为评估优化算法的性能，我们使用了 Goldstein-Price 函数。为了增强其数值稳定性和适应性，我们对该函数进行了对数化和归一化处理。

Goldstein-Price 函数的标准形式为：

和定义域为 [−2,2]，该函数有一个全局最小值点在 = (0,−1)，最小值为 = 3。

Target function为其对数形式：

Source function 1 对输入变量进行了平移和缩放处理：

Source function 2 对进行了取反处理：

Source function 3 为单独设计的其他函数：

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | **Datasets 1** | | | | **Datasets 2** | | | |
|  | **Inputs and output** | **Min** | **Max** | **Mean** | **Standard deviation** | **Min** | **Max** | **Mean** | **Standard deviation** |
| **Inputs** | **Solution treatment time (h)** | 0.5 | 5 | 2.6 | 1.21 | 0 | 2 | 0.8 | 0.93 |
|  | **Solution treatment temperature (℃)** | 899 | 1348 | 1176.6 | 106.68 | 0 | 1080 | 685.48 | 484.04 |
|  | **Solution cooling way** | 0 | 4 | 1.38 | 1.37 | 0 | 3 | 0.74 | 0.63 |
|  | **Aging treatment time (h)** | 1 | 24 | 11.1 | 8.68 | 0 | 50 | 2.77 | 8.44 |
|  | **Aging treatment temperature (℃)** | 704 | 1145 | 934.1 | 148.73 | 0 | 770 | 467.01 | 330.43 |
|  | **Aging cooling way** | 0 | 4 | 0.85 | 0.97 | 0 | 1 | 0.67 | 0.47 |
|  | **2nd aging treatment time (h)** | 0 | 32 | 11.41 | 9.16 | 0 | 50 | 1.14 | 7.49 |
|  | **2nd aging treatment temperature (℃)** | 0 | 899 | 507.62 | 401.12 | 0 | 610 | 13.86 | 91.43 |
|  | **2nd aging cooling way** | 0 | 1 | 0.26 | 0.44 | 0 | 1 | 0.02 | 0.15 |
|  | **C (mass%)** | 0 | 0.43 | 0.09 | 0.11 | 0 | 0.1 | 0.06 | 0.03 |
|  | **Si (mass%)** | 0 | 0.86 | 0.2 | 0.27 | 0 | 0.46 | 0.24 | 0.17 |
|  | **Ni (mass%)** | 10.35 | 77.26 | 50.7 | 20.34 | 0 | 0.7 | 0.15 | 0.29 |
|  | **Mo (mass%)** | 0 | 4.4 | 1.74 | 1.57 | 0 | 0.8 | 0.36 | 0.25 |
|  | **W (mass%)** | 0 | 18.6 | 2.92 | 3.09 | 0 | 1 | 0.07 | 0.25 |
|  | **Al (mass%)** | 0 | 7.5 | 2.78 | 2.4 | 5.75 | 6.61 | 5.97 | 0.24 |
|  | **N (mass%)** | 0 | 0.16 | 0.01 | 0.03 | 0 | 0.05 | 0.01 | 0.01 |
|  | **Nb+Ta (mass%)** | 0 | 12 | 3.08 | 3.33 | 0 | 1.4 | 0.55 | 0.42 |
|  | **B (mass%)** | 0 | 0.05 | 0.01 | 0.01 | 0 | 0.11 | 0.01 | 0.02 |
|  | **V (mass%)** | 0 | 0.32 | 0.03 | 0.09 | 0 | 4.23 | 1.25 | 1.89 |
|  | **Ti (mass%)** | 0 | 5 | 1.41 | 1.3 | 82.95 | 89.74 | 85.95 | 2.15 |
|  | **Fe (mass%)** | 0 | 53.18 | 9.98 | 16.72 | 0 | 1.18 | 0.16 | 0.34 |
|  | **Zr (mass%)** | 0 | 0.04 | 0 | 0.01 | 0 | 4 | 2.44 | 1.64 |
|  | **Sn (mass%)** | 0 | 0 | 0 | 0 | 0 | 4.02 | 2.74 | 1.84 |
|  | **Mn (mass%)** | 0 | 1.91 | 0.4 | 0.61 | 0 | 0 | 0 | 0 |
|  | **P (mass%)** | 0 | 0.02 | 0 | 0.01 | 0 | 0 | 0 | 0 |
|  | **S (mass%)** | 0 | 0.02 | 0 | 0.01 | 0 | 0 | 0 | 0 |
|  | **Cr (mass%)** | 0.6 | 25.43 | 13.75 | 6.07 | 0 | 0 | 0 | 0 |
|  | **Cu (mass%)** | 0 | 0.08 | 0.02 | 0.02 | 0 | 0 | 0 | 0 |
|  | **Co (mass%)** | 0 | 54.71 | 11.72 | 13.01 | 0 | 0 | 0 | 0 |
|  | **Re (mass%)** | 0 | 7.5 | 1.04 | 1.85 | 0 | 0 | 0 | 0 |
|  | **Y (mass%)** | 0 | 0.05 | 0 | 0.01 | 0 | 0 | 0 | 0 |
|  | **Hf (mass%)** | 0 | 5.6 | 0.09 | 0.44 | 0 | 0 | 0 | 0 |
|  | **Test temperature (℃)** | 204 | 1800 | 847.62 | 201.87 | 475 | 675 | 603.41 | 47.67 |
|  | **Test stress (MPa)** | 10 | 800 | 253.86 | 173.62 | 97 | 550 | 283.86 | 90.27 |
|  | **Creep rupture life (h)** | 1.2 | 151536 | 5467.77 | 15470 | 0 | 4770 | 299 | 796.87 |
| **Output** | **Solution treatment time (h)** | 0.5 | 5 | 2.6 | 1.21 | 0 | 2 | 0.8 | 0.93 |

测试函数

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Iterations** | **0** | **5** | **10** | **15** | **20** | **25** | **30** |
| **Standard BO** | 3.46 ± 0.77 | 3.08 ± 1.04 | 2.24 ± 1.0 | 1.79 ± 0.79 | 1.47 ± 0.57 | 1.42 ± 0.54 | 1.35 ± 0.48 |
| **Transfer BO 1** | 3.44 ± 0.79 | 2.45 ± 0.53 | 1.83 ± 0.52 | 1.44 ± 0.33 | 1.27 ± 0.13 | 1.24 ± 0.04 | 1.23 ± 0.0 |
| **Transfer BO 2** | 3.62 ± 1.08 | 3.33 ± 1.17 | 2.31 ± 1.06 | 1.75 ± 0.92 | 1.58 ± 0.81 | 1.42 ± 0.66 | 1.38 ± 0.61 |
| **Transfer BO 3** | 3.31 ± 0.93 | 2.83 ± 1.04 | 2.11 ± 1.05 | 1.58 ± 0.65 | 1.38 ± 0.54 | 1.24 ± 0.02 | 1.23 ± 0.0 |

钯催化数据集

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Iterations** | **0** | **5** | **10** | **15** | **20** | **25** | **30** |
| **Aryl-1** | | | | | | | |
| **Random** | 36.34 ± 5.63 | 40.67 ± 4.75 | 42.36 ± 3.93 | 43.58 ± 3.06 | 44.05 ± 2.67 | 44.32 ± 2.24 | 44.65 ± 1.76 |
| **LHS** | 34.99 ± 5.46 | 39.31 ± 4.67 | 42.64 ± 3.72 | 43.25 ± 3.37 | 44.25 ± 2.42 | 44.38 ± 2.15 | 44.45 ± 2.13 |
| **EDS** | 36.3 ± 3.57 | 39.93 ± 4.44 | 42.88 ± 3.69 | 43.53 ± 3.19 | 43.98 ± 2.68 | 44.78 ± 0.99 | 45.05 ± 0.0 |
| **Aryl-9** | | | | | | | |
| **Random** | 82.24 ± 2.6 | 83.53 ± 2.07 | 84.65 ± 1.56 | 85.19 ± 0.99 | 85.54 ± 0.7 | 85.68 ± 0.53 | 85.82 ± 0.34 |
| **LHS** | 80.23 ± 3.2 | 83.4 ± 1.81 | 84.55 ± 1.43 | 85.1 ± 1.06 | 85.38 ± 0.94 | 85.62 ± 0.66 | 85.78 ± 0.44 |
| **EDS** | 82.86 ± 1.31 | 83.7 ± 0.81 | 84.26 ± 0.82 | 84.9 ± 0.97 | 85.26 ± 0.9 | 85.51 ± 0.72 | 85.82 ± 0.34 |
| **Aryl-15** | | | | | | | |
| **Random** | 92.41 ± 4.14 | 94.81 ± 3.76 | 95.86 ± 2.6 | 96.75 ± 1.95 | 97.0 ± 1.79 | 97.48 ± 1.53 | 97.66 ± 1.39 |
| **LHS** | 91.38 ± 4.11 | 94.03 ± 4.0 | 95.62 ± 2.41 | 96.78 ± 1.89 | 97.03 ± 1.74 | 97.57 ± 1.46 | 97.75 ± 1.3 |
| **EDS** | 93.46 ± 1.77 | 94.8 ± 1.41 | 95.61 ± 1.79 | 96.32 ± 1.9 | 97.19 ± 1.71 | 97.83 ± 1.22 | 98.29 ± 0.0 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Iterations** | **0** | **10** | **20** | **30** | **40** | **50** |
| **Aryl-1** | | | | | | |
| **Standard BO** | 32.27 ± 4.33 | 38.83 ± 4.94 | 41.77 ± 4.33 | 42.6 ± 3.79 | 43.25 ± 3.37 | 43.78 ± 2.88 |
| **Transfer BO 2** | 32.6 ± 4.46 | 40.49 ± 4.99 | 42.82 ± 3.71 | 43.85 ± 2.88 | 44.05 ± 2.67 | 44.65 ± 1.76 |
| **Transfer BO 4** | 31.21 ± 5.57 | 38.92 ± 5.29 | 41.88 ± 4.09 | 43.4 ± 3.35 | 44.05 ± 2.67 | 44.38 ± 2.15 |
| **Transfer BO 7** | 32.17 ± 4.3 | 37.84 ± 5.66 | 41.84 ± 4.5 | 43.66 ± 3.03 | 44.19 ± 2.6 | 44.4 ± 2.33 |
| **Aryl-1** | | | | | | |
| **Standard BO** | 76.98 ± 6.15 | 82.17 ± 2.74 | 83.23 ± 2.09 | 83.58 ± 2.27 | 84.6 ± 1.5 | 85.18 ± 1.13 |
| **Transfer BO 2** | 78.54 ± 6.06 | 83.45 ± 1.29 | 84.29 ± 0.88 | 84.53 ± 0.97 | 84.89 ± 0.92 | 85.26 ± 0.9 |
| **Transfer BO 8** | 81.62 ± 5.27 | 85.06 ± 0.76 | 85.45 ± 0.54 | 85.72 ± 0.38 | 85.84 ± 0.22 | 85.87 ± 0.16 |
| **Transfer BO 14** | 76.13 ± 5.61 | 83.13 ± 1.52 | 84.98 ± 1.22 | 85.43 ± 0.84 | 85.6 ± 0.73 | 85.72 ± 0.54 |
| **Aryl-1** | | | | | | |
| **Standard BO** | 79.04 ± 13.6 | 92.48 ± 4.4 | 94.39 ± 2.79 | 95.17 ± 2.35 | 95.59 ± 1.85 | 95.97 ± 1.83 |
| **Transfer BO 7** | 85.31 ± 7.6 | 92.07 ± 4.59 | 94.18 ± 2.69 | 95.87 ± 1.81 | 96.18 ± 1.83 | 96.38 ± 1.84 |
| **Transfer BO 8** | 89.57 ± 9.7 | 94.05 ± 1.81 | 98.06 ± 1.01 | 98.07 ± 1.0 | 98.07 ± 1.0 | 98.07 ± 1.0 |
| **Transfer BO 11** | 90.24 ± 8.39 | 94.83 ± 1.16 | 95.45 ± 1.58 | 96.31 ± 1.81 | 96.58 ± 1.82 | 97.12 ± 1.71 |

合金数据集

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Iterations** | **0** | **5** | **10** | **15** | **20** | **25** | **30** |
| **Dataset 1** | | | | | | | |
| **Random** | 10.71 ± 0.78 | 11.22 ± 0.55 | 11.55 ± 0.43 | 11.71 ± 0.29 | 11.73 ± 0.26 | 11.79 ± 0.19 | 11.82 ± 0.18 |
| **Standard BO** | 10.96 ± 0.67 | 11.51 ± 0.39 | 11.76 ± 0.29 | 11.84 ± 0.11 | 11.84 ± 0.11 | 11.88 ± 0.09 | 11.89 ± 0.08 |
| **Transfer BO** | 10.57 ± 0.92 | 11.55 ± 0.38 | 11.76 ± 0.27 | 11.8 ± 0.24 | 11.87 ± 0.11 | 11.9 ± 0.06 | 11.91 ± 0.04 |
| **Dataset 2** | | | | | | | |
| **Random** | 6.29 ± 1.09 | 7.3 ± 0.98 | 7.97 ± 0.64 | 8.15 ± 0.5 | 8.27 ± 0.45 | 8.27 ± 0.45 | 8.44 ± 0.14 |
| **Standard BO** | 5.96 ± 1.23 | 7.26 ± 1.15 | 8.04 ± 0.86 | 8.23 ± 0.68 | 8.38 ± 0.39 | 8.45 ± 0.1 | 8.47 ± 0.0 |
| **Transfer BO** | 6.09 ± 1.02 | 7.55 ± 1.19 | 8.26 ± 0.57 | 8.4 ± 0.33 | 8.47 ± 0.0 | 8.47 ± 0.0 | 8.47 ± 0.0 |