{\partial x_2} = \left(1 + \frac{\rho\sigma_1}{\sigma_2}\right)$

Denote $\mathrm{A} = \frac{\sigma_2}{\sigma_1}$, $\mathrm{M} = \frac{1+\rho\mathrm{A}}{1+\rho/\mathrm{A}}$.

Applying AS methodology we find:

$\Lambda = [(1 + \rho\mathrm{A})^2 + (1 + \frac{\rho}{\mathrm{A}})^2, 0]$,

$$W = \begin{bmatrix} \frac{M}{\sqrt{1 + M^2}} & -\frac{1}{M\sqrt{1 + (1/M)^2}} \\ \frac{1}{\sqrt{1 + M^2}} & \frac{1}{\sqrt{1 + (1/M)^2}} \end{bmatrix}$$

$y = W_1^T x = \frac{M}{\sqrt{1+M^2}} x_1 + \frac{\mathbf{1}}{\sqrt{1+M^2}} x_2$ - active direction

$z = W_2^T x = -\frac{1}{M\sqrt{1+(1/M)^2}} x_1 + \frac{1}{\sqrt{1+(1/M)^2}} x_2$ - not active direction

Linear model with correlated inputs. AS, Sobol SI and DGSM

$$S_1 = \frac{(\sigma_1 + \rho\sigma_2)^2}{\sigma_1^2 + \sigma_2^2 + 2\rho\sigma_1\sigma_2}, S_1^T = \frac{\sigma_1^2(1-\rho^2)}{\sigma_1^2 + \sigma_2^2 + 2\rho\sigma_1\sigma_2},$$

$$S_2 = \frac{(\sigma_2 + \rho\sigma_1)^2}{\sigma_1^2 + \sigma_2^2 + 2\rho\sigma_1\sigma_2}, S_2^T = \frac{\sigma_2^2(1-\rho^2)}{\sigma_1^2 + \sigma_2^2 + 2\rho\sigma_1\sigma_2}$$

$$\nu_1 = (1 + \rho \mathrm{A})^2, \nu_2 = (1 + \rho/\mathrm{A})^2$$

Extreme case 1. ρ=0.0, → M=1

$$\Lambda = [2, 0], \qquad W = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

$y = W_1^T x = \frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$ - active direction

$z = W_2^T x = -\frac{1}{\sqrt{2}} x_1 + \frac{1}{\sqrt{2}} x_2$ - not active direction

$$S_1 = S_1^T = \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2 + 2\sigma_1\sigma_2}, S_2 = S_2^T = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2 + 2\sigma_1\sigma_2}$$

$$\nu_1 = \nu_2 = 1$$

Linear model with correlated inputs. AS, Sobol SI and DGSM

Extreme case 2. $\sigma_2 \rightarrow 0$, $\mathrm{A} = 0$, M=0

$$\Lambda = [\rightarrow \propto, 0], \qquad W = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$y = W_1^T x = x_2$ - active direction

$z = W_2^T x = -x_1$ - not active direction

$S_1 = 1,\ S_1^T = (1 - \rho^2),$
$S_2 = \rho^2,\ S_2^T = 0$

$\nu_1 = 1,\ \nu_2 \rightarrow \propto$

Ref.: *S. Kucherenko, S. Tarantola, P. Annoni. Estimation of global sensitivity indices for models with dependent variables, Comp. Physics Comm., 183 (2012) 937–946*

Ishigami function (a=1, b=0.01) with correlated inputs

$$x \sim \mathcal{N}\left(0, \begin{bmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 \end{bmatrix}\right)$$

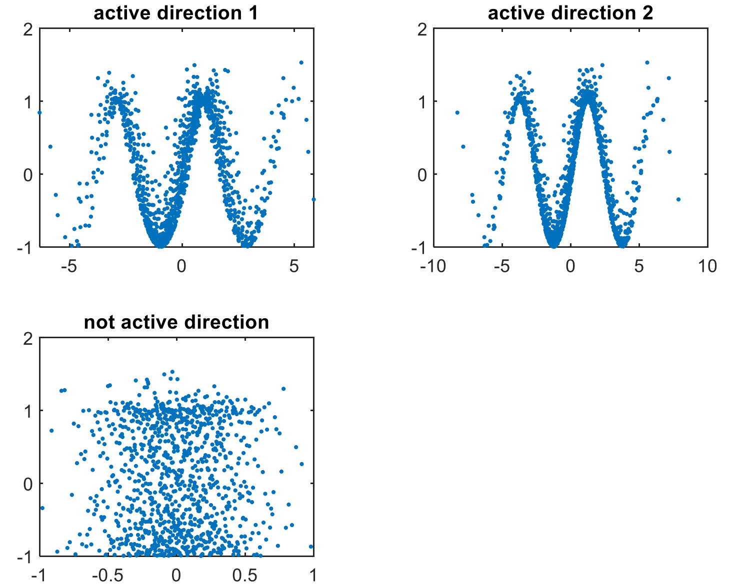
σ_1^2=10, σ_2^2=0.1, σ_3^2=0.1,

ρ_{12}=0.1, ρ_{13}= ρ_{23}=0

Λ = [1.15; 0.12; 0.0],

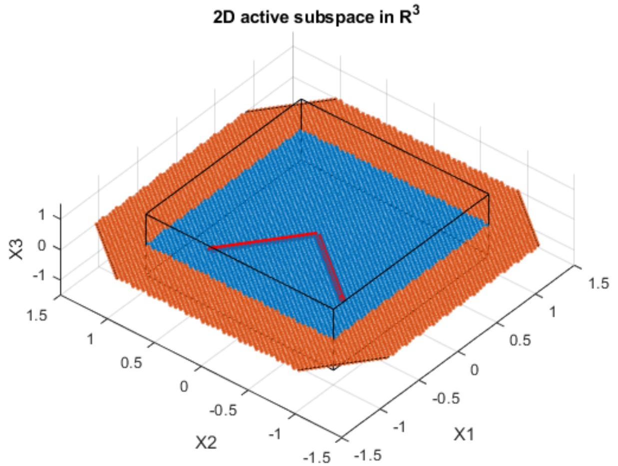
$\lambda_1, \lambda_2 \gg \lambda_3$ − 2D active subspace is defined by

$$\Lambda_1 = [1.15; 0.12], \; W_1 = \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \\ 0.0 & 0.0 \end{bmatrix}$$

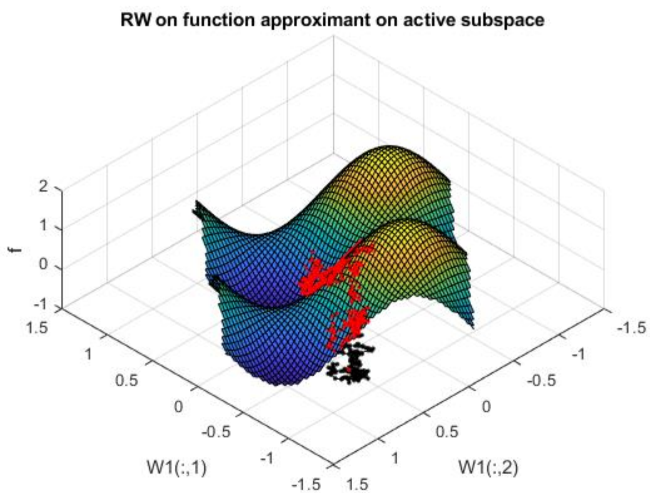


Scatter plots in the active dimensional space

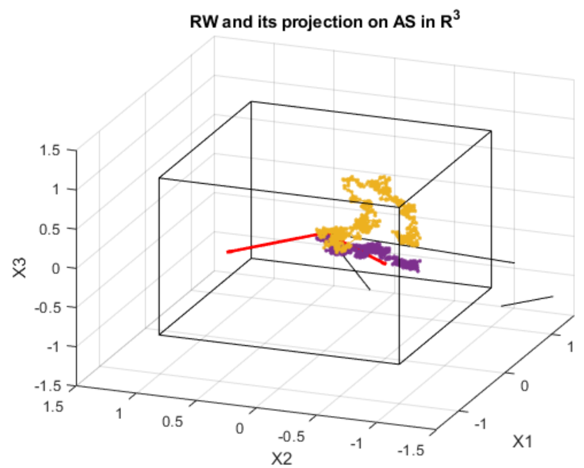
Ishigami function (a=1, b=0.01) with correlated inputs



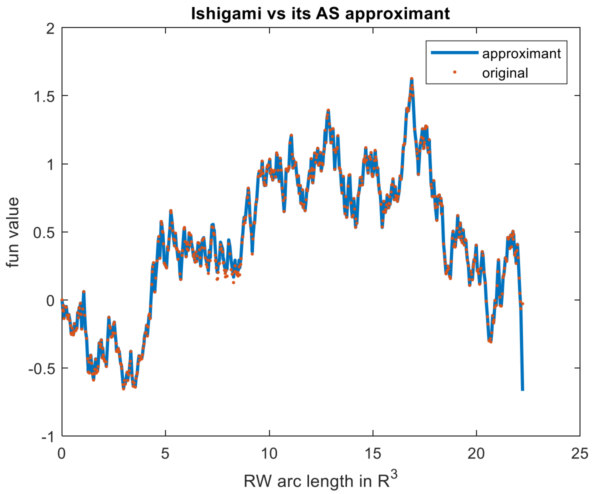
Active directions



Random walk on 2D function approximant on active subspace



Random walk (RW) in R^3 (yellow line) and its projection on 2D AS



RW on full model (red dots) and its projection on 2D AS (blue line)

Summary

1. The AS method is capable of finding new directions in which parameters have the same importance regardless of their space orientation.

2. Sobol' and DGSM methods are unable to identify directions and rank parameters in active subspaces rather than in original directions.

3. The AS method allows dimension reduction by ingoring inactive variables.

4. We generalised the AS methodology for the case of models with dependent variables and showed its efficiency

Link between DGSM and Active subspaces

Constantine et al. introduced the so-called activity score defined as

$$a_i(k) = \sum_{j=1}^{k} \lambda_j w_{i,j}^2, \qquad i = 1, \dots, n$$

- a combined reflection of the contribution of each input variable to the active subspace.

A link between the activity score and DGSM:

$$a_i(n) = \sum_{j=1}^{n} \lambda_j w_{i,j}^2 = \nu_i, \qquad i = 1, \dots, n$$

Ref.: *Paul G. Constantine, Paul Diaz, Global sensitivity metrics from active subspaces, Reliability Engineering and System Safety 162 (2017) 1–13.*

Models with correlated inputs. Derivatives

Linear function: $f(x) = x_1 + x_2 + x_3$,

$$x \sim \mathcal{N}\left(0, \begin{bmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 \end{bmatrix}\right).$$

Model (x_1, x_2, x_3) as follows: $(x_2, x_3) = r_1(x_1, Z_2, Z_3)$,

$$\begin{cases} X_2 = \dfrac{\rho_{12}\sigma_2}{\sigma_1} X_1 + \sqrt{1-\rho_{12}^2} Z_2 \\ X_3 = \dfrac{\rho_{13}\sigma_3}{\sigma_1} X_1 + \dfrac{\sigma_3(\rho_{23}-\rho_{12}\rho_{13})}{\sigma_2\sqrt{1-\rho_{12}^2}} Z_2 + \sqrt{\dfrac{1-\rho_{12}^2-\rho_{13}^2-\rho_{23}^2+2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{12}^2}} Z_3 , \end{cases}$$

$Z_j \sim \mathcal{N}(0, I), j = 2, 3,\ Z_2, Z_3, X_1$ are independent.

Thus,

$$f(X_1, r_1(x_1, Z_2, Z_3)) = \left(1 + \frac{\rho_{12}\sigma_2}{\sigma_1} + \frac{\rho_{13}\sigma_3}{\sigma_1}\right) X_1 + \left(\sqrt{1-\rho_{12}^2} + \frac{\sigma_3(\rho_{23}-\rho_{12}\rho_{13})}{\sigma_2\sqrt{1-\rho_{12}^2}}\right) Z_2 + \sqrt{\frac{1-\rho_{12}^2-\rho_{13}^2-\rho_{23}^2+2\rho_{12}\rho_{13}\rho_{23}}{1-\rho_{12}^2}} Z_3$$

then $\dfrac{\partial f}{\partial x_1} = \left(1 + \dfrac{\rho_{12}\sigma_2}{\sigma_1} + \dfrac{\rho_{13}\sigma_3}{\sigma_1}\right)$

Similarly we find $f(x_2, r_2(x_2, Z_1, Z_3)), \dfrac{\partial f}{\partial x_2}, \ldots$.