Benchmark Functions for Bayesian Optimization

Jungtaek Kim

Pohang University of Science and Technology, Pohang 37673, Republic of Korea

`jtkim@postech.ac.kr`

July 30, 2020

Revised on November 7, 2020
Revised on February 10, 2021
Revised on January 12, 2022

Introduction

In these notes, we cover benchmark functions for Bayesian optimization. Since Bayesian optimization is used to solve a global optimization problem, the benchmark functions described in these notes are utilized in diverse problems on mathematical optimization.

Benchmark Functions for Bayesian Optimization

All functions are implemented in `https://github.com/jungtaekkim/bayeso-benchmarks`. We refer to [Surjanovic and Bingham, 2013] for specific forms of many benchmark functions, which are described in `https://www.sfu.ca/~ssurjano`. The details of `BayesO` [Kim and Choi, 2017] and `BayesO Benchmarks` are introduced in `http://bayeso.org`.

We will introduce the following benchmark functions in this article.

1. Ackley

2. Beale

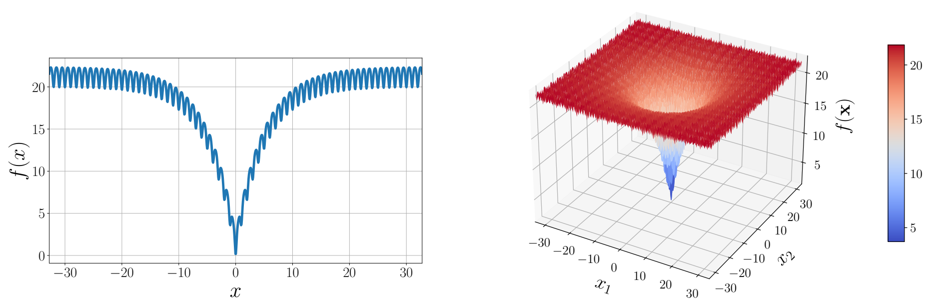
3. Bohachevsky

4. Branin

5. Cosines

6. De Jong 5
7. Drop-Wave
8. Eggholder
9. Goldstein-Price
10. Gramacy & Lee (2012)
11. Hartmann 3D
12. Hartmann 6D
13. Holder Table
14. Kim1
15. Kim2
16. Kim3
17. Michalewicz
18. Rosenbrock
19. Six-Hump Camel
20. Sphere
21. Three-Hump Camel

1 Ackley Function



(a) $d = 1$ (b) $d = 2$

Figure 1: Ackley function.

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-32.768, 32.768]^d$,

$$f(\mathbf{x}) = -20 \exp\left(-0.2\sqrt{\frac{1}{d}\sum_{i=1}^{d} x_i^2}\right) - \exp\left(\frac{1}{d}\sum_{i=1}^{d}\cos(2\pi x_i)\right) + 20 + \exp(1). \tag{1}$$

A global optimum is 0, at $\mathbf{x}^\star = [0, \ldots, 0] \in \mathbb{R}^d$.

2 Beale Function

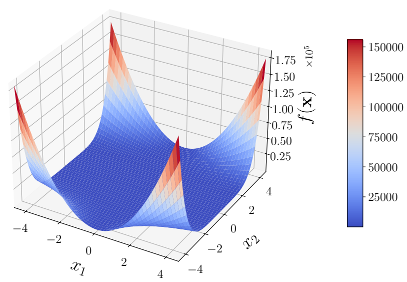


Figure 2: Beale function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-4.5, 4.5]^2$,

$$f(\mathbf{x}) = (1.5 - x_1 + x_1 x_2)^2 + (2.25 - x_1 + x_1 x_2^2)^2 + (2.625 - x_1 + x_1 x_2^3)^2. \tag{2}$$

A global optimum is 0, at $\mathbf{x}^\star = [3.0, 0.5]$.

3 Bohachevsky Function

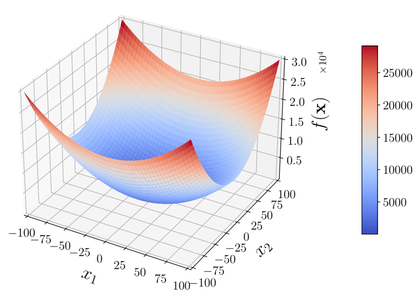


Figure 3: Bohachevsky function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-100, 100]^2$,

$$f(\mathbf{x}) = x_1^2 + 2x_2^2 - 0.3\cos(3\pi x_1) - 0.4\cos(4\pi x_2) + 0.7. \tag{3}$$

A global optimum is 0, at $\mathbf{x}^\star = [0, 0]$.

4 Branin Function

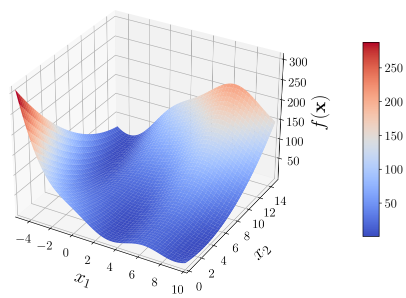


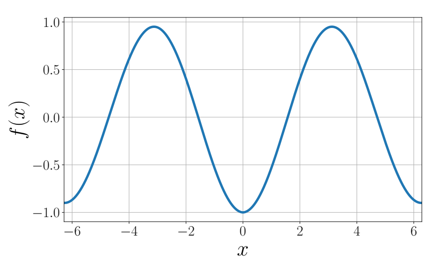
Figure 4: Branin function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2]$ for $-5 \leq x_1 \leq 10$, $0 \leq x_2 \leq 15$,

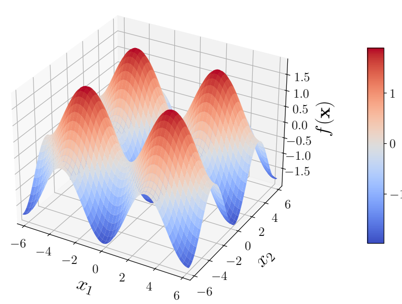
$$f(\mathbf{x}) = \left(x_2 - \frac{5.1}{4\pi^2} x_1^2 + \frac{5}{\pi} x_1 - 6 \right)^2 + 10 \left(1 - \frac{1}{8\pi} \right) \cos(x_1) + 10. \tag{4}$$

Global optima are 0, at $\mathbf{x}^\star = [-\pi, 12.275]$, $[\pi, 2.275]$, and $[9.42478, 2.475]$.

5 Cosines Function



(a) $d = 1$



(b) $d = 2$

Figure 5: Cosines function.

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \dots, x_d] \in [-2\pi, 2\pi]^d$,

$$f(\mathbf{x}) = \sum_{i=1}^{d} \cos(x_i) \left(\frac{0.1}{2\pi} |x_i| - 1 \right). \tag{5}$$

A global optimum is $-d$, at $\mathbf{x}^\star = [0, \dots, 0] \in \mathbb{R}^d$.

6 De Jong 5 Function

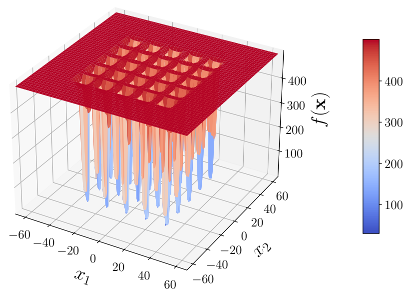


Figure 6: De Jong 5 function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-65.536, 65.536]^2$,

$$f(\mathbf{x}) = \left(0.002 + \sum_{i=1}^{25} \frac{1}{i + (x_1 - A_{1i})^6 + (x_2 - A_{2i})^6} \right)^{-1}, \tag{6}$$

where

$$\boldsymbol{A} = \begin{pmatrix} \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} \\ -\mathbf{b} & -0.5\mathbf{b} & 0\mathbf{b} & 0.5\mathbf{b} & \mathbf{b} \end{pmatrix} \in \mathbb{R}^{2 \times 25}, \tag{7}$$

$\mathbf{a} = [-32, -16, 0, 16, 32]$, and $\mathbf{b} = [32, 32, 32, 32, 32]$.

A global optimum is 0.998004, at $\mathbf{x}^\star = [-32.104282, -32.137058]$ or many other points.

7 Drop-Wave Function

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-5.12, 5.12]^2$,

$$f(\mathbf{x}) = -\frac{1 + \cos\left(12\sqrt{x_1^2 + x_2^2}\right)}{0.5\,(x_1^2 + x_2^2) + 2}. \tag{8}$$

A global optimum is -1, at $\mathbf{x}^\star = [0, 0]$.

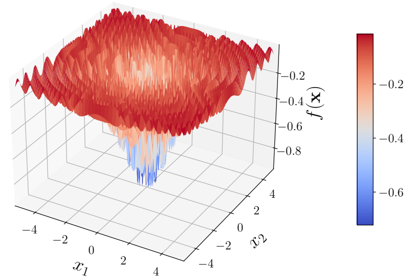


Figure 7: Drop-Wave function.

8 Eggholder Function

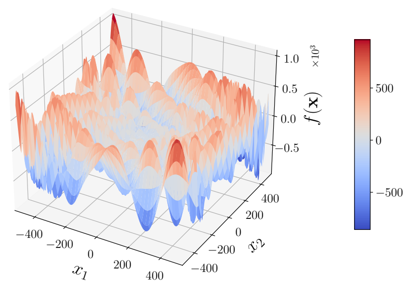


Figure 8: Eggholder function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-512, 512]^2$,

$$f(\mathbf{x}) = -(x_2 + 47) \sin\left(\sqrt{|x_2 + 0.5x_1 + 47|}\right) - x_1 \sin\left(\sqrt{|x_1 - (x_2 + 47)|}\right). \tag{9}$$

A global optimum is -959.6407, at $\mathbf{x}^\star = [512.0, 404.2319]$.

9 Goldstein-Price Function

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-2, 2]^2$,

$$f(\mathbf{x}) = \left[1 + A(B - 14x_2 + 6x_1x_2 + 3x_2^2)\right] \left[30 + C(D + 48x_2 - 36x_1x_2 + 27x_2^2)\right], \tag{10}$$

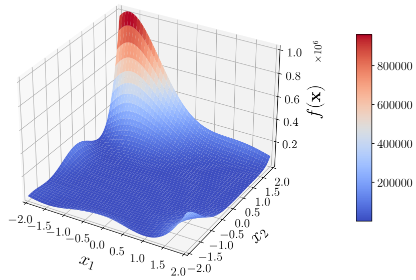


Figure 9: Goldstein-Price function.

where

$$A = (x_1 + x_2 + 1)^2, \tag{11}$$

$$B = 19 - 14x_1 + 3x_1^2, \tag{12}$$

$$C = (2x_1 - 3x_2)^2, \tag{13}$$

$$D = 18 - 32x_1 + 12x_1^2. \tag{14}$$

A global optimum is 3, at $\mathbf{x}^\star = [0, -1]$.

10 Gramacy & Lee (2012) Function

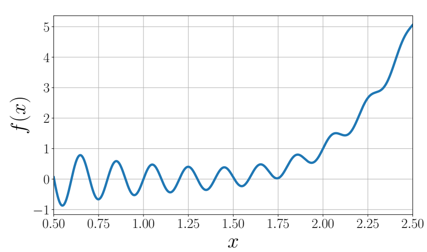


Figure 10: Gramacy & Lee (2012) function.

Given a one-dimensional input, $x \in [0.5, 2.5]$,

$$f(x) = \frac{\sin(10\pi x)}{2x} + (x-1)^4. \tag{15}$$

A global optimum is 0.54856405, at $x^\star = -0.86901113$.

11 Hartmann 3D Function

Given a three-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2, x_3] \in [0,1]^3$,

$$f(\mathbf{x}) = -\sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{3} A_{ij}(x_j - P_{ij})^2\right), \tag{16}$$

where $\boldsymbol{\alpha} = [1.0, 1.2, 3.0, 3.2]^\top$,

$$\boldsymbol{A} = \begin{pmatrix} 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \end{pmatrix}, \tag{17}$$

$$\boldsymbol{P} = 10^{-4} \begin{pmatrix} 3689 & 1170 & 2673 \\ 4699 & 4387 & 7470 \\ 1091 & 8732 & 5547 \\ 381 & 5743 & 8828 \end{pmatrix}. \tag{18}$$

A global optimum is -3.86278, at $\mathbf{x}^\star = [0.114614, 0.555649, 0.852547]$.

12 Hartmann 6D Function

Given a six-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_6] \in [0,1]^6$,

$$f(\mathbf{x}) = -\sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{6} A_{ij}(x_j - P_{ij})^2\right), \tag{19}$$

where $\boldsymbol{\alpha} = [1.0, 1.2, 3.0, 3.2]^\top$,

$$\boldsymbol{A} = \begin{pmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{pmatrix}, \tag{20}$$

$$\boldsymbol{P} = 10^{-4} \begin{pmatrix} 1312 & 1696 & 5569 & 124 & 8283 & 5886 \\ 2329 & 4135 & 8307 & 3736 & 1004 & 9991 \\ 2348 & 1451 & 3522 & 2883 & 3047 & 6650 \\ 4047 & 8828 & 8732 & 5743 & 1091 & 381 \end{pmatrix}. \tag{21}$$

A global optimum is -3.32237, at $\mathbf{x}^\star = [0.20169, 0.150011, 0.476874, 0.275332, 0.311652, 0.6573]$.

13 Holder Table Function

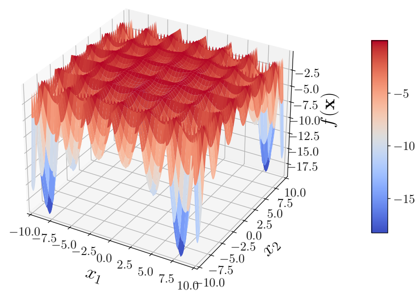


Figure 11: Holder Table function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-10, 10]^2$,

$$f(\mathbf{x}) = -\left| \sin(x_1) \cos(x_2) \exp\left(\left| 1 - \frac{\sqrt{x_1^2 + x_2^2}}{\pi} \right| \right) \right|. \tag{22}$$

Global optima are -19.2085, at $\mathbf{x}^\star = [8.05502, 9.66459]$, $[8.05502, -9.66459]$, $[-8.05502, 9.66459]$, and $[-8.05502, -9.66459]$.

14 Kim1 Function

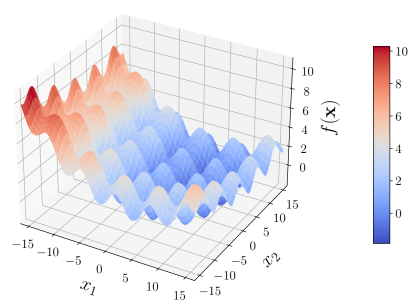


Figure 12: Kim1 function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-16, 16]^2$,

$$f(\mathbf{x}) = \sin(x_1) + \cos(x_2) + 0.016(x_1 - 5)^2 + 0.008(x_2 - 5)^2. \tag{23}$$

A global optimum is -1.97152323, at $\mathbf{x}^\star = [4.72130726, 3.17086303]$.

15 Kim2 Function

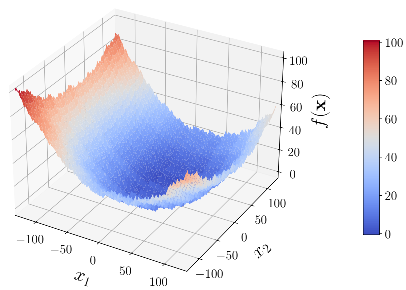


Figure 13: Kim2 function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-128, 128]^2$,

$$f(\mathbf{x}) = \sum_{i=0}^{4} \left(\sin\left(\frac{x_1}{2^i}\right) + \cos\left(\frac{x_2}{2^i}\right) \right) + 0.0032(x_1 - 20)^2 + 0.0016(x_2 - 20)^2. \tag{24}$$

A global optimum is -3.45438747, at $\mathbf{x}^\star = [-2.10134660, 34.14526252]$.

16 Kim3 Function

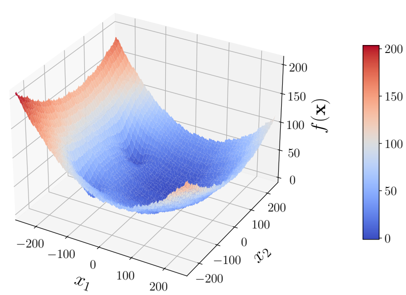


Figure 14: Kim3 function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-256, 256]^2$,

$$\begin{aligned} f(\mathbf{x}) = &\sum_{i=0}^{4} \left(\sin\left(\frac{x_1}{2^i}\right) + \cos\left(\frac{x_2}{2^i}\right) \right) \\ &+ 0.0016(x_1 - 40)^2 + 0.0008(x_2 - 40)^2 \\ &- 25600(\phi(\mathbf{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + \phi(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)), \end{aligned} \tag{25}$$

where $\phi(\cdot; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ is a probability density function of multivariate Gaussian distribution defined with a mean vector $\boldsymbol{\mu}$ and a covariance matrix $\boldsymbol{\Sigma}$, $\boldsymbol{\mu}_1 = [-120, -120]$, $\boldsymbol{\mu}_2 = [-120, 120]$, and

$$\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \begin{bmatrix} 1000 & 0 \\ 0 & 1000 \end{bmatrix}. \tag{26}$$

A global optimum is -4.94396792, at $\mathbf{x}^\star = [48.12477173, 34.19859065]$.

17 Michalewicz Function

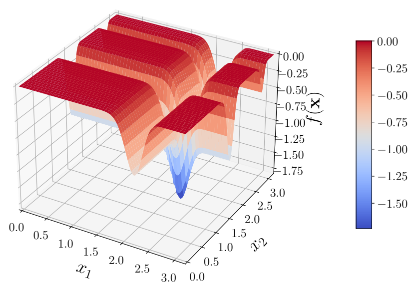


Figure 15: Michalewicz function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [0, \pi]^2$,

$$f(\mathbf{x}) = -\sum_{i=1}^{2} \sin(x_i) \sin^{20}\left(\frac{i x_i^2}{\pi}\right). \tag{27}$$

A global optimum is -1.801302197, at $\mathbf{x}^\star = [2.20279089, 1.57063923]$.

18 Rosenbrock Function

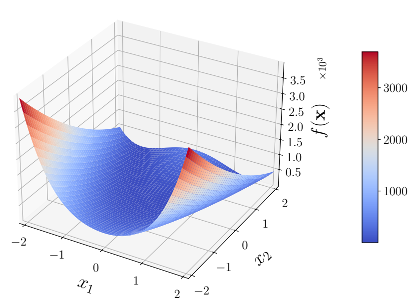


Figure 16: Rosenbrock function ($d = 2$).

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-2.048, 2.048]^d$,

$$f(\mathbf{x}) = \sum_{i=1}^{d-1} \left[100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2\right], \tag{28}$$

where $d \geq 2$. A global optimum is 0, at $\mathbf{x}^\star = [1, \ldots, 1] \in \mathbb{R}^d$.

19 Six-Hump Camel Function

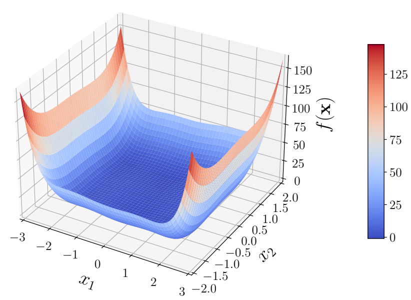


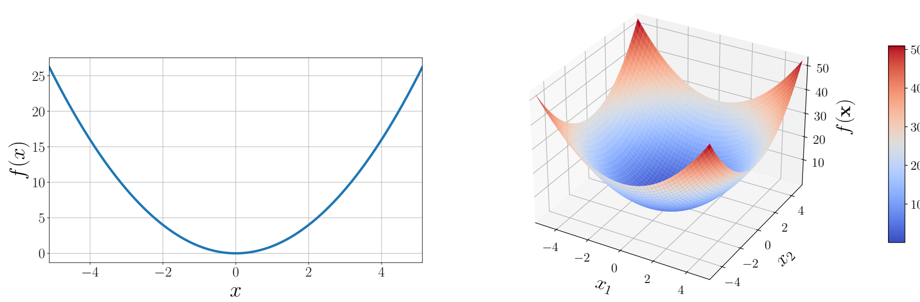
Figure 17: Six-Hump Camel function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2]$ for $-3 \leq x_1 \leq 3$, $-2 \leq x_2 \leq 2$,

$$f(\mathbf{x}) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right) x_1^2 + x_1 x_2 + (-4 + 4x_2^2) x_2^2. \tag{29}$$

Global optima are -1.0316, at $\mathbf{x}^\star = [0.0898, -0.7126]$ and $[-0.0898, 0.7126]$.

20 Sphere Function



(a) $d = 1$

(b) $d = 2$

Figure 18: Sphere function.

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-5.12, 5.12]^d$,

$$f(\mathbf{x}) = \sum_{i=1}^{d} x_i^2. \tag{30}$$

A global optimum is 0, at $\mathbf{x}^\star = [0, \ldots, 0] \in \mathbb{R}^d$.

21 Three-Hump Camel Function

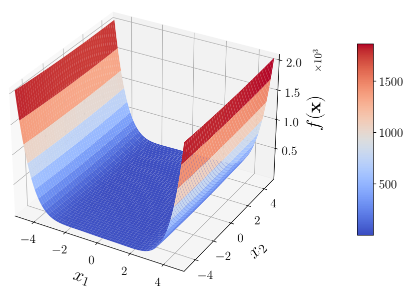


Figure 19: Three-Hump Camel function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2] \in [-5, 5]^2$,

$$f(\mathbf{x}) = 2x_1^2 - 1.05x_1^4 + \frac{x_1^6}{6} + x_1 x_2 + x_2^2. \tag{31}$$

A global optimum is 0, at $\mathbf{x}^\star = [0, 0]$.

References

J. Kim and S. Choi. BayesO: A Bayesian optimization framework in Python. `https://bayeso.org`, 2017.

S. Surjanovic and D. Bingham. Virtual library of simulation experiments: Test functions and datasets. `http://www.sfu.ca/~ssurjano`, 2013.