

# Modern approaches for component-wise boosting:

Automation, efficiency, and distributed computing with application to the medical domain

---

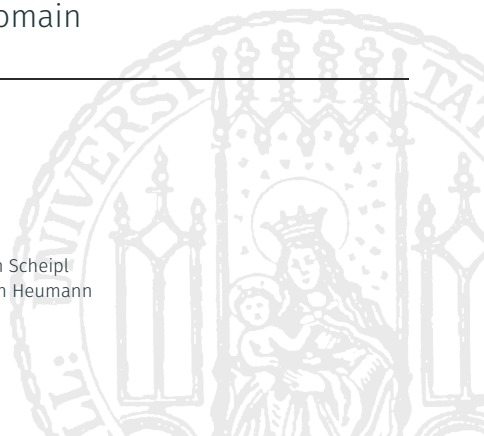
**Daniel Schalk**

March 24, 2023

**Supervisor:** Prof. Dr. Bernd Bischl

**Referees:** Prof. Dr. Matthias Schmid, PD Dr. Fabian Scheipl

**Chair of the examination panel:** Prof. Dr. Christian Heumann



Bla

---

Bla (see, e.g., Pepe, 2003), or DeLong et al. (1988)

## References

---

- Abadi, M., Chu, A., Goodfellow, I., McMahan, H. B., Mironov, I., Talwar, K., and Zhang, L. (2016). Deep learning with differential privacy. In *Proceedings of the 2016 ACM SIGSAC conference on computer and communications security*, pages 308–318.
- Arrieta, A. B., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., García, S., Gil-López, S., Molina, D., Benjamins, R., et al. (2020). Explainable artificial intelligence (xai): Concepts, taxonomies, opportunities and challenges toward responsible ai. *Information fusion*, 58:82–115.
- Audet, C. and Hare, W. (2017). *Derivative-free and blackbox optimization*, volume 2. Springer.
- Barrett, R., Berry, M., Chan, T. F., Demmel, J., Donato, J., Dongarra, J., Eijkhout, V., Pozo, R., Romine, C., and Van der Vorst, H. (1994). *Templates for the solution of linear systems: building blocks for iterative methods*. SIAM.
- Bates, D., Maechler, M., and Jagan, M. (2022). *Matrix: Sparse and Dense Matrix Classes and Methods*. R package version 1.5-1.
- Bekkerman, R., Bilenko, M., and Langford, J. (2011). *Scaling up machine learning: Parallel and distributed approaches*. Cambridge University Press.
- Biau, G., Cadre, B., and Rouvière, L. (2019). Accelerated gradient boosting. *Machine Learning*, 108(6):971–992.

# References ii

- Bischl, B., Binder, M., Lang, M., Pielok, T., Richter, J., Coors, S., Thomas, J., Ullmann, T., Becker, M., Boulesteix, A.-L., et al. (2021). Hyperparameter optimization: Foundations, algorithms, best practices and open challenges. *arXiv preprint arXiv:2107.05847*.
- Bischl, B., Mersmann, O., Trautmann, H., and Weihs, C. (2012). Resampling methods for meta-model validation with recommendations for evolutionary computation. *Evolutionary computation*, 20:249–75.
- Bost, R., Popa, R. A., Tu, S., and Goldwasser, S. (2014). Machine learning classification over encrypted data. Cryptology ePrint Archive, Paper 2014/331. <https://eprint.iacr.org/2014/331>.
- Breiman, L. (2001). Random forests. *Machine learning*, 45(1):5–32.
- Brier, G. W. et al. (1950). Verification of forecasts expressed in terms of probability. *Monthly weather review*, 78(1):1–3.
- Brockhaus, S., Rügamer, D., and Greven, S. (2020). Boosting functional regression models with fdboost. *Journal of Statistical Software*, 94(10):1–50.
- Browne, M. W. (2000). Cross-validation methods. *Journal of Mathematical Psychology*, 44(1):108–132.
- Bühlmann, P., Hothorn, T., et al. (2007). Boosting algorithms: Regularization, prediction and model fitting. *Statistical science*, 22(4):477–505.
- Bühlmann, P. and Yu, B. (2003). Boosting with the L2 loss: regression and classification. *Journal of the American Statistical Association*, 98(462):324–339.
- Buluc, A. and Gilbert, J. R. (2008). Challenges and advances in parallel sparse matrix-matrix multiplication. In *2008 37th International Conference on Parallel Processing*, pages 503–510.

## References iii

- Casalicchio, G. (2019). *On benchmark experiments and visualization methods for the evaluation and interpretation of machine learning models*. PhD dissertation, LMU Munich.
- Chen, Y.-R., Rezapour, A., and Tzeng, W.-G. (2018). Privacy-preserving ridge regression on distributed data. *Information Sciences*, 451:34–49.
- Choi, J., Walker, D. W., and Dongarra, J. J. (1994). Pumma: Parallel universal matrix multiplication algorithms on distributed memory concurrent computers. *Concurrency: Practice and Experience*, 6(7):543–570.
- Coors, S., Schalk, D., Bischl, B., and Rügamer, D. (2021). Automatic componentwise boosting: An interpretable automl system. *ECML-PKDD Workshop on Automating Data Science*.
- Cunha, M., Mendes, R., and Vilela, J. P. (2021). A survey of privacy-preserving mechanisms for heterogeneous data types. *Computer Science Review*, 41:100403.
- Dagum, L. and Menon, R. (1998). Openmp: an industry standard api for shared-memory programming. *Computational Science & Engineering, IEEE*, 5(1):46–55.
- Davis, T. A. (2006). *Direct methods for sparse linear systems*. SIAM.
- DeLong, E. R., DeLong, D. M., and Clarke-Pearson, D. L. (1988). Comparing the areas under two or more correlated receiver operating characteristic curves: a nonparametric approach. *Biometrics*, pages 837–845.
- Drozdal, J., Weisz, J., Wang, D., Dass, G., Yao, B., Zhao, C., Muller, M., Ju, L., and Su, H. (2020). Trust in automl: Exploring information needs for establishing trust in automated machine learning systems. In *Proceedings of the 25th International Conference on Intelligent User Interfaces, IUI '20*, page 297–307, New York, NY, USA. Association for Computing Machinery.

# References iv

- Duff, I. S., Grimes, R. G., and Lewis, J. G. (1989). Sparse matrix test problems. *ACM Transactions on Mathematical Software (TOMS)*, 15(1):1–14.
- Dwork, C. (2006). Differential privacy. In *International Colloquium on Automata, Languages, and Programming*, pages 1–12. Springer.
- Dwork, C., Kenthapadi, K., McSherry, F., Mironov, I., and Naor, M. (2006a). Our data, ourselves: Privacy via distributed noise generation. In *Annual International Conference on the Theory and Applications of Cryptographic Techniques*, pages 486–503. Springer.
- Dwork, C., McSherry, F., Nissim, K., and Smith, A. (2006b). Calibrating noise to sensitivity in private data analysis. In *Theory of cryptography conference*, pages 265–284. Springer.
- Dwork, C., Roth, A., et al. (2014). The algorithmic foundations of differential privacy. *Found. Trends Theor. Comput. Sci.*, 9(3-4):211–407.
- Eilers, P. H. and Marx, B. D. (1996). Flexible smoothing with B-splines and penalties. *Statistical science*, pages 89–102.
- Fang, H. and Qian, Q. (2021). Privacy preserving machine learning with homomorphic encryption and federated learning. *Future Internet*, 13(4).
- Fawcett, T. (2006). An introduction to roc analysis. *Pattern recognition letters*, 27(8):861–874.
- Feurer, M. and Hutter, F. (2019). Hyperparameter optimization. In *Automated machine learning*, pages 3–33. Springer, Cham.
- Feurer, M., Klein, A., Eggenberger, K., Springenberg, J., Blum, M., and Hutter, F. (2015). Efficient and robust automated machine learning. *Advances in neural information processing systems*, 28.

# References v

- Flach, P. (2012). *Machine learning: the art and science of algorithms that make sense of data*. Cambridge university press.
- Freitas, A. A. (2019). Automated machine learning for studying the trade-off between predictive accuracy and interpretability. In Holzinger, A., Kieseberg, P., Tjoa, A. M., and Weippl, E., editors, *Machine Learning and Knowledge Extraction*, pages 48–66, Cham. Springer International Publishing.
- Freund, Y. and Schapire, R. E. (1997). A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of computer and system sciences*, 55(1):119–139.
- Friedman, J. H. (2001). Greedy function approximation: a gradient boosting machine. *Annals of statistics*, pages 1189–1232.
- Gambs, S., Kégl, B., and Aïmeur, E. (2007). Privacy-preserving boosting. *Data Mining and Knowledge Discovery*, 14(1):131–170.
- Gaye, A., Marcon, Y., Isaeva, J., LaFlamme, P., Turner, A., Jones, E. M., Minion, J., Boyd, A. W., Newby, C. J., Nuotio, M.-L., et al. (2014). Datashield: taking the analysis to the data, not the data to the analysis. *International journal of epidemiology*, 43(6):1929–1944.
- Gong, M., Xie, Y., Pan, K., Feng, K., and Qin, A. (2020). A survey on differentially private machine learning [review article]. *IEEE Computational Intelligence Magazine*, 15(2):49–64.
- Gordon, D. F. and Desjardins, M. (1995). Evaluation and selection of biases in machine learning. *Machine learning*, 20(1):5–22.
- Hastie, T. J. (2017). Generalized additive models. In *Statistical models in S*, pages 249–307. Routledge.



- Hofner, B., Hothorn, T., Kneib, T., and Schmid, M. (2011). A framework for unbiased model selection based on boosting. *Journal of Computational and Graphical Statistics*, 20(4):956–971.
- Hofner, B., Mayr, A., and Schmid, M. (2016). gamboostLSS: An R package for model building and variable selection in the GAMLSS framework. *Journal of Statistical Software*, 74(1).
- Hothorn, T., Bühlmann, P., Kneib, T., Schmid, M., and Hofner, B. (2010). Model-based boosting 2.0. *The Journal of Machine Learning Research*, 11:2109–2113.
- Hothorn, T., Bühlmann, P., Kneib, T., Schmid, M., and Hofner, B. (2020). *mboost: Model-based boosting*. R package version 2.9-7.
- Hutter, F., Kotthoff, L., and Vanschoren, J. (2019). *Automated machine learning: methods, systems, challenges*. Springer Nature.
- Jayaraman, B. and Evans, D. (2019). Evaluating differentially private machine learning in practice. In *28th USENIX Security Symposium (USENIX Security 19)*, pages 1895–1912.
- John, G. H. (1995). Robust decision trees: Removing outliers from databases. In *KDD*, volume 95, pages 174–179.
- Karr, A. F., Lin, X., Sanil, A. P., and Reiter, J. P. (2005). Secure regression on distributed databases. *Journal of Computational and Graphical Statistics*, 14(2):263–279.
- Kingma, D. P. and Ba, J. (2014). Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*.
- Kotthoff, L., Thornton, C., Hoos, H. H., Hutter, F., and Leyton-Brown, K. (2017). Auto-weka 2.0: Automatic model selection and hyperparameter optimization in weka. *Journal of Machine Learning Research*, 18(25):1–5.

- Kotthoff, L., Thornton, C., Hoos, H. H., Hutter, F., and Leyton-Brown, K. (2019). Auto-weka: Automatic model selection and hyperparameter optimization in weka. In *Automated machine learning*, pages 81–95. Springer, Cham.
- Lang, S., Umlauf, N., Wechselberger, P., Harttgen, K., and Kneib, T. (2014). Multilevel structured additive regression. *Statistics and Computing*, 24(2):223–238.
- Lazarevic, A. and Obradovic, Z. (2001). The distributed boosting algorithm. In *Proceedings of the seventh ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 311–316.
- Li, J., Kuang, X., Lin, S., Ma, X., and Tang, Y. (2020). Privacy preservation for machine learning training and classification based on homomorphic encryption schemes. *Information Sciences*, 526:166–179.
- Li, Y., Jiang, X., Wang, S., Xiong, H., and Ohno-Machado, L. (2016). Vertical grid logistic regression (vertigo). *Journal of the American Medical Informatics Association*, 23(3):570–579.
- Li, Z. and Wood, S. N. (2020). Faster model matrix crossproducts for large generalized linear models with discretized covariates. *Statistics and Computing*, 30(1):19–25.
- Liew, B. X., Rügamer, D., Abichandani, D., and De Nunzio, A. M. (2020a). Classifying individuals with and without patellofemoral pain syndrome using ground force profiles – Development of a method using functional data boosting. *Gait & Posture*, 80:90–95.
- Liew, B. X., Rügamer, D., Stocker, A., and De Nunzio, A. M. (2020b). Classifying neck pain status using scalar and functional biomechanical variables – Development of a method using functional data boosting. *Gait & posture*, 76:146–150.

# References viii

- Liu, W. and Vinter, B. (2014). An efficient gpu general sparse matrix-matrix multiplication for irregular data. In *2014 IEEE 28th International Parallel and Distributed Processing Symposium*, pages 370–381.
- Lu, H., Karimireddy, S. P., Ponomareva, N., and Mirrokni, V. (2020). Accelerating gradient boosting machines. In *International Conference on Artificial Intelligence and Statistics*, pages 516–526. PMLR.
- Lundberg, S. M. and Lee, S.-I. (2017). A unified approach to interpreting model predictions. In Guyon, I., Luxburg, U. V., Bengio, S., Wallach, H., Fergus, R., Vishwanathan, S., and Garnett, R., editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc.
- Luo, C., Islam, M., Sheils, N. E., Buresh, J., Reps, J., Schuemie, M. J., Ryan, P. B., Edmondson, M., Duan, R., Tong, J., et al. (2022). Dlmm as a lossless one-shot algorithm for collaborative multi-site distributed linear mixed models. *Nature Communications*, 13(1):1–10.
- Machanavajjhala, A., Kifer, D., Gehrke, J., and Venkitasubramaniam, M. (2007). l-diversity: Privacy beyond k-anonymity. *ACM Transactions on Knowledge Discovery from Data (TKDD)*, 1(1):3–es.
- McMahan, B., Moore, E., Ramage, D., Hampson, S., and Arcas, B. A. y. (2017). Communication-Efficient Learning of Deep Networks from Decentralized Data. In Singh, A. and Zhu, J., editors, *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, volume 54 of *Proceedings of Machine Learning Research*, pages 1273–1282. PMLR.
- Mohassel, P. and Zhang, Y. (2017). Secureml: A system for scalable privacy-preserving machine learning. In *2017 IEEE symposium on security and privacy (SP)*, pages 19–38. IEEE.
- Molnar, C. (2020). *Interpretable machine learning*. Lulu. com.

# References ix

- Nesterov, Y. (1983). A method for solving the convex programming problem with convergence rate  $O(1/k^2)$ .
- Nori, H., Jenkins, S., Koch, P., and Caruana, R. (2019). Interpretml: A unified framework for machine learning interpretability. *arXiv preprint arXiv:1909.09223*.
- Pepe, M. S. (2000). An interpretation for the roc curve and inference using glm procedures. *Biometrics*, 56(2):352–359.
- Pepe, M. S. (2003). The statistical evaluation of medical tests for classification and prediction. *Journal of the American Statistical Association*.
- Pfisterer, F. (2022). *Democratizing Machine Learning – Contributions in AutoML and Fairness*. PhD thesis, LMU Munich.
- Pfisterer, F., Thomas, J., and Bischl, B. (2019). Towards human centered automl. *arXiv preprint arXiv:1911.02391*.
- Prasser, F., Kohlbacher, O., Mansmann, U., Bauer, B., and Kuhn, K. A. (2018). Data integration for future medicine (difuture). *Methods Inf Med*, 57(S01):e57–e65.
- R Core Team (2022). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.
- Ribeiro, M. T., Singh, S., and Guestrin, C. (2016). "why should i trust you?" explaining the predictions of any classifier. In *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*, pages 1135–1144.
- Ruder, S. (2016). An overview of gradient descent optimization algorithms. *arXiv preprint arXiv:1609.04747*.

# References x

- Rudin, C. (2019). Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature Machine Intelligence*, 1(5):206–215.
- Rügamer, D., Brockhaus, S., Gentsch, K., Scherer, K., and Greven, S. (2018). Boosting factor-specific functional historical models for the detection of synchronization in bioelectrical signals. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 67(3):621–642.
- Saintigny, P., Zhang, L., Fan, Y.-H., El-Naggar, A. K., Papadimitrakopoulou, V. A., Feng, L., Lee, J. J., Kim, E. S., Hong, W. K., and Mao, L. (2011). Gene expression profiling predicts the development of oral cancer. *Cancer Prevention Research*, 4(2):218–229.
- Samarati, P. and Sweeney, L. (1998). Protecting privacy when disclosing information: k-anonymity and its enforcement through generalization and suppression.
- Sanderson, C. and Curtin, R. (2016). Armadillo: a template-based c++ library for linear algebra. *Journal of Open Source Software*, 1(2):26.
- Sanderson, C. and Curtin, R. (2018). A user-friendly hybrid sparse matrix class in c++. In *International Congress on Mathematical Software*, pages 422–430. Springer.
- Schalk, D., Bischl, B., and Rügamer, D. (2022a). Accelerated componentwise gradient boosting using efficient data representation and momentum-based optimization. *Journal of Computational and Graphical Statistics*.
- Schalk, D., Bischl, B., and Rügamer, D. (2022b). Privacy-preserving and lossless distributed estimation of high-dimensional generalized additive mixed models. *arXiv preprint arXiv:2210.07723*. Currently under review in the *Journal of Computational and Graphical Statistics*.

- Schalk, D., Hoffmann, V. S., Bischl, B., and Mansmann, U. (2022c). Distributed non-disclosive validation of predictive models by a modified roc-glm. *arXiv preprint arXiv:2203.10828*.
- Schalk, D., Hoffmann, V. S., Bischl, B., and Mansmann, U. (2022d). dsBinVal: Conducting distributed ROC analysis using DataSHIELD. *Currently under review in the Journal of Open Source Software*, [github.com/openjournals/joss-reviews/issues/4545](https://github.com/openjournals/joss-reviews/issues/4545).
- Schalk, D., Thomas, J., and Bischl, B. (2018). compboost: Modular framework for component-wise boosting. *Journal of Open Source Software*, 3(30):967.
- Schmid, M. and Hothorn, T. (2008). Boosting additive models using component-wise p-splines. *Computational Statistics & Data Analysis*, 53(2):298–311.
- Shahnaz, R., Usman, A., and Chughtai, I. R. (2005). Review of storage techniques for sparse matrices. In *2005 Pakistan Section Multitopic Conference*, pages 1–7.
- Stehman, S. V. (1997). Selecting and interpreting measures of thematic classification accuracy. *Remote sensing of Environment*, 62(1):77–89.
- Sun, X., Zhang, P., Liu, J. K., Yu, J., and Xie, W. (2020). Private machine learning classification based on fully homomorphic encryption. *IEEE Transactions on Emerging Topics in Computing*, 8(2):352–364.
- Sweeney, L. (2002). k-anonymity: A model for protecting privacy. *International journal of uncertainty, fuzziness and knowledge-based systems*, 10(05):557–570.
- Thomas, J., Coors, S., and Bischl, B. (2018). Automatic gradient boosting. *ICML AutoML Workshop*.
- Thomas, J., Hepp, T., Mayr, A., and Bischl, B. (2017). Probing for sparse and fast variable selection with model-based boosting. *Computational and mathematical methods in medicine*, 2017.

## References xii

- Thornton, C., Hutter, F., Hoos, H. H., and Leyton-Brown, K. (2013). Auto-weka: Combined selection and hyperparameter optimization of classification algorithms. In *Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 847–855.
- Tutz, G. and Gertheiss, J. (2016). Regularized regression for categorical data. *Statistical Modelling*, 16(3):161–200.
- Van Buuren, S. (2018). *Flexible imputation of missing data*. CRC press.
- Verbraeken, J., Wolting, M., Katzy, J., Kloppenburg, J., Verbelen, T., and Rellermeyer, J. S. (2020). A survey on distributed machine learning. *Acm computing surveys (csur)*, 53(2):1–33.
- Vuk, M. and Curk, T. (2006). Roc curve, lift chart and calibration plot. *Metodoloski zvezki*, 3(1):89.
- Wang, Q. and Kurz, D. (2022). Reconstructing training data from diverse ml models by ensemble inversion. In *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*, pages 2909–2917.
- Wood, S. N. (2017). *Generalized additive models: an introduction with R*. Chapman and Hall/CRC.
- Wood, S. N., Li, Z., Shaddick, G., and Augustin, N. H. (2017). Generalized additive models for gigadata: Modeling the u.k. black smoke network daily data. *Journal of the American Statistical Association*, 112(519):1199–1210.
- Xanthopoulos, I., Tsamardinos, I., Christophides, V., Simon, E., and Salinger, A. (2020). Putting the human back in the automl loop. In *EDBT/ICDT Workshops*.
- Yan, Z., Zachrisson, K. S., Schwamm, L. H., Estrada, J. J., and Duan, R. (2022). Fed-glmm: A privacy-preserving and computation-efficient federated algorithm for generalized linear mixed models to analyze correlated electronic health records data. *medRxiv*.

Zhu, R., Jiang, C., Wang, X., Wang, S., Zheng, H., and Tang, H. (2020). Privacy-preserving construction of generalized linear mixed model for biomedical computation. *Bioinformatics*, 36(Supplement\_1):i128–i135.



## Backup slides

---

bla