**Evaluation of machine learning and empirical models for concrete creep compliance prediction**

Viet-Linh Tran1,2 and Jin-Kook Kim1\*

1 Department of Civil Engineering, Seoul National University of Science and Technology, 232 Gongneung-ro, Nowon-gu, Seoul 01811, Republic of Korea

2 Department of Civil Engineering, Vinh University, Vinh 461010, Vietnam

\* Corresponding author : [jinkook.kim@seoultech.ac.kr](mailto:jinkook.kim@seoultech.ac.kr).

**1. Dataset CT1**

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-1.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 50.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-2.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 100.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-3.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 150.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-4.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 200.

A picture containing screenshot, colorfulness, rectangle, line

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-5.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 250.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-6.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 300.

**Table S-1** Performance of GWO-LGB models on the training set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 0.996 | 44 | 0.951 | 43 | 3.019 | 44 | 1.498 | 35 | 166 |
|  | 0.60 | 0.995 | 10 | 0.943 | 9 | 3.276 | 19 | 1.658 | 10 | 48 |
|  | 0.65 | 0.995 | 10 | 0.945 | 13 | 3.145 | 31 | 1.551 | 24 | 78 |
|  | 0.70 | 0.995 | 10 | 0.945 | 13 | 3.132 | 34 | 1.559 | 22 | 79 |
|  | 0.75 | 0.995 | 10 | 0.952 | 48 | 3.056 | 41 | 1.462 | 43 | 142 |
|  | 0.80 | 0.995 | 10 | 0.95 | 39 | 3.029 | 43 | 1.424 | 45 | 137 |
|  | 0.85 | 0.995 | 10 | 0.947 | 25 | 3.244 | 21 | 1.532 | 27 | 83 |
|  | 0.90 | 0.994 | 1 | 0.946 | 19 | 3.442 | 2 | 1.576 | 19 | 41 |
| 100 | 0.55 | 0.994 | 1 | 0.94 | 3 | 3.392 | 5 | 1.762 | 1 | 10 |
|  | 0.60 | 0.995 | 10 | 0.946 | 19 | 3.094 | 40 | 1.538 | 26 | 95 |
|  | 0.65 | 0.995 | 10 | 0.946 | 19 | 3.105 | 38 | 1.529 | 28 | 95 |
|  | 0.70 | 0.995 | 10 | 0.949 | 34 | 3.046 | 42 | 1.462 | 43 | 129 |
|  | 0.75 | 0.996 | 44 | 0.95 | 39 | 2.987 | 46 | 1.41 | 47 | 176 |
|  | 0.80 | 0.995 | 10 | 0.947 | 25 | 3.176 | 27 | 1.563 | 20 | 82 |
|  | 0.85 | 0.995 | 10 | 0.948 | 30 | 3.16 | 28 | 1.477 | 39 | 107 |
|  | **0.90** | **0.994** | **1** | **0.948** | **30** | **3.358** | **10** | **1.559** | **22** | **63** |
| 150 | 0.55 | 0.995 | 10 | 0.946 | 19 | 3.128 | 37 | 1.581 | 17 | 83 |
|  | 0.60 | 0.995 | 10 | 0.94 | 3 | 3.365 | 8 | 1.683 | 7 | 28 |
|  | 0.65 | 0.995 | 10 | 0.946 | 19 | 3.098 | 39 | 1.526 | 29 | 97 |
|  | 0.70 | 0.994 | 1 | 0.941 | 7 | 3.384 | 7 | 1.706 | 5 | 20 |
|  | 0.75 | 0.996 | 44 | 0.951 | 43 | 2.972 | 47 | 1.385 | 48 | 182 |
|  | 0.80 | 0.995 | 10 | 0.948 | 30 | 3.157 | 29 | 1.512 | 32 | 101 |
|  | 0.85 | 0.995 | 10 | 0.945 | 13 | 3.3 | 16 | 1.599 | 15 | 54 |
|  | 0.90 | 0.994 | 1 | 0.947 | 25 | 3.401 | 4 | 1.563 | 20 | 50 |
| 200 | 0.55 | 0.995 | 10 | 0.943 | 9 | 3.338 | 11 | 1.713 | 4 | 34 |
|  | 0.60 | 0.994 | 1 | 0.937 | 1 | 3.492 | 1 | 1.752 | 2 | 5 |
|  | 0.65 | 0.995 | 10 | 0.945 | 13 | 3.18 | 26 | 1.579 | 18 | 67 |
|  | 0.70 | 0.995 | 10 | 0.947 | 25 | 3.131 | 35 | 1.506 | 33 | 103 |
|  | 0.75 | 0.995 | 10 | 0.949 | 34 | 3.133 | 33 | 1.488 | 37 | 114 |
|  | 0.80 | 0.995 | 10 | 0.945 | 13 | 3.293 | 17 | 1.599 | 15 | 55 |
|  | 0.85 | 0.994 | 1 | 0.947 | 25 | 3.39 | 6 | 1.62 | 14 | 46 |
|  | 0.90 | 0.995 | 10 | 0.951 | 43 | 3.208 | 22 | 1.465 | 42 | 117 |
| 250 | 0.55 | 0.995 | 10 | 0.943 | 9 | 3.315 | 13 | 1.686 | 6 | 38 |
|  | 0.60 | 0.995 | 10 | 0.94 | 3 | 3.289 | 18 | 1.623 | 13 | 44 |
|  | 0.65 | 0.994 | 1 | 0.939 | 2 | 3.414 | 3 | 1.715 | 3 | 9 |
|  | 0.70 | 0.996 | 44 | 0.951 | 43 | 2.954 | 48 | 1.423 | 46 | 181 |
|  | 0.75 | 0.995 | 10 | 0.949 | 34 | 3.134 | 32 | 1.501 | 34 | 110 |
|  | 0.80 | 0.995 | 10 | 0.95 | 39 | 3.131 | 35 | 1.491 | 36 | 120 |
|  | 0.85 | 0.994 | 1 | 0.945 | 13 | 3.36 | 9 | 1.626 | 12 | 35 |
|  | 0.90 | 0.995 | 10 | 0.951 | 43 | 3.189 | 24 | 1.467 | 41 | 118 |
| 300 | 0.55 | 0.995 | 10 | 0.943 | 9 | 3.264 | 20 | 1.682 | 8 | 47 |
|  | 0.60 | 0.995 | 10 | 0.94 | 3 | 3.308 | 15 | 1.636 | 11 | 39 |
|  | 0.65 | 0.995 | 10 | 0.941 | 7 | 3.33 | 12 | 1.674 | 9 | 38 |
|  | 0.70 | 0.996 | 44 | 0.95 | 39 | 2.999 | 45 | 1.471 | 40 | 168 |
|  | 0.75 | 0.995 | 10 | 0.946 | 19 | 3.204 | 23 | 1.548 | 25 | 77 |
|  | 0.80 | 0.995 | 10 | 0.948 | 30 | 3.189 | 24 | 1.521 | 31 | 95 |
|  | 0.85 | 0.995 | 10 | 0.949 | 34 | 3.152 | 30 | 1.485 | 38 | 112 |
|  | 0.90 | 0.995 | 10 | 0.949 | 34 | 3.313 | 14 | 1.526 | 29 | 87 |

**Table S-2** Performance of GWO-LGB models on the test set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 0.976 | 2 | 0.874 | 6 | 6.798 | 5 | 3.439 | 6 | 19 |
|  | 0.60 | 0.977 | 6 | 0.869 | 5 | 6.657 | 7 | 3.406 | 7 | 25 |
|  | 0.65 | 0.979 | 19 | 0.885 | 13 | 6.285 | 31 | 3.209 | 13 | 76 |
|  | 0.70 | 0.979 | 19 | 0.89 | 20 | 6.368 | 21 | 3.136 | 19 | 79 |
|  | 0.75 | 0.979 | 19 | 0.895 | 25 | 6.33 | 29 | 3.061 | 35 | 108 |
|  | 0.80 | 0.978 | 12 | 0.894 | 24 | 6.495 | 14 | 3.122 | 20 | 70 |
|  | 0.85 | 0.981 | 39 | 0.902 | 41 | 6.118 | 40 | 3.031 | 41 | 161 |
|  | 0.90 | 0.981 | 39 | 0.909 | 45 | 5.754 | 46 | 2.805 | 48 | 178 |
| 100 | 0.55 | 0.976 | 2 | 0.867 | 1 | 6.845 | 2 | 3.494 | 3 | 8 |
|  | 0.60 | 0.977 | 6 | 0.882 | 12 | 6.579 | 10 | 3.285 | 11 | 39 |
|  | 0.65 | 0.979 | 19 | 0.892 | 22 | 6.206 | 37 | 3.12 | 21 | 99 |
|  | 0.70 | 0.979 | 19 | 0.896 | 26 | 6.274 | 32 | 3.086 | 30 | 107 |
|  | 0.75 | 0.978 | 12 | 0.893 | 23 | 6.425 | 16 | 3.102 | 26 | 77 |
|  | 0.80 | 0.978 | 12 | 0.888 | 15 | 6.522 | 13 | 3.205 | 14 | 54 |
|  | 0.85 | 0.98 | 35 | 0.9 | 39 | 6.224 | 34 | 3.042 | 38 | 146 |
|  | **0.90** | **0.982** | **47** | **0.911** | **46** | **5.694** | **48** | **2.807** | **47** | **188** |
| 150 | 0.55 | 0.977 | 6 | 0.874 | 6 | 6.705 | 6 | 3.447 | 5 | 23 |
|  | 0.60 | 0.978 | 12 | 0.876 | 8 | 6.542 | 12 | 3.273 | 12 | 44 |
|  | 0.65 | 0.979 | 19 | 0.889 | 18 | 6.226 | 33 | 3.099 | 28 | 98 |
|  | 0.70 | 0.98 | 35 | 0.889 | 18 | 6.218 | 35 | 3.15 | 18 | 106 |
|  | 0.75 | 0.978 | 12 | 0.897 | 30 | 6.406 | 18 | 3.066 | 34 | 94 |
|  | 0.80 | 0.979 | 19 | 0.898 | 37 | 6.361 | 22 | 3.101 | 27 | 105 |
|  | 0.85 | 0.981 | 39 | 0.897 | 30 | 6.06 | 42 | 2.997 | 42 | 153 |
|  | 0.90 | 0.982 | 47 | 0.908 | 44 | 5.737 | 47 | 2.814 | 45 | 183 |
| 200 | 0.55 | 0.976 | 2 | 0.868 | 3 | 6.817 | 4 | 3.532 | 2 | 11 |
|  | 0.60 | 0.977 | 6 | 0.878 | 11 | 6.571 | 11 | 3.315 | 9 | 37 |
|  | 0.65 | 0.979 | 19 | 0.888 | 15 | 6.332 | 28 | 3.155 | 17 | 79 |
|  | 0.70 | 0.979 | 19 | 0.897 | 30 | 6.327 | 30 | 3.097 | 29 | 108 |
|  | 0.75 | 0.979 | 19 | 0.897 | 30 | 6.347 | 24 | 3.059 | 37 | 110 |
|  | 0.80 | 0.979 | 19 | 0.897 | 30 | 6.422 | 17 | 3.16 | 16 | 82 |
|  | 0.85 | 0.981 | 39 | 0.896 | 26 | 6.118 | 40 | 3.041 | 39 | 144 |
|  | 0.90 | 0.981 | 39 | 0.912 | 48 | 5.799 | 44 | 2.81 | 46 | 177 |
| 250 | 0.55 | 0.976 | 2 | 0.868 | 3 | 6.831 | 3 | 3.462 | 4 | 12 |
|  | 0.60 | 0.977 | 6 | 0.876 | 8 | 6.632 | 8 | 3.316 | 8 | 30 |
|  | 0.65 | 0.98 | 35 | 0.887 | 14 | 6.138 | 38 | 3.112 | 24 | 111 |
|  | 0.70 | 0.979 | 19 | 0.898 | 37 | 6.333 | 26 | 3.104 | 25 | 107 |
|  | 0.75 | 0.979 | 19 | 0.896 | 26 | 6.337 | 25 | 3.086 | 30 | 100 |
|  | 0.80 | 0.979 | 19 | 0.897 | 30 | 6.432 | 15 | 3.117 | 22 | 86 |
|  | 0.85 | 0.981 | 39 | 0.902 | 41 | 6.128 | 39 | 3.033 | 40 | 159 |
|  | 0.90 | 0.981 | 39 | 0.907 | 43 | 5.882 | 43 | 2.897 | 43 | 168 |
| 300 | 0.55 | 0.975 | 1 | 0.867 | 1 | 6.936 | 1 | 3.549 | 1 | 4 |
|  | 0.60 | 0.977 | 6 | 0.876 | 8 | 6.605 | 9 | 3.314 | 10 | 33 |
|  | 0.65 | 0.978 | 12 | 0.888 | 15 | 6.36 | 23 | 3.201 | 15 | 65 |
|  | 0.70 | 0.978 | 12 | 0.891 | 21 | 6.375 | 20 | 3.116 | 23 | 76 |
|  | 0.75 | 0.979 | 19 | 0.897 | 30 | 6.333 | 26 | 3.073 | 33 | 108 |
|  | 0.80 | 0.979 | 19 | 0.901 | 40 | 6.391 | 19 | 3.079 | 32 | 110 |
|  | 0.85 | 0.98 | 35 | 0.896 | 26 | 6.212 | 36 | 3.06 | 36 | 133 |
|  | 0.90 | 0.981 | 39 | 0.911 | 46 | 5.78 | 45 | 2.852 | 44 | 174 |

**2. Dataset CT2**

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, text, graphics

Description automatically generated

**Fig. S-1.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 50.

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, colorfulness, graphics

Description automatically generated

**Fig. S-2.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 100.

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, text, graphics

Description automatically generated

**Fig. S-3.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 150.

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, colorfulness, graphics

Description automatically generated

**Fig. S-4.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 200.

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, colorfulness, graphics

Description automatically generated

**Fig. S-5.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 250.

A picture containing screenshot, text, line, font

Description automatically generated

A picture containing screenshot, line, colorfulness, graphics

Description automatically generated

**Fig. S-6.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 300.

**Table S-1** Performance of GWO-LGB models on the training set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 0.536 | 40 | 0.444 | 24 | 31.337 | 43 | 17.837 | 33 | 140 |
|  | 0.60 | 0.528 | 7 | 0.44 | 16 | 31.727 | 3 | 18.011 | 18 | 44 |
|  | 0.65 | 0.527 | 3 | 0.43 | 2 | 31.636 | 11 | 18.195 | 2 | 18 |
|  | 0.70 | 0.524 | 1 | 0.431 | 3 | 31.587 | 17 | 18.158 | 3 | 24 |
|  | 0.75 | 0.538 | 44 | 0.455 | 34 | 31.299 | 47 | 17.768 | 36 | 161 |
|  | 0.80 | 0.538 | 44 | 0.458 | 36 | 31.309 | 46 | 17.72 | 37 | 163 |
|  | 0.85 | 0.534 | 25 | 0.49 | 48 | 31.513 | 25 | 17.344 | 45 | 143 |
|  | **0.90** | **0.534** | **25** | **0.489** | **45** | **31.616** | **14** | **17.211** | **48** | **132** |
| 100 | 0.55 | 0.534 | 25 | 0.443 | 22 | 31.401 | 37 | 17.912 | 27 | 111 |
|  | 0.60 | 0.532 | 20 | 0.453 | 32 | 31.606 | 15 | 17.85 | 31 | 98 |
|  | 0.65 | 0.529 | 14 | 0.432 | 5 | 31.56 | 19 | 18.126 | 5 | 43 |
|  | 0.70 | 0.528 | 7 | 0.438 | 11 | 31.442 | 31 | 18.043 | 10 | 59 |
|  | 0.75 | 0.538 | 44 | 0.449 | 28 | 31.329 | 44 | 17.829 | 34 | 150 |
|  | 0.80 | 0.535 | 36 | 0.451 | 31 | 31.407 | 36 | 17.869 | 28 | 131 |
|  | 0.85 | 0.534 | 25 | 0.489 | 45 | 31.515 | 24 | 17.358 | 44 | 138 |
|  | 0.90 | 0.534 | 25 | 0.486 | 40 | 31.641 | 9 | 17.379 | 41 | 115 |
| 150 | 0.55 | 0.536 | 40 | 0.444 | 24 | 31.346 | 42 | 17.857 | 30 | 136 |
|  | 0.60 | 0.53 | 17 | 0.449 | 28 | 31.661 | 7 | 17.926 | 24 | 76 |
|  | 0.65 | 0.529 | 14 | 0.431 | 3 | 31.566 | 18 | 18.077 | 6 | 41 |
|  | 0.70 | 0.527 | 3 | 0.437 | 10 | 31.473 | 28 | 18.062 | 8 | 49 |
|  | 0.75 | 0.535 | 36 | 0.443 | 22 | 31.419 | 35 | 17.948 | 20 | 113 |
|  | 0.80 | 0.539 | 48 | 0.461 | 37 | 31.286 | 48 | 17.663 | 38 | 171 |
|  | 0.85 | 0.534 | 25 | 0.488 | 43 | 31.519 | 22 | 17.382 | 40 | 130 |
|  | 0.90 | 0.533 | 21 | 0.483 | 39 | 31.651 | 8 | 17.443 | 39 | 107 |
| 200 | 0.55 | 0.535 | 36 | 0.436 | 9 | 31.379 | 40 | 17.932 | 23 | 108 |
|  | 0.60 | 0.528 | 7 | 0.438 | 11 | 31.722 | 5 | 18.013 | 17 | 40 |
|  | 0.65 | 0.53 | 17 | 0.435 | 8 | 31.558 | 20 | 18.036 | 11 | 56 |
|  | 0.70 | 0.527 | 3 | 0.441 | 20 | 31.492 | 26 | 18.025 | 14 | 63 |
|  | 0.75 | 0.536 | 40 | 0.439 | 15 | 31.372 | 41 | 17.947 | 21 | 117 |
|  | 0.80 | 0.534 | 25 | 0.45 | 30 | 31.442 | 31 | 17.923 | 25 | 111 |
|  | 0.85 | 0.534 | 25 | 0.488 | 43 | 31.516 | 23 | 17.372 | 42 | 133 |
|  | 0.90 | 0.534 | 25 | 0.487 | 41 | 31.63 | 12 | 17.327 | 46 | 124 |
| 250 | 0.55 | 0.533 | 21 | 0.433 | 6 | 31.429 | 33 | 17.966 | 19 | 79 |
|  | 0.60 | 0.528 | 7 | 0.44 | 16 | 31.723 | 4 | 18.018 | 16 | 43 |
|  | 0.65 | 0.528 | 7 | 0.425 | 1 | 31.595 | 16 | 18.204 | 1 | 25 |
|  | 0.70 | 0.527 | 3 | 0.44 | 16 | 31.489 | 27 | 18.068 | 7 | 53 |
|  | 0.75 | 0.538 | 44 | 0.446 | 26 | 31.325 | 45 | 17.866 | 29 | 144 |
|  | 0.80 | 0.535 | 36 | 0.456 | 35 | 31.399 | 38 | 17.838 | 32 | 141 |
|  | 0.85 | 0.525 | 2 | 0.446 | 26 | 31.827 | 1 | 18.152 | 4 | 33 |
|  | 0.90 | 0.534 | 25 | 0.487 | 41 | 31.638 | 10 | 17.362 | 43 | 119 |
| 300 | 0.55 | 0.533 | 21 | 0.438 | 11 | 31.427 | 34 | 17.945 | 22 | 88 |
|  | 0.60 | 0.528 | 7 | 0.44 | 16 | 31.745 | 2 | 18.034 | 12 | 37 |
|  | 0.65 | 0.53 | 17 | 0.434 | 7 | 31.533 | 21 | 18.045 | 9 | 54 |
|  | 0.70 | 0.528 | 7 | 0.441 | 20 | 31.465 | 30 | 18.025 | 14 | 71 |
|  | 0.75 | 0.533 | 21 | 0.438 | 11 | 31.472 | 29 | 18.032 | 13 | 74 |
|  | 0.80 | 0.536 | 40 | 0.453 | 32 | 31.381 | 39 | 17.825 | 35 | 146 |
|  | 0.85 | 0.529 | 14 | 0.462 | 38 | 31.706 | 6 | 17.92 | 26 | 84 |
|  | 0.90 | 0.534 | 25 | 0.489 | 45 | 31.629 | 13 | 17.311 | 47 | 130 |

**Table S-2** Performance of GWO-LGB models on the test set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 0.485 | 13 | 0.401 | 11 | 32.906 | 14 | 19.249 | 31 | 69 |
|  | 0.60 | 0.494 | 29 | 0.397 | 6 | 32.432 | 35 | 19.308 | 22 | 92 |
|  | 0.65 | 0.491 | 22 | 0.406 | 23 | 32.679 | 30 | 19.233 | 34 | 109 |
|  | 0.70 | 0.5 | 34 | 0.398 | 7 | 32.762 | 24 | 19.464 | 7 | 72 |
|  | 0.75 | 0.47 | 3 | 0.41 | 26 | 33.167 | 1 | 19.56 | 5 | 35 |
|  | 0.80 | 0.469 | 1 | 0.423 | 34 | 33.128 | 6 | 19.451 | 11 | 52 |
|  | 0.85 | 0.513 | 44 | 0.433 | 43 | 31.094 | 39 | 18.43 | 42 | 168 |
|  | **0.90** | **0.508** | **37** | **0.437** | **47** | **29.682** | **48** | **18.072** | **48** | **180** |
| 100 | 0.55 | 0.486 | 15 | 0.405 | 20 | 32.896 | 16 | 19.249 | 31 | 82 |
|  | 0.60 | 0.492 | 25 | 0.407 | 24 | 32.493 | 31 | 19.303 | 25 | 105 |
|  | 0.65 | 0.491 | 22 | 0.411 | 29 | 32.704 | 29 | 19.287 | 28 | 108 |
|  | 0.70 | 0.499 | 31 | 0.396 | 1 | 32.782 | 20 | 19.423 | 17 | 69 |
|  | 0.75 | 0.471 | 4 | 0.408 | 25 | 33.154 | 3 | 19.556 | 6 | 38 |
|  | 0.80 | 0.471 | 4 | 0.423 | 34 | 33.093 | 9 | 19.462 | 8 | 55 |
|  | 0.85 | 0.512 | 43 | 0.425 | 37 | 31.105 | 37 | 18.465 | 39 | 156 |
|  | 0.90 | 0.506 | 37 | 0.429 | 41 | 29.696 | 45 | 18.146 | 43 | 166 |
| 150 | 0.55 | 0.485 | 13 | 0.402 | 14 | 32.907 | 13 | 19.263 | 29 | 69 |
|  | 0.60 | 0.493 | 26 | 0.401 | 11 | 32.466 | 32 | 19.305 | 24 | 93 |
|  | 0.65 | 0.491 | 22 | 0.412 | 30 | 32.705 | 28 | 19.182 | 36 | 116 |
|  | 0.70 | 0.5 | 34 | 0.403 | 17 | 32.773 | 22 | 19.448 | 12 | 85 |
|  | 0.75 | 0.472 | 11 | 0.398 | 7 | 33.119 | 7 | 19.595 | 4 | 29 |
|  | 0.80 | 0.469 | 1 | 0.417 | 31 | 33.144 | 5 | 19.431 | 14 | 51 |
|  | 0.85 | 0.513 | 44 | 0.428 | 39 | 31.092 | 40 | 18.45 | 41 | 164 |
|  | 0.90 | 0.506 | 37 | 0.436 | 45 | 29.691 | 46 | 18.113 | 46 | 174 |
| 200 | 0.55 | 0.486 | 15 | 0.4 | 9 | 32.898 | 15 | 19.291 | 26 | 65 |
|  | 0.60 | 0.493 | 26 | 0.396 | 1 | 32.443 | 34 | 19.312 | 21 | 82 |
|  | 0.65 | 0.489 | 19 | 0.41 | 26 | 32.743 | 25 | 19.239 | 33 | 103 |
|  | 0.70 | 0.499 | 31 | 0.404 | 18 | 32.779 | 21 | 19.427 | 16 | 86 |
|  | 0.75 | 0.471 | 4 | 0.402 | 14 | 33.147 | 4 | 19.61 | 2 | 24 |
|  | 0.80 | 0.471 | 4 | 0.426 | 38 | 33.069 | 12 | 19.459 | 10 | 64 |
|  | 0.85 | 0.513 | 44 | 0.428 | 39 | 31.095 | 38 | 18.451 | 40 | 161 |
|  | 0.90 | 0.506 | 37 | 0.44 | 48 | 29.687 | 47 | 18.105 | 47 | 179 |
| 250 | 0.55 | 0.486 | 15 | 0.396 | 1 | 32.882 | 18 | 19.291 | 26 | 60 |
|  | 0.60 | 0.493 | 26 | 0.396 | 1 | 32.446 | 33 | 19.329 | 19 | 79 |
|  | 0.65 | 0.49 | 20 | 0.402 | 14 | 32.71 | 27 | 19.328 | 20 | 81 |
|  | 0.70 | 0.499 | 31 | 0.401 | 11 | 32.787 | 19 | 19.444 | 13 | 74 |
|  | 0.75 | 0.471 | 4 | 0.404 | 18 | 33.156 | 2 | 19.597 | 3 | 27 |
|  | 0.80 | 0.471 | 4 | 0.424 | 36 | 33.084 | 10 | 19.462 | 8 | 58 |
|  | 0.85 | 0.517 | 48 | 0.421 | 33 | 30.956 | 42 | 18.604 | 37 | 160 |
|  | 0.90 | 0.506 | 37 | 0.433 | 43 | 29.697 | 44 | 18.127 | 44 | 168 |
| 300 | 0.55 | 0.486 | 15 | 0.405 | 20 | 32.893 | 17 | 19.251 | 30 | 82 |
|  | 0.60 | 0.494 | 29 | 0.396 | 1 | 32.428 | 36 | 19.307 | 23 | 89 |
|  | 0.65 | 0.49 | 20 | 0.41 | 26 | 32.721 | 26 | 19.205 | 35 | 107 |
|  | 0.70 | 0.5 | 34 | 0.405 | 20 | 32.772 | 23 | 19.411 | 18 | 95 |
|  | 0.75 | 0.472 | 11 | 0.4 | 9 | 33.106 | 8 | 19.618 | 1 | 29 |
|  | 0.80 | 0.471 | 4 | 0.429 | 41 | 33.078 | 11 | 19.431 | 14 | 70 |
|  | 0.85 | 0.516 | 47 | 0.417 | 31 | 31 | 41 | 18.533 | 38 | 157 |
|  | 0.90 | 0.506 | 37 | 0.436 | 45 | 29.701 | 43 | 18.124 | 45 | 170 |

**3. Dataset CT3**

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-1.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 50.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-2.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 100.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-3.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 150.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-4.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 200.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-5.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 250.

A picture containing screenshot, colorfulness, line, rectangle

Description automatically generated

A picture containing text, screenshot, font, line

Description automatically generated

**Fig. S-6.** Effect of training-test ratios on the GWO-LGB model’s performance with population size of 300.

**Table S-1** Performance of GWO-LGB models on the training set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 1 | 5 | 1 | 2 | 0.555 | 17 | 0.372 | 19 | 43 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.466 | 26 | 0.315 | 27 | 60 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.362 | 41 | 0.225 | 40 | 88 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.565 | 16 | 0.412 | 15 | 38 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.615 | 10 | 0.454 | 10 | 27 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.508 | 21 | 0.362 | 21 | 49 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.603 | 12 | 0.434 | 12 | 31 |
|  | 0.90 | 1 | 5 | 1 | 2 | 0.597 | 13 | 0.431 | 13 | 33 |
| 100 | 0.55 | 1 | 5 | 1 | 2 | 0.463 | 27 | 0.292 | 28 | 62 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.383 | 38 | 0.242 | 37 | 82 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.399 | 35 | 0.262 | 34 | 76 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.364 | 40 | 0.241 | 38 | 85 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.423 | 31 | 0.28 | 30 | 68 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.476 | 24 | 0.344 | 24 | 55 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.476 | 24 | 0.332 | 25 | 56 |
|  | 0.90 | 0.999 | 1 | 1 | 2 | 0.759 | 4 | 0.567 | 3 | 10 |
| 150 | 0.55 | 1 | 5 | 1 | 2 | 0.38 | 39 | 0.216 | 41 | 87 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.432 | 29 | 0.286 | 29 | 65 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.503 | 23 | 0.366 | 20 | 50 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.658 | 6 | 0.486 | 7 | 20 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.427 | 30 | 0.28 | 30 | 67 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.403 | 34 | 0.262 | 34 | 75 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.35 | 42 | 0.21 | 42 | 91 |
|  | 0.90 | 0.999 | 1 | 1 | 2 | 0.766 | 3 | 0.566 | 4 | 10 |
| 200 | 0.55 | 1 | 5 | 1 | 2 | 0.521 | 19 | 0.345 | 23 | 49 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.413 | 32 | 0.271 | 32 | 71 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.28 | 47 | 0.142 | 47 | 101 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.295 | 46 | 0.165 | 46 | 99 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.521 | 19 | 0.383 | 18 | 44 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.455 | 28 | 0.322 | 26 | 61 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.683 | 5 | 0.502 | 5 | 17 |
|  | 0.90 | 0.999 | 1 | 0.999 | 1 | 0.832 | 1 | 0.61 | 1 | 4 |
| 250 | 0.55 | 1 | 5 | 1 | 2 | 0.584 | 15 | 0.395 | 16 | 38 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.303 | 45 | 0.171 | 45 | 97 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.327 | 43 | 0.191 | 43 | 93 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.324 | 44 | 0.19 | 44 | 95 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.592 | 14 | 0.43 | 14 | 35 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.398 | 36 | 0.257 | 36 | 79 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.631 | 8 | 0.463 | 9 | 24 |
|  | 0.90 | 1 | 5 | 1 | 2 | 0.387 | 37 | 0.238 | 39 | 83 |
| 300 | 0.55 | 1 | 5 | 1 | 2 | 0.28 | 47 | 0.124 | 48 | 102 |
|  | 0.60 | 1 | 5 | 1 | 2 | 0.408 | 33 | 0.266 | 33 | 73 |
|  | 0.65 | 1 | 5 | 1 | 2 | 0.541 | 18 | 0.391 | 17 | 42 |
|  | 0.70 | 1 | 5 | 1 | 2 | 0.505 | 22 | 0.359 | 22 | 51 |
|  | 0.75 | 1 | 5 | 1 | 2 | 0.653 | 7 | 0.488 | 6 | 20 |
|  | 0.80 | 1 | 5 | 1 | 2 | 0.629 | 9 | 0.476 | 8 | 24 |
|  | 0.85 | 1 | 5 | 1 | 2 | 0.606 | 11 | 0.439 | 11 | 29 |
|  | **0.90** | **0.999** | **1** | **1** | **2** | **0.773** | **2** | **0.572** | **2** | **7** |

**Table S-2** Performance of GWO-LGB models on the test set

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Pop** | **Tr.atio** | **R2** | **Score** | **A10** | **Score** | **RMSE** | **Score** | **MAE** | **Score** | **Total** |
| 50 | 0.55 | 0.992 | 1 | 0.923 | 1 | 3.024 | 3 | 2.132 | 3 | 8 |
|  | 0.60 | 0.993 | 8 | 0.951 | 15 | 2.848 | 10 | 1.96 | 9 | 42 |
|  | 0.65 | 0.994 | 22 | 0.949 | 13 | 2.703 | 20 | 1.804 | 19 | 74 |
|  | 0.70 | 0.993 | 8 | 0.978 | 46 | 2.645 | 26 | 1.79 | 21 | 101 |
|  | 0.75 | 0.994 | 22 | 0.977 | 45 | 2.528 | 36 | 1.672 | 43 | 146 |
|  | 0.80 | 0.993 | 8 | 0.948 | 11 | 2.722 | 16 | 1.763 | 31 | 66 |
|  | 0.85 | 0.995 | 38 | 0.962 | 27 | 2.455 | 42 | 1.76 | 32 | 139 |
|  | 0.90 | 0.995 | 38 | 0.963 | 31 | 2.53 | 34 | 1.833 | 14 | 117 |
| 100 | 0.55 | 0.992 | 1 | 0.927 | 3 | 2.92 | 6 | 2.005 | 8 | 18 |
|  | 0.60 | 0.993 | 8 | 0.955 | 21 | 2.797 | 11 | 1.947 | 12 | 52 |
|  | 0.65 | 0.994 | 22 | 0.96 | 26 | 2.65 | 25 | 1.781 | 24 | 97 |
|  | 0.70 | 0.994 | 22 | 0.972 | 41 | 2.574 | 33 | 1.77 | 28 | 124 |
|  | 0.75 | 0.993 | 8 | 0.959 | 25 | 2.664 | 22 | 1.715 | 38 | 93 |
|  | 0.80 | 0.994 | 22 | 0.972 | 41 | 2.651 | 24 | 1.703 | 40 | 127 |
|  | 0.85 | 0.995 | 38 | 0.981 | 47 | 2.426 | 43 | 1.723 | 37 | 165 |
|  | 0.90 | 0.995 | 38 | 0.963 | 31 | 2.354 | 45 | 1.676 | 42 | 156 |
| 150 | 0.55 | 0.992 | 1 | 0.927 | 3 | 2.996 | 5 | 2.088 | 4 | 13 |
|  | 0.60 | 0.993 | 8 | 0.958 | 23 | 2.771 | 13 | 1.948 | 11 | 55 |
|  | 0.65 | 0.994 | 22 | 0.952 | 17 | 2.618 | 28 | 1.78 | 25 | 92 |
|  | 0.70 | 0.994 | 22 | 0.969 | 35 | 2.529 | 35 | 1.74 | 34 | 126 |
|  | 0.75 | 0.993 | 8 | 0.962 | 27 | 2.762 | 14 | 1.746 | 33 | 82 |
|  | 0.80 | 0.993 | 8 | 0.953 | 18 | 2.727 | 15 | 1.771 | 27 | 68 |
|  | 0.85 | 0.995 | 38 | 0.962 | 27 | 2.488 | 39 | 1.779 | 26 | 130 |
|  | 0.90 | 0.995 | 38 | 0.953 | 18 | 2.468 | 41 | 1.705 | 39 | 136 |
| 200 | 0.55 | 0.992 | 1 | 0.935 | 6 | 3.069 | 2 | 2.141 | 1 | 10 |
|  | 0.60 | 0.993 | 8 | 0.955 | 21 | 2.88 | 8 | 2.012 | 7 | 44 |
|  | 0.65 | 0.994 | 22 | 0.946 | 10 | 2.68 | 21 | 1.79 | 21 | 74 |
|  | 0.70 | 0.994 | 22 | 0.969 | 35 | 2.592 | 29 | 1.767 | 30 | 116 |
|  | 0.75 | 0.992 | 1 | 0.974 | 43 | 2.873 | 9 | 1.805 | 18 | 71 |
|  | 0.80 | 0.993 | 8 | 0.958 | 23 | 2.721 | 17 | 1.782 | 23 | 71 |
|  | 0.85 | 0.995 | 38 | 0.969 | 35 | 2.312 | 47 | 1.668 | 44 | 164 |
|  | 0.90 | 0.995 | 38 | 0.944 | 9 | 2.361 | 44 | 1.65 | 46 | 137 |
| 250 | 0.55 | 0.992 | 1 | 0.929 | 5 | 3.075 | 1 | 2.134 | 2 | 9 |
|  | 0.60 | 0.993 | 8 | 0.941 | 8 | 2.889 | 7 | 2.062 | 5 | 28 |
|  | 0.65 | 0.994 | 22 | 0.954 | 20 | 2.627 | 27 | 1.793 | 20 | 89 |
|  | 0.70 | 0.994 | 22 | 0.966 | 33 | 2.585 | 30 | 1.768 | 29 | 114 |
|  | 0.75 | 0.994 | 22 | 0.97 | 40 | 2.503 | 38 | 1.681 | 41 | 141 |
|  | 0.80 | 0.993 | 8 | 0.948 | 11 | 2.661 | 23 | 1.733 | 35 | 77 |
|  | 0.85 | 0.995 | 38 | 0.969 | 35 | 2.34 | 46 | 1.639 | 47 | 166 |
|  | 0.90 | 0.995 | 38 | 0.935 | 6 | 2.516 | 37 | 1.821 | 17 | 98 |
| 300 | 0.55 | 0.992 | 1 | 0.923 | 1 | 3.002 | 4 | 2.055 | 6 | 12 |
|  | 0.60 | 0.993 | 8 | 0.951 | 15 | 2.782 | 12 | 1.952 | 10 | 45 |
|  | 0.65 | 0.994 | 22 | 0.968 | 34 | 2.707 | 19 | 1.827 | 15 | 90 |
|  | 0.70 | 0.994 | 22 | 0.969 | 35 | 2.575 | 31 | 1.834 | 13 | 101 |
|  | 0.75 | 0.994 | 22 | 0.974 | 43 | 2.48 | 40 | 1.659 | 45 | 150 |
|  | 0.80 | 0.993 | 8 | 0.962 | 27 | 2.721 | 17 | 1.729 | 36 | 88 |
|  | 0.85 | 0.994 | 22 | 0.95 | 14 | 2.575 | 31 | 1.825 | 16 | 83 |
|  | **0.90** | **0.996** | **48** | **0.991** | **48** | **2.135** | **48** | **1.529** | **48** | **192** |