

## DAFTAR PUSTAKA

- Abimanyu, C., 2020, Implementasi Machine Learning untuk Memprediksi Energi Atomisasi Molekul dengan Algoritma Boosted Regression Tree dan Neural Network, *Skripsi*, FMIPA UGM.
- Alkahfi, C., 2022, Python : Random Forest untuk Model Klasifikasi Menggunakan Scikit-Learn, <https://sainsdata.id/machine-learning/893/python-random-forest-untuk-model-klasifikasi-menggunakan-scikitlearn/>, diakses 13 Juni 2023.
- Balabin, R. & M., Lomakina, E. I., 2009, Neural network approach to quantumchemistry data: Accurate prediction of density functional theory energies, *Journal of Chemical Physics*, 131, 074104.
- Balabin, R. M., & Lomakina, E. I., 2011, Support vector machine regression (LSSVM)—an alternative to artificial neural networks (ANNs) for the analysis of quantum chemistry data, *Physical Chemistry Chemical Physics*, 13, pp. 11710-11718.
- Bevans, R., 2020, Simple Linear Regression | An Easy Introduction & Examples, <https://www.scribbr.com/statistics/simple-linear-regression/>, diakses 13 Juni 2023.
- Carleo, G., & Troyer, M., 2017, Solving the quantum many-body problem with artificial neural networks, *Science*, 355(6325), pp. 602-606.
- Chatfield, C., 1995, *Problem Solving: A Statistician's Guide (2nd ed.)*, Chapman and Hall.
- Chen, T., & Guestrin C., 2016, XGBoost: A Scalable Tree Boosting System, *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* 785–94.
- Géron, A., 2019, *Hands-on Machine Learning with Scikit-Learn, Keras, and TensorFlow (Second ed.)*, O'Reilly Media.
- Haqqi, M. F., 2021, Penerapan Algoritma XGBoost Dan Random Forest Untuk Estimasi Porositas Efektif Data LOG Sumur, *Skripsi*, FMIPA UGM.

- Hansen, K., Montavon, G., Biegler, F., Fazli, S., Rupp, M., Scheffer, M., Lilienfeld, A., Tkatchenko, & A., Muller, K., 2013, Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies, *Journal of Chemical Theory and Computation*, 9, pp. 3404-3419.
- Himmetoglu, B., 2015, Tree based machine learning framework for predicting ground state energies of molecules, *Journal of Chemical Physics*, 145, 134101.
- Ho, T.K., 1995, Random decision forests, *Proceedings of 3rd International Conference on Document Analysis and Recognition, IEEE*, Vol. 1, pp. 278-282.
- Holmes, Mark H., 2013, *Introduction to Perturbation Methods*, Springer.
- James, G., Witten, D., Hastie, T., & Tibshirani, R., 2013, *An Introduction to Statistical Learning*, Springer.
- Ke, G., Meng, Q., Finley T., Wang T., Chen W., Ma W., Ye Q., & Liu Y., 2017, LightGBM: A Highly Efficient Gradient Boosting Decision Tree, *31st Conference on Neural Information Processing Systems (NIPS 2017)*, 3149–3157.
- Kim S., Thiessen P.A., Bolton E.E., Chen J., Fu G., Gindulyte A., Han L., He J., He S., Shoemaker B.A., Wang J., Yu B., Zhang J., & Bryant S.H., 2016, PubChem Substance and Compound databases. *Nucleic acids research* vol. 44, D1 : D1202–D1213.
- Meredig, B., Agrawal, A., Kirklin, S., Saal, J. E., Doak, J. W., Thompson, A., Zhang, K., Choudhary, A., & Wolverton, C., 2014, Combinatorial screening for new materials in unconstrained composition space with machine learning, *Phys. Rev. B*, 89, 094104.
- Ojala and Garriga., 2010. *Permutation Tests for Studying Classifier Performance*, J. Mach. Learn. Res
- Mithcell, T., 1997, *Machine Learning*, McGraw Hill.
- Patel, B., Patil, H., Hembram, J., & Jaswal, S., 2020, Loan default forecasting using data mining. *Proceedings of the 2020 International Conference for Emerging Technology*, 1–4.

- Pedregosa, F., Varoquax, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhonfer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, & M., Duchesnay, E., 2011, Scikit-learn: Machine Learning in Python, *Journal of Machine Learning*, 12, pp. 2825-2830.
- Pizzi, G., Cepelloti, A., Sabatini, R., Marzani, N., & Kozinsky, B., 2016, AiiDA: automated interactive infrastructure and database for computational science, *Elsevier: Computational Materials Science*, Vol. 111, pp. 218 - 230.
- Pongajow, N., Juliandri, & Hastiawan, I., 2017, Penentuan Geometri Dan Karakteristik Ikatan Senyawa Kompleks Ni(Ii)-Dibutilditiokarbamat Dengan Metode Density Functional Theory, *JAS*, 7(2), 33.
- Pyle, D., 1999, *Data Preparation for Data Mining*, Morgan Kaufmann Publishers, Los Altos, California.
- Raschka, S., 2018, MLxtend: Providing machine learning and data science utilities and extensions to Python's scientific computing stack. *Journal of Open Source Software*, 3(24), 638.
- Rupp, M., Tkatchenko, A., Muller, K.R., & Lilienfeld, O. A. V., 2012, Fast and accurate modeling of molecular atomization energies with machine learning, *Physical Review Letters*, 108(5), 058301.
- Russel, S. J., & Norvig, P., 2010, *Artificial Intelligence: A Modern Approach (Third ed.)*, Prentice Hall.
- Sagert, I., Fann, G. I., Fattoyev, F. J., Postnikov, S., & Horowitz, C. J., 2016, Quantum simulations of nuclei and nuclear pasta with the multiresolution adaptive numerical environment for scientific simulations, *Phys. Rev. C*, 93, 055801.
- Samuel, A., 1959, Some Studies in Machine Learning Using the Game of Checkers, *IBM Journal of Research and Development*, 3(3), pp. 210-229.
- Sandi, K., Habibi, R., & Fauzan, M. N., *Tutorial PHP Machine Learning Menggunakan Regresi Linear Berganda pada Aplikasi Bank Sampah Istimewa Versi 2.0 Berbasis Web*, Penerbit Industri Nusantara, Bandung.

- Shirangi, Mehrdad G., Durlofsky, & Louis J., 2016, A general method to select representative models for decision making and optimization under uncertainty, *Computers and Geosciences*, 96, pp. 109-123.
- Sumanto, M., Martoprawiro, M. A., & Ivansyah, A. L., 2021, The prediction of molecule atomization energy using neural network and extreme gradient boosting *Journal of Physics: Conference Series*, 2072(1), 012005.
- Tchagang, A. B., & Valdés, J. J., 2019, Prediction of the Atomization Energy of Molecules Using Coulomb Matrix and Atomic Composition in a Bayesian Regularized Neural Networks. *Artificial Neural Networks and Machine Learning – ICANN 2019: Workshop and Special Sessions. ICANN 2019. Lecture Notes in Computer Science()*, vol 11731, Springer.
- Wang, R., 2018, Significantly Improving the Prediction of Molecular Atomization Energies by an Ensemble of Machine Learning Algorithms and Rescanning Input Space: A Stacked Generalization Approach, *The Journal of Physical Chemistry C*, 122 (16), 8868-8873
- Wijayandanu, N. H., 2021, Deteksi Serangan Distributed Denial Of Service Menggunakan Komparasi Metode LightGBM, XGBoost, Dan CatBoost, *Skripsi, FMIPA UGM*
- Wolpert, D., 1992, Stacked Generalization, *Neural Networks*, Vol. 5, 1992, pp. 241-259.
- Yadav, S. S., Shukla, S., 2016, Analysis of k-Fold Cross-Validation over HoldOut Validation on Colossal Datasets for Quality Classification, *IEEE 6th International Conference on Advanced Computing (IACC)*, pp. 78-83.