Benchmark Functions for Bayesian Optimization

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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 can be utilized in diverse problems on mathematical optimization.

Benchmark Functions for Bayesian Optimization

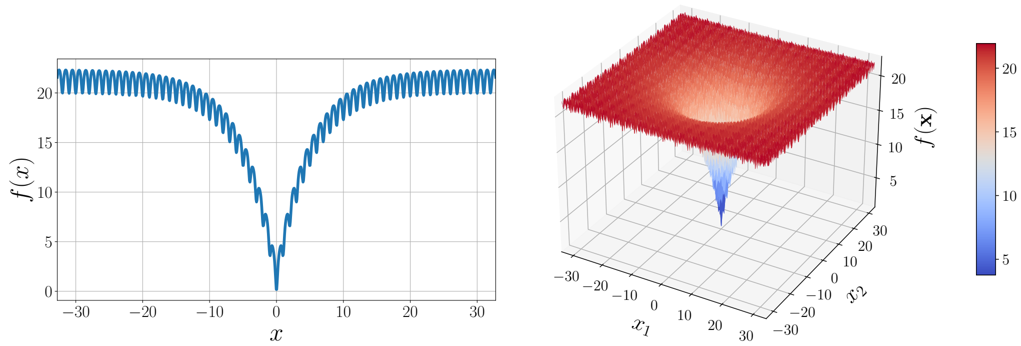
All functions are implemented in `https://github.com/jungtaekkim/bayeso-benchmarks`. We refer to [Surjanovic and Bingham, 2013] for specific forms of many benchmark functions, which are described in `https://www.sfu.ca/~ssurjano`. The details of `BayesO` [Kim and Choi, 2017] and `BayesO Benchmarks` are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

We will introduce the following benchmark functions in this article.

1. Ackley
2. Beale
3. Bohachevsky
4. Branin
5. Bukin 6
6. Colville
7. Cosines
8. De Jong 5

9. Drop-Wave
10. Easom
11. Eggholder
12. Goldstein-Price
13. Gramacy & Lee (2012)
14. Griewank
15. Hartmann 3D
16. Hartmann 6D
17. Holder Table
18. Kim1
19. Kim2
20. Kim3
21. Levy
22. Michalewicz
23. Rastrigin
24. Rosenbrock
25. Shubert
26. Six-Hump Camel
27. Sphere
28. Three-Hump Camel
29. Zakharov

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

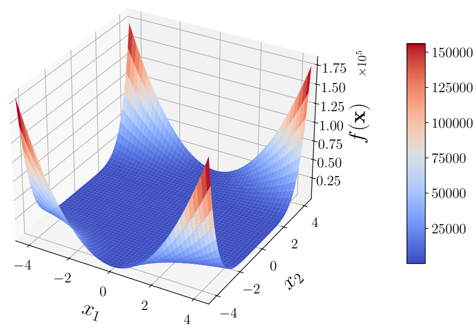


Figure 2: Beale function.

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

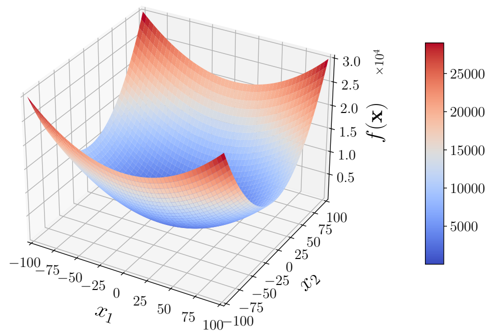


Figure 3: Bohachevsky function.

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

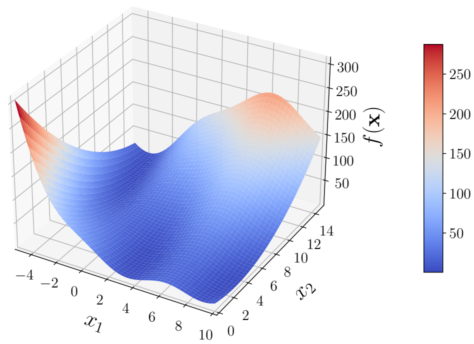


Figure 4: Branin function.

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 Bukin 6 Function

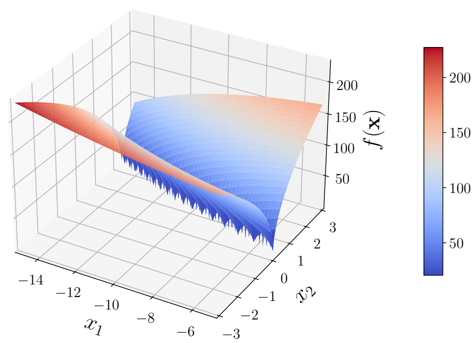


Figure 5: Bukin 6 function.

Given a two-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2]$ for $-15 \leq x_1 \leq -5$, $-3 \leq x_2 \leq 3$,

$$f(\mathbf{x}) = 100\sqrt{|x_2 - 0.01x_1^2|} + 0.01|x_1 + 10|. \tag{5}$$

A global optimum is 0, at $\mathbf{x}^\star = [-10, 1]$.

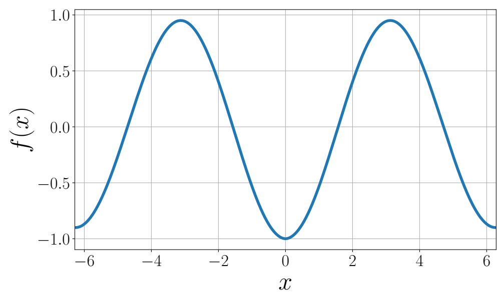
6 Colville Function

Given a four-dimensional input, $\mathbf{x} \coloneqq [x_1, x_2, x_3, x_4] \in [-10, 10]^4$,

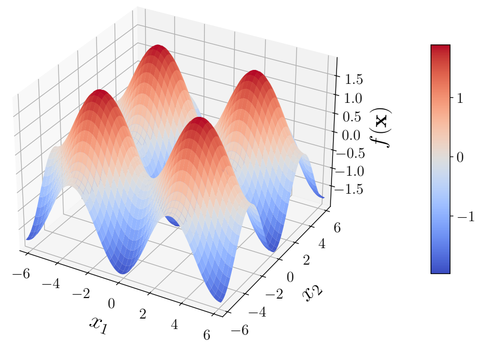
$$\begin{aligned} f(\mathbf{x}) = 100(x_1^2 - x_2)^2 + (x_1 - 1)^2 + (x_3 - 1)^2 + 90(x_3^2 - x_4)^2 \\ + 10.1((x_2 - 1)^2 + (x_4 - 1)^2) + 19.8(x_2 - 1)(x_4 - 1). \end{aligned} \tag{6}$$

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

7 Cosines Function



(a) $d = 1$



(b) $d = 2$

Figure 6: Cosines function.

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

$$f(\mathbf{x}) = \sum_{i=1}^{d} \cos(x_i) \left(\frac{0.1}{2\pi} |x_i| - 1 \right). \tag{7}$$

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

8 De Jong 5 Function

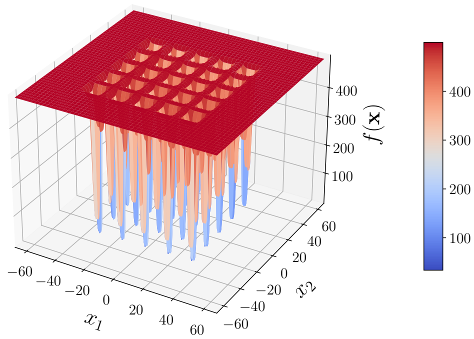


Figure 7: De Jong 5 function.

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

$$f(\mathbf{x}) = \left(0.002 + \sum_{i=1}^{25} \frac{1}{i + (x_1 - A_{1i})^6 + (x_2 - A_{2i})^6}\right)^{-1}, \tag{8}$$

where

$$\boldsymbol{A} = \begin{pmatrix} \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} & \mathbf{a} \\ -\mathbf{b} & -0.5\mathbf{b} & 0\mathbf{b} & 0.5\mathbf{b} & \mathbf{b} \end{pmatrix} \in \mathbb{R}^{2 \times 25}, \tag{9}$$

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

9 Drop-Wave Function

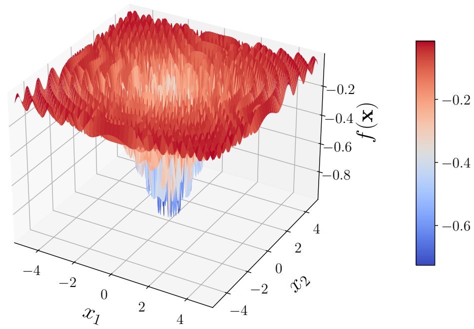


Figure 8: Drop-Wave function.

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

$$f(\mathbf{x}) = -\frac{1 + \cos\left(12\sqrt{x_1^2 + x_2^2}\right)}{0.5\left(x_1^2 + x_2^2\right) + 2}. \tag{10}$$

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

10 Easom Function

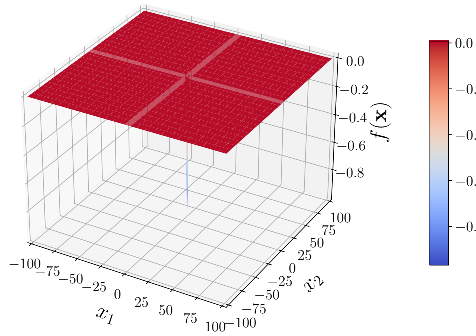


Figure 9: Easom function.

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

$$f(\mathbf{x}) = -\cos(x_1)\cos(x_2)\exp\left(-(x_1-\pi)^2-(x_2-\pi)^2\right). \tag{11}$$

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

11 Eggholder Function

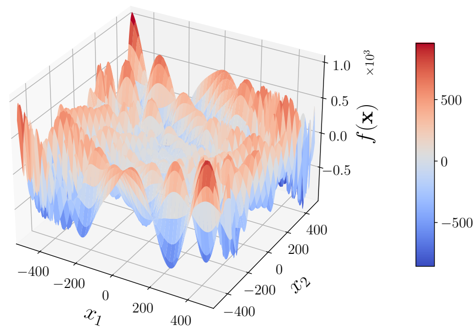


Figure 10: Eggholder function.

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

$$f(\mathbf{x}) = -(x_2 + 47)\sin\left(\sqrt{|x_2 + 0.5x_1 + 47|}\right) - x_1 \sin\left(\sqrt{|x_1 - (x_2 + 47)|}\right). \tag{12}$$

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

12 Goldstein-Price Function

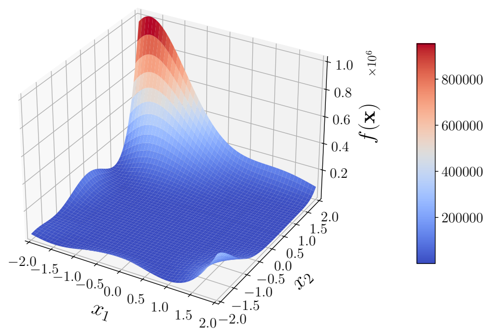


Figure 11: Goldstein-Price function.

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

$$f(\mathbf{x}) = \left[1 + A(B - 14x_2 + 6x_1x_2 + 3x_2^2)\right]\left[30 + C(D + 48x_2 - 36x_1x_2 + 27x_2^2)\right], \tag{13}$$

where

$$A = (x_1 + x_2 + 1)^2, \tag{14}$$

$$B = 19 - 14x_1 + 3x_1^2, \tag{15}$$

$$C = (2x_1 - 3x_2)^2, \tag{16}$$

$$D = 18 - 32x_1 + 12x_1^2. \tag{17}$$

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

13 Gramacy & Lee (2012) Function

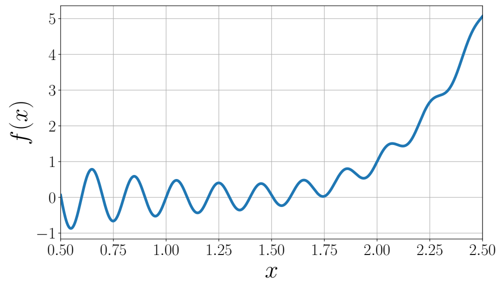


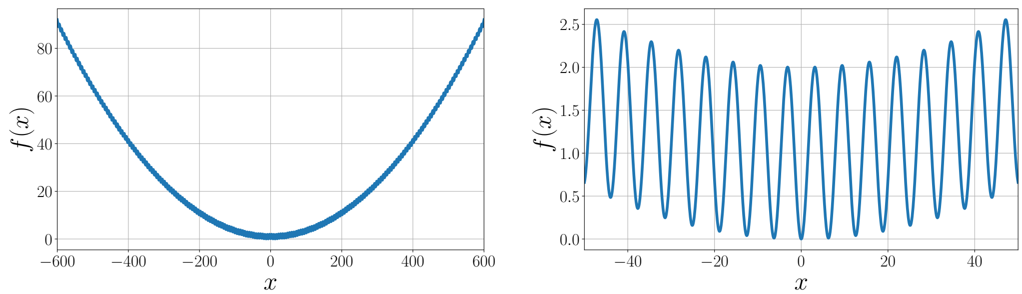
Figure 12: Gramacy & Lee (2012) function.

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

$$f(x) = \frac{\sin(10\pi x)}{2x} + (x-1)^4. \tag{18}$$

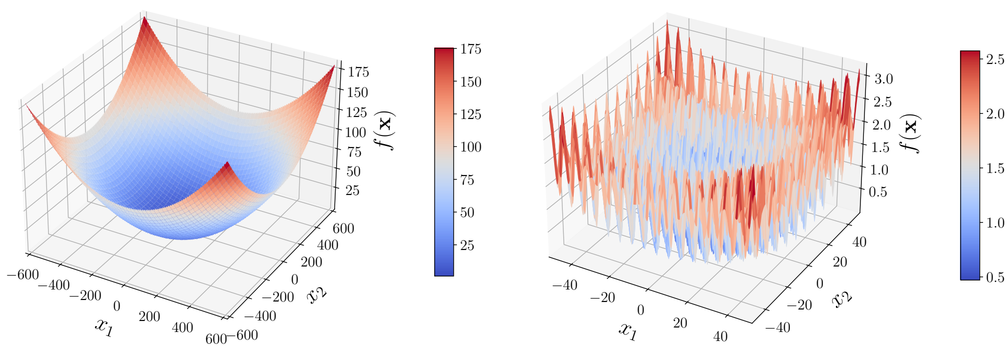
A global optimum is 0.54856405, at $x^\star = -0.86901113$.

14 Griewank Function



(a) $-600 \leq x \leq 600$ (b) $-50 \leq x \leq 50$

Figure 13: Griewank function ($d = 1$).



(a) $-600 \leq x_1 \leq 600$, $-600 \leq x_2 \leq 600$ (b) $-50 \leq x_1 \leq 50$, $-50 \leq x_2 \leq 50$

Figure 14: Griewank function ($d = 2$).

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-600, 600]^d$,

$$f(\mathbf{x}) = \sum_{i=1}^{d} \frac{x_i^2}{4000} - \prod_{i=1}^{d} \cos\left(\frac{x_i}{\sqrt{i}}\right) + 1. \tag{19}$$

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

15 Hartmann 3D Function

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

$$f(\mathbf{x}) = -\sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{3} A_{ij}(x_j - P_{ij})^2\right), \tag{20}$$

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

$$\boldsymbol{A} = \begin{pmatrix} 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \end{pmatrix}, \tag{21}$$

$$\boldsymbol{P} = 10^{-4} \begin{pmatrix} 3689 & 1170 & 2673 \\ 4699 & 4387 & 7470 \\ 1091 & 8732 & 5547 \\ 381 & 5743 & 8828 \end{pmatrix}. \tag{22}$$

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

16 Hartmann 6D Function

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

$$f(\mathbf{x}) = -\sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{6} A_{ij}(x_j - P_{ij})^2\right), \tag{23}$$

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

$$\boldsymbol{A} = \begin{pmatrix} 10 & 3 & 17 & 3.5 & 1.7 & 8 \\ 0.05 & 10 & 17 & 0.1 & 8 & 14 \\ 3 & 3.5 & 1.7 & 10 & 17 & 8 \\ 17 & 8 & 0.05 & 10 & 0.1 & 14 \end{pmatrix}, \tag{24}$$

$$\boldsymbol{P} = 10^{-4} \begin{pmatrix} 1312 & 1696 & 5569 & 124 & 8283 & 5886 \\ 2329 & 4135 & 8307 & 3736 & 1004 & 9991 \\ 2348 & 1451 & 3522 & 2883 & 3047 & 6650 \\ 4047 & 8828 & 8732 & 5743 & 1091 & 381 \end{pmatrix}. \tag{25}$$

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

17 Holder Table Function

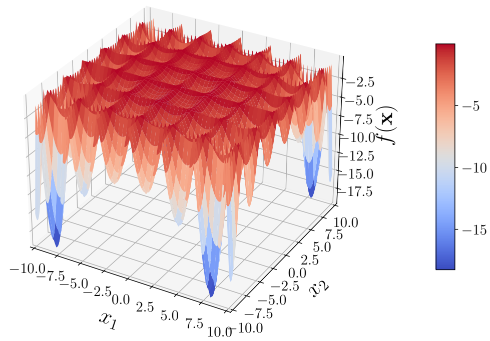


Figure 15: Holder Table function.

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

$$f(\mathbf{x}) = -\left|\sin(x_1)\cos(x_2)\exp\left(\left|1 - \frac{\sqrt{x_1^2 + x_2^2}}{\pi}\right|\right)\right|. \tag{26}$$

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

18 Kim1 Function

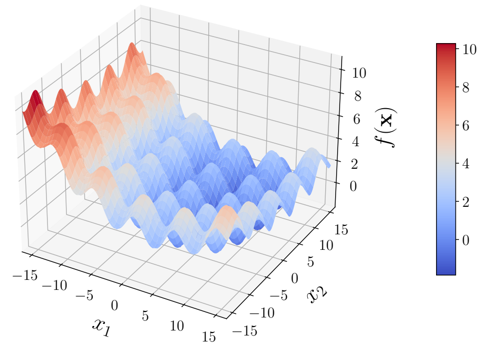


Figure 16: Kim1 function.

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

$$f(\mathbf{x}) = \sin(x_1) + \cos(x_2) + 0.016(x_1 - 5)^2 + 0.008(x_2 - 5)^2. \tag{27}$$

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

19 Kim2 Function

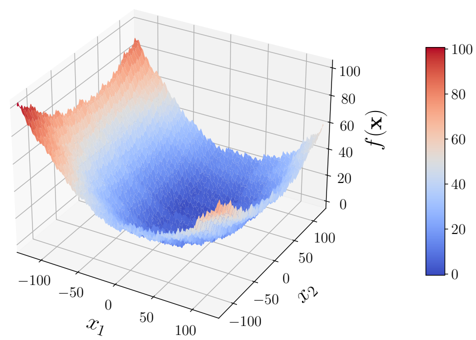


Figure 17: Kim2 function.

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

$$f(\mathbf{x}) = \sum_{i=0}^{4} \left(\sin\left(\frac{x_1}{2^i}\right) + \cos\left(\frac{x_2}{2^i}\right) \right) + 0.0032(x_1 - 20)^2 + 0.0016(x_2 - 20)^2. \tag{28}$$

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

20 Kim3 Function

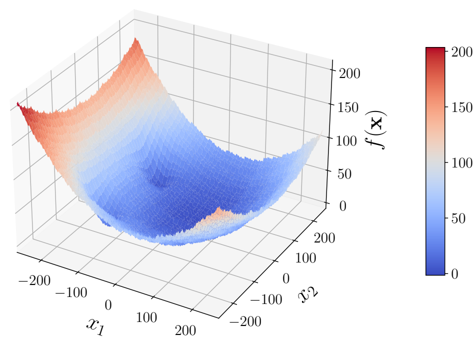


Figure 18: Kim3 function.

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

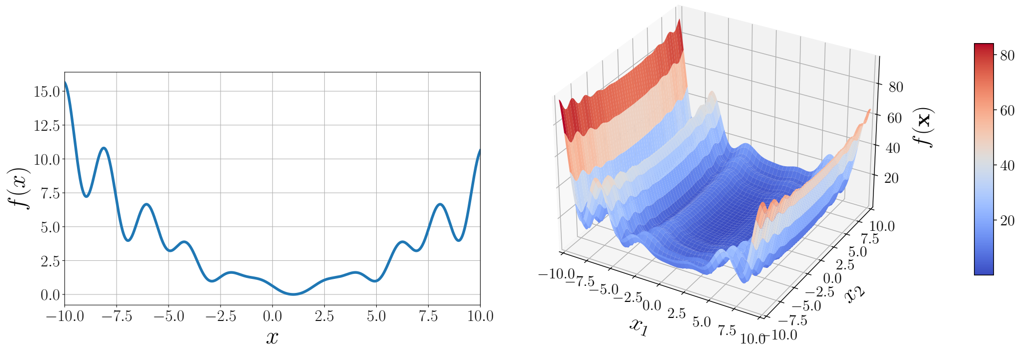
$$\begin{aligned} f(\mathbf{x}) = &\sum_{i=0}^{4} \left(\sin\left(\frac{x_1}{2^i}\right) + \cos\left(\frac{x_2}{2^i}\right) \right) \\ &+ 0.0016(x_1 - 40)^2 + 0.0008(x_2 - 40)^2 \\ &- 25600(\phi(\mathbf{x}; \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + \phi(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)), \end{aligned} \tag{29}$$

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

$$\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \begin{bmatrix} 1000 & 0 \\ 0 & 1000 \end{bmatrix}. \tag{30}$$

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

21 Levy Function



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

Figure 19: Levy function.

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-10, 10]^d$,

$$f(\mathbf{x}) = \sin^2\left(\frac{\pi(x_1+3)}{4}\right) + \sum_{i=1}^{d-1}\left(\frac{x_i-1}{4}\right)^2\left(1 + 10\sin^2\left(\frac{\pi(x_i+3)}{4}+1\right)\right)$$
$$+\left(\frac{x_d-1}{4}\right)^2\left(1+\sin^2\left(\frac{\pi(x_d+3)}{2}\right)\right). \tag{31}$$

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

22 Michalewicz Function

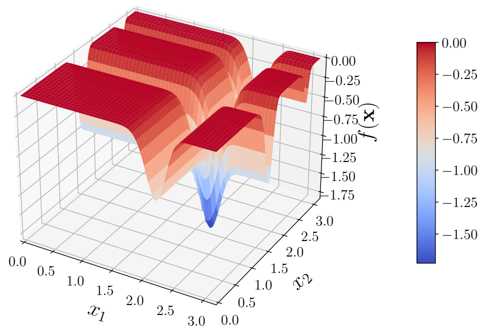


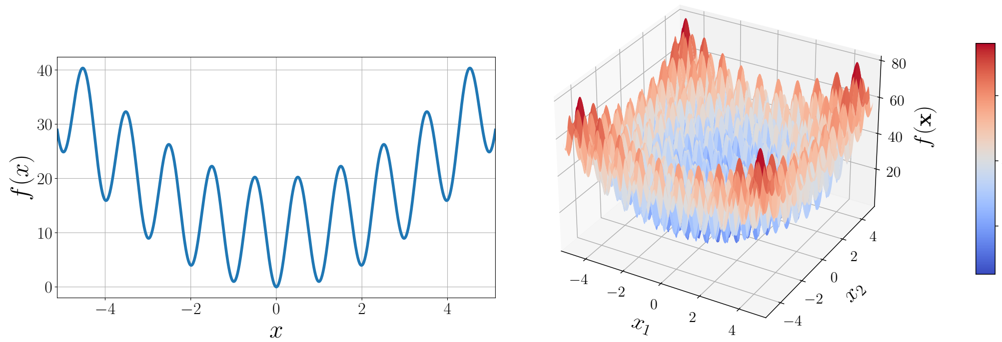
Figure 20: Michalewicz function.

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

$$f(\mathbf{x}) = -\sum_{i=1}^{2} \sin(x_i) \sin^{20}\left(\frac{ix_i^2}{\pi}\right). \tag{32}$$

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

23 Rastrigin Function



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

Figure 21: Rastrigin function.

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

$$f(\mathbf{x}) = 10d + \sum_{i=1}^{d} \left(x_i^2 - 10 \cos(2\pi x_i) \right). \tag{33}$$

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

24 Rosenbrock Function

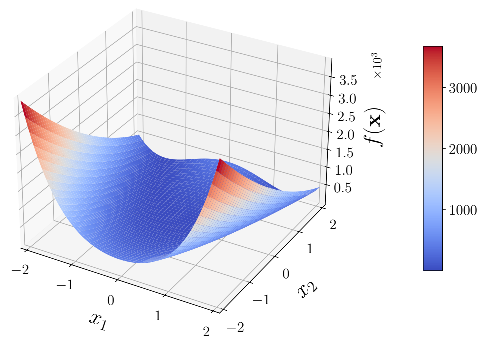


Figure 22: Rosenbrock function ($d = 2$).

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

$$f(\mathbf{x}) = \sum_{i=1}^{d-1} \left[100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2\right], \tag{34}$$

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

25 Shubert Function

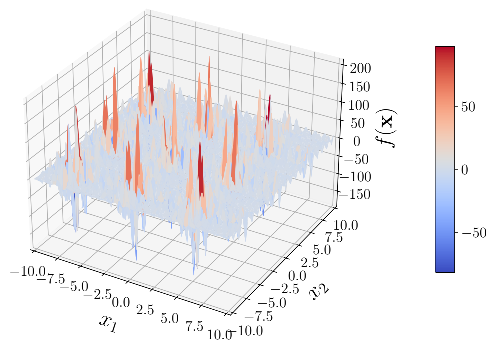


Figure 23: Shubert function.

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

$$f(\mathbf{x}) = \left(\sum_{i=1}^{5} i \cos((i+1)x_1 + i) \right) \left(\sum_{i=1}^{5} i \cos((i+1)x_2 + i) \right). \tag{35}$$

A global optimum is -186.73090883, at $\mathbf{x}^\star = [-7.08350641, -7.70831374]$.

26 Six-Hump Camel Function

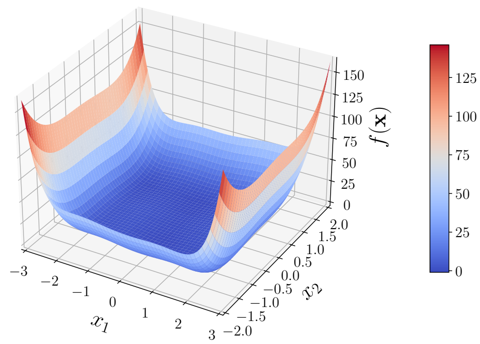


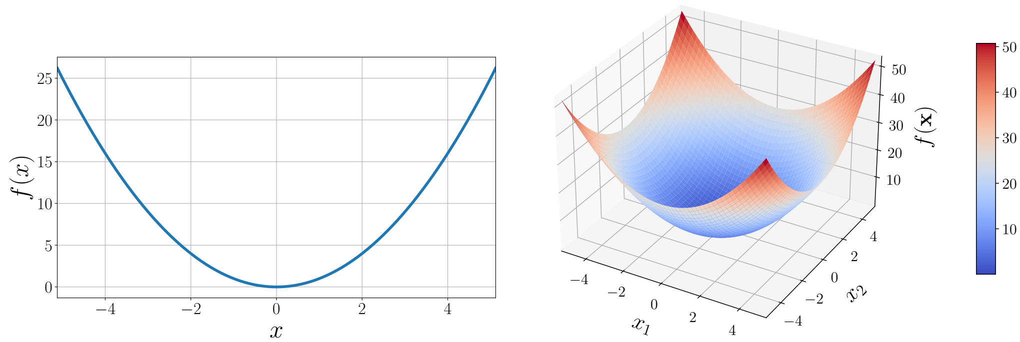
Figure 24: Six-Hump Camel function.

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

$$f(\mathbf{x}) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3}\right) x_1^2 + x_1 x_2 + (-4 + 4x_2^2)x_2^2. \tag{36}$$

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

27 Sphere Function



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

Figure 25: Sphere function.

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

$$f(\mathbf{x}) = \sum_{i=1}^{d} x_i^2. \tag{37}$$

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

28 Three-Hump Camel Function

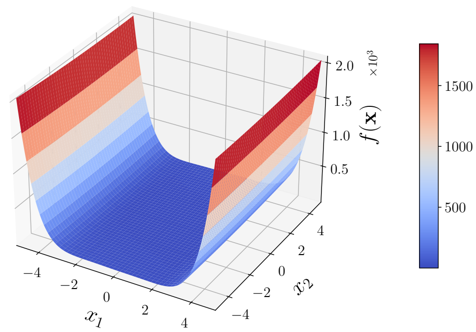


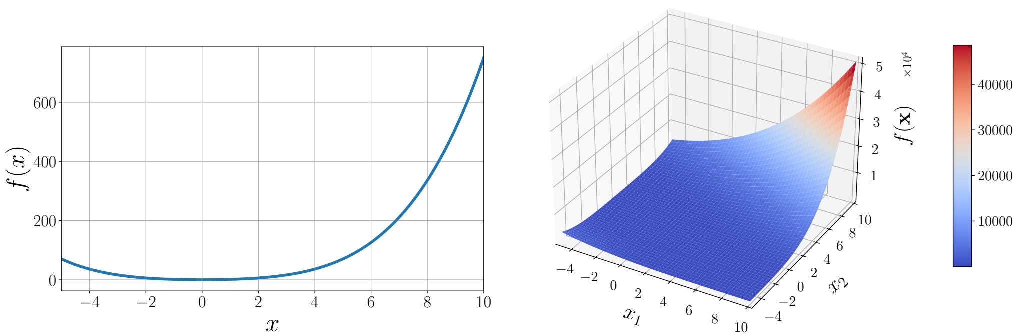
Figure 26: Three-Hump Camel function.

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

$$f(\mathbf{x}) = 2x_1^2 - 1.05x_1^4 + \frac{x_1^6}{6} + x_1 x_2 + x_2^2. \tag{38}$$

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

29 Zakharov Function



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

Figure 27: Zakharov function.

Given a d-dimensional input, $\mathbf{x} \coloneqq [x_1, \ldots, x_d] \in [-5, 10]^d$,

$$f(\mathbf{x}) = \sum_{i=1}^{d} x_i^2 + \left(\sum_{i=1}^{d} 0.5 i x_i \right)^2 + \left(\sum_{i=1}^{d} 0.5 i x_i \right)^4 . \tag{39}$$

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

References

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