Supplementary Material

## A Novel Modeling Optimization Approach for a Seven-channel Titania Ceramic Membrane in an Oily Wastewater Filtration System Based on Experimentation, Full Factorial Design, and Machine Learning

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Graphical user interface

Description automatically generated with medium confidence

**Figure S1.** Ceramic membrane dimensions: (**a**) the complete illustration, (**b**) cross-sectional area, (**c**) ceramic membrane internal channels and walls.



**Figure S2.** Contact angles of a Bakken oil droplet at the ceramic membrane surface.



**Figure S3.** Contact angles of a water droplet at the ceramic membrane surface.



**Figure S4.** LabBrain crossflow ceramic membrane filtration unit.

Diagram

Description automatically generated

**Figure S5.** LabBrain P&I control loop schematic diagram unit.

**Graphical user interface, application, email

Description automatically generated**

**Figure S6**. Multiple linear regression models

Chart, line chart

Description automatically generated

**Figure S7.** Machine learning flux regression models analysis

**All runs for MLR analysis**

**Table S1.** Algorithms models and their training functions fitted for the experimental run 1

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 28.429 | 0.67 | 808.2 | 22.747 | 6.907 |
| 2 | Linear regression | Interactions linear | 28.501 | 0.67 | 812.32 | 22.788 | 26.614 |
| 3 | Linear regression | Robust Linear | 35.131 | 0.49 | 1234.2 | 20.255 | 24.223 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 28.515 | 0.67 | 813.12 | 22.783 | 23.455 |
| 5 | Tree | Fine Tree | 0.69536 | 0.99 | 0.48352 | 0.40585 | 22.87 |
| 6 | Tree | Medium Tree | 1.4311 | 0.99 | 2.0479 | 0.73886 | 21.765 |
| 7 | Tree | Coarse Tree | 3.9243 | 0.99 | 15.4 | 1.9125 | 21.301 |
| 8 | SVM | Linear SVM | 33.464 | 0.54 | 1119.9 | 20.08 | 20.574 |
| 9 | SVM | Quadratic SVM | 14.445 | 0.91 | 208.66 | 9.1763 | 17.922 |
| 10 | SVM | Cubic SVM | 4.484 | 0.99 | 20.106 | 3.3184 | 17.086 |
| 11 | SVM | Fine Gaussian SVM | 11.473 | 0.95 | 131.63 | 5.4515 | 16.651 |
| 12 | SVM | Medium Gaussian SVM | 5.9821 | 0.99 | 35.785 | 3.2133 | 16.014 |
| 13 | SVM | Coarse Gaussian SVM | 20.482 | 0.83 | 419.51 | 10.48 | 15.245 |
| 14 | Ensemble | Boosted Trees | 13.048 | 0.93 | 170.25 | 12.85 | 14.343 |
| 15 | Ensemble | Bagged Trees | 8.3093 | 0.97 | 69.045 | 4.7875 | 13.822 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.11847 | 0.99 | 0.014036 | 0.078545 | 177.84 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.22 | 0.99 | 0.039999 | 0.078125 | 344.26 |
| 18 | Gaussian Process Regression | Exponential GPR | 2.0966 | 0.99 | 4.3958 | 0.66784 | 172.35 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.11581** | **0.99** | **0.013412** | **0.076448** | **632.7** |

**Table S2.** Algorithms models and their training functions fitted for the experimental run 2

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 43.758 | 0.69 | 1914.8 | 35.093 | 1.2577 |
| 2 | Linear regression | Interactions linear | 43.833 | 0.69 | 1921.3 | 35.102 | 3.5282 |
| 3 | Linear regression | Robust Linear | 52.554 | 0.55 | 2761.9 | 32.171 | 3.3376 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 43.396 | 0.69 | 1930.4 | 35.174 | 3.6711 |
| 5 | Tree | Fine Tree | 1.64412 | 0.99 | 2.6936 | 0.90334 | 3.04441 |
| 6 | Tree | Medium Tree | 3.4007 | 0.99 | 11.565 | 1.727 | 2.7862 |
| 7 | Tree | Coarse Tree | 8.2559 | 0.99 | 68.161 | 4.2186 | 2.5456 |
| 8 | SVM | Linear SVM | 51.327 | 0.57 | 2634.5 | 31.43 | 3.295 |
| 9 | SVM | Quadratic SVM | 21.204 | 0.93 | 449.62 | 13.653 | 4.7413 |
| 10 | SVM | Cubic SVM | 0.244 | 0.99 | 38.988 | 4.8416 | 3.8689 |
| 11 | SVM | Fine Gaussian SVM | 22.668 | 0.92 | 513.83 | 10.961 | 1.7156 |
| 12 | SVM | Medium Gaussian SVM | 10.514 | 0.98 | 110.54 | 5.3972 | 1.0433 |
| 13 | SVM | Coarse Gaussian SVM | 33.249 | 0.82 | 1105.5 | 17.154 | 2.2603 |
| 14 | Ensemble | Boosted Trees | 9.5902 | 0.99 | 91.972 | 8.8499 | 8.3556 |
| 15 | Ensemble | Bagged Trees | 15.807 | 0.96 | 249.87 | 9.2271 | 10.743 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.22253 | 0.99 | 0.04952 | 0.16429 | 117.31 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.3335 | 0.99 | 0.11122 | 0.14526 | 188.22 |
| 18 | Gaussian Process Regression | Exponential GPR | 3.7225 | 0.99 | 13.857 | 1.3026 | 111.69 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.20797** | **0.99** | **0.043251** | **0.14847** | **284.6** |

**Table S3.** Algorithms models and their training functions fitted for the experimental run 3

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 29.504 | 0.80 | 870.47 | 24.387 | 5.8006 |
| 2 | Linear regression | Interactions linear | 29.561 | 0.79 | 873.84 | 24.379 | 5.5124 |
| 3 | Linear regression | Robust Linear | 30.104 | 0.79 | 906.24 | 23.305 | 4.8347 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 29.579 | 0.79 | 874.94 | 24.416 | 8.074 |
| 5 | Tree | Fine Tree | 1.0089 | 0.99 | 1.0179 | 0.66786 | 7.8541 |
| 6 | Tree | Medium Tree | 2.2571 | 0.99 | 5.0945 | 1.2932 | 7.5005 |
| 7 | Tree | Coarse Tree | 5.8136 | 0.99 | 33.798 | 3.4576 | 7.2166 |
| 8 | SVM | Linear SVM | 33.02 | 0.74 | 1090.3 | 22.623 | 6.8945 |
| 9 | SVM | Quadratic SVM | 10.047 | 0.98 | 100.95 | 7.5186 | 9.1211 |
| 10 | SVM | Cubic SVM | 4.1641 | 0.99 | 17.34 | 3.7413 | 8.8379 |
| 11 | SVM | Fine Gaussian SVM | 14.83 | 0.95 | 219.92 | 8.7513 | 8.5498 |
| 12 | SVM | Medium Gaussian SVM | 5.6381 | 0.99 | 31.788 | 3.6645 | 8.3157 |
| 13 | SVM | Coarse Gaussian SVM | 16.427 | 0.94 | 269.83 | 9.6486 | 8.0373 |
| 14 | Ensemble | Boosted Trees | 12.389 | 0.96 | 153.49 | 12.018 | 9.6828 |
| 15 | Ensemble | Bagged Trees | 12.113 | 0.97 | 146.73 | 7.2512 | 10.084 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.14564 | 0.99 | 0.02121 | 0.098603 | 61.78 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.22425 | 0.99 | 0.050287 | 0.092411 | 90.139 |
| 18 | Gaussian Process Regression | Exponential GPR | 2.3813 | 0.99 | 5.6708 | 0.78877 | 62.477 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.14351** | **0.99** | **0.020595** | **0.097105** | **123.38** |

**Table S4.** Algorithms models and their training functions fitted for the experimental run 4

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 27.781 | 0.67 | 771.8 | 22.21 | 4.8178 |
| 2 | Linear regression | Interactions linear | 27.878 | 0.67 | 777.18 | 22.261 | 7.4377 |
| 3 | Linear regression | Robust Linear | 34.061 | 0.50 | 1160.1 | 19.672 | 7.1827 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 27.814 | 0.67 | 773.64 | 22.226 | 8.0331 |
| 5 | Tree | Fine Tree | 0.66027 | 0.99 | 0.43595 | 0..39209 | 6.9139 |
| 6 | Tree | Medium Tree | 1.2826 | 0.99 | 1.645 | 0.67065 | 6.6744 |
| 7 | Tree | Coarse Tree | 3.9155 | 0.99 | 15.331 | 1.9036 | 7.7719 |
| 8 | SVM | Linear SVM | 32.766 | 0.54 | 1073.6 | 19.633 | 8.3373 |
| 9 | SVM | Quadratic SVM | 14.079 | 0.91 | 198.21 | 8.9187 | 8.8662 |
| 10 | SVM | Cubic SVM | 4.3986 | 0.99 | 19.348 | 3.2432 | 10.936 |
| 11 | SVM | Fine Gaussian SVM | 11.359 | 0.94 | 129.02 | 5.3948 | 9.8362 |
| 12 | SVM | Medium Gaussian SVM | 5.9736 | 0.98 | 35.684 | 3.1058 | 8.6073 |
| 13 | SVM | Coarse Gaussian SVM | 19.986 | 0.83 | 399.45 | 10.193 | 9.2706 |
| 14 | Ensemble | Boosted Trees | 13.23 | 0.92 | 175.03 | 13.037 | 12.266 |
| 15 | Ensemble | Bagged Trees | 8.3314 | 0.97 | 69.412 | 4.7482 | 13.767 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.11418 | 0.99 | 0.013038 | 0.07809 | 209.58 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.19434 | 0.99 | 0.037768 | 0.075552 | 349.54 |
| 18 | Gaussian Process Regression | Exponential GPR | 2.013 | 0.99 | 4.052 | 0.63274 | 203.29 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.11066** | **0.99** | **0.12246** | **0.075797** | **507.21** |

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 25.713 | 0.59 | 661.15 | 19.97 | 6.0469 |
| 2 | Linear regression | Interactions linear | 25.753 | 0.59 | 663.21 | 19.963 | 5.3005 |
| 3 | Linear regression | Robust Linear | 36.029 | 0.19 | 1298.1 | 177.644 | 9.6615 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 25.819 | 0.59 | 666.61 | 20.016 | 9.325 |
| 5 | Tree | Fine Tree | 0.53494 | 0.99 | 0.28616 | 0.29344 | 9.0115 |
| 6 | Tree | Medium Tree | 1.0473 | 0.99 | 1.0969 | 0.49271 | 8.72998 |
| 7 | Tree | Coarse Tree | 2.9843 | 0.99 | 8.9062 | 1.2966 | 8.494 |
| 8 | SVM | Linear SVM | 31.131 | 0.40 | 969.11 | 16.998 | 8.0144 |
| 9 | SVM | Quadratic SVM | 15.707 | 0.85 | 246.72 | 9.1192 | 7.406 |
| 10 | SVM | Cubic SVM | 6.2853 | 0.98 | 39.504 | 3.8657 | 10.884 |
| 11 | SVM | Fine Gaussian SVM | 10.149 | 0.94 | 103.01 | 3.9022 | 10.735 |
| 12 | SVM | Medium Gaussian SVM | 6.9883 | 0.97 | 48.836 | 3.113 | 10.565 |
| 13 | SVM | Coarse Gaussian SVM | 21.11 | 0.72 | 445.64 | 10.09 | 10.39 |
| 14 | Ensemble | Boosted Trees | 13.739 | 0.88 | 188.76 | 13.613 | 11.418 |
| 15 | Ensemble | Bagged Trees | 6.4706 | 0.97 | 41.868 | 3.2969 | 11.815 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.1406 | 0.99 | 0.019768 | 0.11035 | 545.17 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 00.17149 | 0.99 | 0.029408 | 0.067625 | 615.09 |
| 18 | Gaussian Process Regression | Exponential GPR | 1.9171 | 0.99 | 3.67511 | 0.54674 | 313.72 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.10319** | **0.99** | **0.010647** | **0.070112** | **113.44** |

**Table S5.** Algorithms models and their training functions fitted for the experimental run 5

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 15.266 | 0.81 | 233.06 | 12.688 | 1.1876 |
| 2 | Linear regression | Interactions linear | 15.277 | 0.81 | 233.4 | 12.654 | 0.95009 |
| 3 | Linear regression | Robust Linear | 15.53 | 0.81 | 241.19 | 12.219 | 0.82172 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 15.278 | 0.81 | 233.43 | 12.69 | 2.986 |
| 5 | Tree | Fine Tree | 0.54347 | 0.99 | 0.29536 | 0.36254 | 0..61165 |
| 6 | Tree | Medium Tree | 1.1196 | 0.99 | 1.2535 | 0.66896 | 2.8324 |
| 7 | Tree | Coarse Tree | 3.0142 | 0.99 | 9.0855 | 1.8007 | 2.7174 |
| 8 | SVM | Linear SVM | 16.962 | 00.77 | 287.71 | 11.817 | 2.6191 |
| 9 | SVM | Quadratic SVM | 4.8753 | 0.98 | 23.769 | 3.7454 | 2.5074 |
| 10 | SVM | Cubic SVM | 2.2937 | 0.99 | 5.2611 | 2.0552 | 2.3825 |
| 11 | SVM | Fine Gaussian SVM | 8.5056 | 0.94 | 72.346 | 5.0542 | 2.2667 |
| 12 | SVM | Medium Gaussian SVM | 2.7675 | 0.99 | 7.6591 | 1.9751 | 2.1536 |
| 13 | SVM | Coarse Gaussian SVM | 8.0278 | 0.95 | 64.445 | 4.8415 | 2.0439 |
| 14 | Ensemble | Boosted Trees | 15.969 | 0.79 | 25 | 155.886 | 4.0774 |
| 15 | Ensemble | Bagged Trees | 6.6427 | 0.96 | 44.125 | 4.292 | 3.8628 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.062457 | 0.99 | 0.0039009 | 0.04504 | 52.072 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.099443 | 0.99 | 0.0098889 | 0.044781 | 69.53 |
| 18 | Gaussian Process Regression | Exponential GPR | 1.0945 | 0.99 | 1.1979 | 0.39418 | 48.874 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.062188** | **0.99** | **0.0038674** | **0.044647** | **97.315** |

**Table S6.** Algorithms models and their training functions ions fitted for the experimental run 6

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 36.739 | 0.65 | 1349.8 | 29.128 | 1.8351 |
| 2 | Linear regression | Interactions linear | 36.633 | 0.65 | 1342 | 28.995 | 1.5596 |
| 3 | Linear regression | Robust Linear | 47.295 | 0.42 | 2236.8 | 25.862 | 1.3992 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 36.732 | 0.65 | 1349.2 | 299.132 | 3.0758 |
| 5 | Tree | Fine Tree | 0.94998 | 0.99 | 0.90245 | 0.52139 | 1.0653 |
| 6 | Tree | Medium Tree | 1.9171 | 0.99 | 3.6753 | 0.91812 | 0.89322 |
| 7 | Tree | Coarse Tree | 5.0678 | 0.99 | 25.683 | 2.4312 | 2..897 |
| 8 | SVM | Linear SVM | 43.596 | 0.50 | 1900.6 | 25.573 | 2.7984 |
| 9 | SVM | Quadratic SVM | 19.843 | 0.90 | 393.73 | 12.194 | 2.7012 |
| 10 | SVM | Cubic SVM | 6.6846 | 0.99 | 44.684 | 4.6318 | 3.3783 |
| 11 | SVM | Fine Gaussian SVM | 15.979 | 0.93 | 255.33 | 7.1442 | 2.5064 |
| 12 | SVM | Medium Gaussian SVM | 8.6115 | 0.98 | 74.158 | 4.3876 | 2.36 |
| 13 | SVM | Coarse Gaussian SVM | 27.982 | 0.880 | 783.01 | 13.956 | 2.8723 |
| 14 | Ensemble | Boosted Trees | 11.121 | 0.97 | 123.67 | 10.745 | 3.0947 |
| 15 | Ensemble | Bagged Trees | 10.075 | 0.97 | 101.51 | 5.663 | 3.0853 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.15389 | 0.99 | 0.023682 | 0.11191 | 159.26 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.2544 | 0.99 | 0.064719 | 0.10792 | 266.67 |
| 18 | Gaussian Process Regression | Exponential GPR | 2.749 | 0.99 | 7.5571 | 0.90354 | 145.66 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.14963** | **0.99** | **0.02239** | **0.10718** | **400.54** |

**Table S7.** Algorithms models and their training functions fitted for the experimental run 7

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 27.758 | 0.67 | 770.49 | 22.207 | 4.3776 |
| 2 | Linear regression | Interactions linear | 27.768 | 0.67 | 771.08 | 22.206 | 8.6775 |
| 3 | Linear regression | Robust Linear | 33.922 | 0.51 | 1150.7 | 19.656 | 8.3485 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 27.814 | 0.67 | 773.6 | 22.226 | 8.0916 |
| 5 | Tree | Fine Tree | 0.65681 | 0.99 | 0.4314 | 0.39461 | 7.8005 |
| 6 | Tree | Medium Tree | 1.2283 | 0.99 | 1.5088 | 0.65118 | 7.3483 |
| 7 | Tree | Coarse Tree | 3.9777 | 0.99 | 15.822 | 1.9508 | 6.8737 |
| 8 | SVM | Linear SVM | 32.941 | 0.53 | 1085.1 | 19.615 | 11.456 |
| 9 | SVM | Quadratic SVM | 14.158 | 0.91 | 200.44 | 8.9564 | 11.137 |
| 10 | SVM | Cubic SVM | 4.3763 | 0.99 | 19.152 | 3.2418 | 10.799 |
| 11 | SVM | Fine Gaussian SVM | 11.314 | 0.95 | 128 | 5.3063 | 10.478 |
| 12 | SVM | Medium Gaussian SVM | 6.1635 | 0..98 | 37.988 | 3.1359 | 9.8724 |
| 13 | SVM | Coarse Gaussian SVM | 20.03 | 0.83 | 401.18 | 10.223 | 9.4104 |
| 14 | Ensemble | Boosted Trees | 13.207 | 0.93 | 174.43 | 13.019 | 12.467 |
| 15 | Ensemble | Bagged Trees | 8.2759 | 0.97 | 68.491 | 4.6454 | 11.834 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.11037 | 0.99 | 0.012181 | 0.077144 | 168.74 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.18257 | 0.99 | 0.03333 | 0.071992 | 280.2 |
| 18 | Gaussian Process Regression | Exponential GPR | 1.9958 | 0.99 | 3.9832 | 0.65374 | 155.7 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.10843** | **0.99** | **0.011757** | **0.074881** | **399.61** |

**Table S8.** Algorithms models and their training functions fitted for the experimental run 8

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 32.667 | 0.81 | 1067.1 | 27.128 | 4.7646 |
| 2 | Linear regression | Interactions linear | 32.708 | 0..81 | 1069.88 | 27.13 | 4.5421 |
| 3 | Linear regression | Robust Linear | 33.311 | 0.80 | 1109.7 | 26.143 | 4.3286 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 32.661 | 0.81 | 1066.8 | 27.117 | 6.7763 |
| 5 | Tree | Fine Tree | 1.1321 | 0..99 | 1.2817 | 0.75576 | 6.5779 |
| 6 | Tree | Medium Tree | 2.3012 | 0.99 | 5.2956 | 1.4001 | 6.3933 |
| 7 | Tree | Coarse Tree | 6.7389 | 0.99 | 45.412 | 4.0861 | 6.1694 |
| 8 | SVM | Linear SVM | 36.259 | 0.77 | 1314.7 | 25.292 | 77.8145 |
| 9 | SVM | Quadratic SVM | 10.523 | 0.98 | 110.73 | 8.006 | 7.6279 |
| 10 | SVM | Cubic SVM | 4.7712 | 0.99 | 22.764 | 4.2537 | 7.4558 |
| 11 | SVM | Fine Gaussian SVM | 16.095 | 0.95 | 259.04 | 9.9045 | 8.2249 |
| 12 | SVM | Medium Gaussian SVM | 5.9298 | 0.99 | 35.163 | 4.2364 | 7.1841 |
| 13 | SVM | Coarse Gaussian SVM | 17.177 | 0.95 | 295.05 | 10.399 | 6.9416 |
| 14 | Ensemble | Boosted Trees | 11.495 | 0.98 | 132.13 | 10.952 | 9.7087 |
| 15 | Ensemble | Bagged Trees | 15.197 | 0.96 | 230.95 | 10.06 | 10.186 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.14689 | 0.99 | 0.021576 | 0.10004 | 57.39 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.22347 | 0.99 | 0.0499937 | 0.096519 | 66.298 |
| 18 | Gaussian Process Regression | Exponential GPR | 2.4836 | 0.99 | 6.1681 | 0.85892 | 62.774 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.14578** | **0.99** | **0.021251** | **0.099163** | **132.73** |

**Table S9.** Algorithms models and their training functions fitted for the experimental run 9

**Table S10.** Algorithms models and their training functions fitted for the experimental run 10

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 44.796 | 0.48 | 2006.6 | 33.015 | 4.6327 |
| 2 | Linear regression | Interactions linear | 44.908 | 0.48 | 2016.7 | 33.063 | 4.4272 |
| 3 | Linear regression | Robust Linear | 65.591 | 0.11 | 4302.2 | 28.354 | 4.2213 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 44.813 | 0.48 | 2008.2 | 33.026 | 6.5623 |
| 5 | Tree | Fine Tree | 0.91438 | 0.99 | 0.8361 | 0.42329 | 6.3459 |
| 6 | Tree | Medium Tree | 2.1937 | 0.99 | 4.8125 | 0.83907 | 6.1669 |
| 7 | Tree | Coarse Tree | 5.2123 | 0.99 | 27.168 | 2.0812 | 5.9854 |
| 8 | SVM | Linear SVM | 55.789 | 0.20 | 3112.4 | 26.17 | 6.8465 |
| 9 | SVM | Quadratic SVM | 34.474 | 0.69 | 1188.5 | 17.14 | 7.1263 |
| 10 | SVM | Cubic SVM | 18.124 | 0.92 | 328.48 | 9.0185 | 8.0766 |
| 11 | SVM | Fine Gaussian SVM | 25.573 | 0.83 | 654 | 8.0496 | 8.572 |
| 12 | SVM | Medium Gaussian SVM | 21.217 | 0.88 | 450.16 | 7.9039 | 7.88 |
| 13 | SVM | Coarse Gaussian SVM | 44.342 | 0.49 | 1966.2 | 18.84 | 8.3659 |
| 14 | Ensemble | Boosted Trees | 8.9627 | 0.98 | 80.33 | 8.4859 | 10.992 |
| 15 | Ensemble | Bagged Trees | 10.478 | 0.97 | 109.79 | 5.0743 | 10.811 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.26835 | 0.99 | 0.072011 | 0.18279 | 586.1 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.5149 | 0.99 | 0.26512 | 0.18982 | 488.06 |
| 18 | Gaussian Process Regression | Exponential GPR | 4.502 | 0.99 | 20.268 | 1.3263 | 268.85 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.16317** | **0.99** | **0.063572** | **0.27709** | **474.03** |

**Table S11.** Algorithms models and their training functions fitted for the experimental run 11

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | **Algorithms models** | **Training Function** | **RMSE** | **R2** | **MSE** | **MAE** | **Training Time, sec** |
| 1 | Linear regression | Linear | 51.235 | 0.44 | 2625 | 36.86 | 3.7994 |
| 2 | Linear regression | Interactions linear | 51.311 | 0.44 | 2632.8 | 36.819 | 3.5066 |
| 3 | Linear regression | Robust Linear | 73.471 | 0.15 | 5398 | 30.335 | 5.5203 |
| 4 | Stepwise Linear Regression | Stepwise Linear | 51.24 | 0.44 | 2625.6 | 36.841 | 5.3291 |
| 5 | Tree | Fine Tree | 1.2376 | 0.99 | 1.5316 | 0.52774 | 5.1203 |
| 6 | Tree | Medium Tree | 2.5712 | 0.99 | 6.6113 | 0.96842 | 4.9658 |
| 7 | Tree | Coarse Tree | 6.0438 | 0.99 | 36.528 | 2.368 | 4.803 |
| 8 | SVM | Linear SVM | 64.328 | 0.12 | 4138.1 | 28.14 | 5.6889 |
| 9 | SVM | Quadratic SVM | 42.652 | 0.61 | 1819.2 | 19.829 | 5.4898 |
| 10 | SVM | Cubic SVM | 24.698 | 0.87 | 610 | 11.473 | 4.0662 |
| 11 | SVM | Fine Gaussian SVM | 35.43 | 0.73 | 1255.3 | 14.495 | 4.915 |
| 12 | SVM | Medium Gaussian SVM | 30.177 | 0.81 | 910.66 | 10.508 | 3.8976 |
| 13 | SVM | Coarse Gaussian SVM | 53.824 | 0.38 | 2897 | 21.698 | 4.6595 |
| 14 | Ensemble | Boosted Trees | 7.2421 | 0.99 | 52.448 | 6.5008 | 7.3543 |
| 15 | Ensemble | Bagged Trees | 12.016 | 0.97 | 144.39 | 5.3114 | 7.6324 |
| 16 | Gaussian Process Regression | Squared Exponential GPR | 0.26505 | 0.99 | 0.070251 | 0.16968 | 697.1 |
| 17 | Gaussian Process Regression | Matern 5/2 GPR | 0.65118 | 0.99 | 0.42404 | 0.28285 | 557.8 |
| 18 | Gaussian Process Regression | Exponential GPR | 5.3675 | 0.99 | 28.81 | 1.6417 | 300.29 |
| **19** | **Gaussian Regression Process** | **Rational Quadratic GPR** | **0.23217** | **0.99** | **0.31526** | **1.15277** | **271.19** |