

University of Groningen

## Intrinsically Interpretable Machine Learning In Computer Aided Diagnosis

S. Ghosh, Sreejita

DOI:  
[10.33612/diss.175627883](https://doi.org/10.33612/diss.175627883)

**IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.**

*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2021

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

S. Ghosh, S. (2021). *Intrinsically Interpretable Machine Learning In Computer Aided Diagnosis*. [Thesis fully internal (DIV), University of Groningen]. University of Groningen.  
<https://doi.org/10.33612/diss.175627883>

### Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

### Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

---

## Bibliography

- Arlt, W., Walker, E. A., Draper, N., Ivison, H. E., Ride, J. P., Hammer, F., Chalder, S. M., Borucka-Mankiewicz, M., Hauffa, B. P., Malunowicz, E. M. et al.: 2004, Congenital adrenal hyperplasia caused by mutant p450 oxidoreductase and human androgen synthesis: analytical study, *The Lancet* **363**(9427), 2128–2135.
- 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.
- Artelt, A. and Hammer, B.: 2019, On the computation of counterfactual explanations—a survey, *arXiv preprint arXiv:1911.07749*.
- Azur, M. J., Stuart, E. A., Frangakis, C. and Leaf, P. J.: 2011, Multiple imputation by chained equations: what is it and how does it work?, *International journal of methods in psychiatric research* **20**(1), 40–49.
- Backhaus, A. and Seiffert, U.: 2014, Classification in high-dimensional spectral data: Accuracy vs. interpretability vs. model size, *Neurocomputing* **131**, 15–22.
- Baranowski, E., Bunte, K., Shackleton, C., Taylor, A., Hughes, B., Biehl, M., Tino, P., Guran, T. and Arlt, W.: 2016, Steroid metabolomics for diagnosis of in-born steroidogenic disorders-bridging the gap between clinician and scientist through computational approaches, *Society for Endocrinology BES 2016*, Vol. 44, BioScientifica.
- Baranowski, E. S., Arlt, W. and Idkowiak, J.: 2018, Monogenic disorders of adrenal steroidogenesis, *Hormone research in paediatrics* **89**(5), 292–310.

- Baranowski, E. S., Ghosh, S., Shackleton, C. H., Taylor, A. E., Hughes, B. A., Gilligan, L. C., Utari, A., Faradz, S. M., der Grinten Hedi, L., Biehl, M. et al.: 2019, Steroid metabolomics: a rapid computational approach for accurate differentiation of inborn disorders of steroidogenesis, *21st European Congress of Endocrinology*, Vol. 63, BioScientifica.
- Bibal, A. and Frénay, B.: 2016, Interpretability of machine learning models and representations: an introduction., *ESANN*.
- Biehl, M., Hammer, B. and Villmann, T.: 2013, Distance measures for prototype based classification, *International Workshop on Brain-Inspired Computing*, Springer, pp. 100–116.
- Breiman, L.: 1996, Bagging predictors, *Machine learning* **24**(2), 123–140.
- Breiman, L.: 2001, Random forests, *Machine learning* **45**(1), 5–32.
- Bunte, K., Baranowski, E., Arlt, W. and Tino, P.: n.d., Relevance learning vector quantization in variable dimensional spaces, in B. Hammer, T. Martinetz and T. Villmann (eds), *NC<sup>2</sup>*, Workshop of the GI-Fachgruppe Neuronale Netze and the German Neural Networks Society in connection to GCPR 2016, Hannover, Germany, pp. 20–23.
- Bunte, K., Hammer, B., Wismüller, A. and Biehl, M.: 2010, Adaptive local dissimilarity measures for discriminative dimension reduction of labeled data, *Neurocomputing* **73**(7-9), 1074–1092.
- Bunte, K., Schneider, P., Hammer, B., Schleif, F., Villmann, T. and Biehl, M.: 2012, Limited rank matrix learning -discriminative dimension reduction and visualization, *Neural Networks* **26**(4), 159–173.  
**URL:** <http://dx.doi.org/10.1016/j.neunet.2011.10.001>
- Bunte, K. and Tino, P.: 2020, Geodesic average over model parameters. In preparation for publishing.  
**URL:** [https://github.com/kbunte/geodesicLVQ\\_toolbox](https://github.com/kbunte/geodesicLVQ_toolbox)
- Carvalho, D. V., Pereira, E. M. and Cardoso, J. S.: 2019, Machine learning interpretability: A survey on methods and metrics, *Electronics* **8**(8), 832.
- Chawla, N. V., Bowyer, K. W., Hall, L. O. and Kegelmeyer, W. P.: 2002, Smote: synthetic minority over-sampling technique, *Journal of artificial intelligence research* **16**, 321–357.
- Chechik, G., Heitz, G., Elidan, G., Abbeel, P. and Koller, D.: 2008, Max-margin classification of data with absent features, *Journal of Machine Learning Research* **9**(Jan), 1–21.

- Doshi-Velez, F. and Kim, B.: 2017, Towards a rigorous science of interpretable machine learning, *arXiv preprint arXiv:1702.08608*.
- Driscoll, T. A., Hale, N. and Trefethen, L. N.: 2014, Chebfun guide.  
**URL:** <https://nl.mathworks.com/matlabcentral/fileexchange/47023-chebfun-current-version>
- Fernández, A., García, S., Galar, M., Prati, R. C., Krawczyk, B. and Herrera, F.: 2018, *Learning from imbalanced data sets*, Springer.
- Fisher, A., Rudin, C. and Dominici, F.: 2019, All models are wrong, but many are useful: Learning a variable's importance by studying an entire class of prediction models simultaneously., *Journal of Machine Learning Research* **20**(177), 1–81.
- Fletcher, P. T., Lu, C., Pizer, S. M. and Joshi, S.: 2004, Principal geodesic analysis for the study of nonlinear statistics of shape, *IEEE Trans. on Medical Imaging* **23**(8), 995–1005.
- García-Laencina, P. J., Sancho-Gómez, J.-L. and Figueiras-Vidal, A. R.: 2010, Pattern classification with missing data: a review, *Neural Computing and Applications* **19**(2), 263–282.  
**URL:** <https://doi.org/10.1007/s00521-009-0295-6>
- Ghosh, S., Baranowski, E., van Veen, R., de Vries, G., Biehl, M., Arlt, W., Tino, P. and Bunte, K.: 2017, Comparison of strategies to learn from imbalanced classes for computer aided diagnosis of inborn steroidogenic disorders, *Proc. of the European Symposium on Artificial Neural Networks*.
- Ghosh, S., Bunte, K., Tino, P., Biehl, M., deHaan, S. and Diaconou, C.: 2021, Probabilistic learning vector quantization with kl divergence.
- Ghosh, S., Tino, P. and Bunte, K.: 2020, Visualisation and knowledge discovery from interpretable models, *International Joint Conference on Neural Networks, IJCNN 2020 Glasgow, UK, July 19-24, 2020*, IEEE.
- Hammer, B., Strickert, M. and Villmann, T.: 2005, On the generalization ability of grlvq networks, *Neural Processing Letters* **21**(2), 109–120.
- Hammer, B. and Villmann, T.: 2002, Generalized relevance learning vector quantization, *Neural Networks* **15**(8–9), 1059 – 1068.  
**URL:** <http://www.sciencedirect.com/science/article/pii/S0893608002000795>
- Hegde, H., Shimpi, N., Panny, A., Glurich, I., Christie, P. and Acharya, A.: 2019, Mice vs ppca: Missing data imputation in healthcare, *Informatics in Medicine Unlocked* **17**, 100275.  
**URL:** <http://www.sciencedirect.com/science/article/pii/S2352914819302783>

- Holzinger, A., Biemann, C., Pattichis, C. S. and Kell, D. B.: 2017, What do we need to build explainable ai systems for the medical domain?, *arXiv preprint arXiv:1712.09923*.
- Hutter, F., Kotthoff, L. and Vanschoren, J.: 2019, *Automated machine learning: methods, systems, challenges*, Springer Nature.
- Janosi, A., Steinbrunn, W., Pfisterer, M. and Detrano, R.: 1988, Heart disease data set, UCI machine learning repository.  
**URL:** <https://archive.ics.uci.edu/ml/datasets/heart+Disease>
- Kahramanli, H. and Allahverdi, N.: 2008, Design of a hybrid system for the diabetes and heart diseases, *Expert systems with applications* **35**(1-2), 82–89.
- Kohonen, T.: 2012, *Self-organizing maps*, Vol. 30, Springer Science & Business Media.
- Kubat, M.: 2017, *An introduction to machine learning*, Springer.
- Lall, U. and Sharma, A.: 1996, A nearest neighbor bootstrap for resampling hydrologic time series, *Water Resources Research* **32**(3), 679–693.
- Little, R. J.: 1988, A test of missing completely at random for multivariate data with missing values, *Journal of the American statistical Association* **83**(404), 1198–1202.
- Little, R. J. and Rubin, D. B.: 2019, *Statistical analysis with missing data*, Vol. 793, John Wiley & Sons.
- Lundberg, S. M. and Lee, S.-I.: 2017, A unified approach to interpreting model predictions, *Advances in neural information processing systems*, pp. 4765–4774.
- Marlin, B. M.: 2008, *Missing Data Problems in Machine Learning*, PhD thesis, Toronto, Ont., Canada, Canada. AAINR57898.
- Minka, T. et al.: 2005, Divergence measures and message passing, *Technical report*, Technical report, Microsoft Research.
- Nahar, J., Imam, T., Tickle, K. S. and Chen, Y.-P. P.: 2013, Computational intelligence for heart disease diagnosis: A medical knowledge driven approach, *Expert Systems with Applications* **40**(1), 96–104.
- Obermeyer, Z., Powers, B., Vogeli, C. and Mullainathan, S.: 2019, Dissecting racial bias in an algorithm used to manage the health of populations, *Science* **366**(6464), 447–453.
- Palaniappan, S. and Awang, R.: 2008, Intelligent heart disease prediction system using data mining techniques, *2008 IEEE/ACS international conference on computer systems and applications*, IEEE, pp. 108–115.

- Parsons, S.: 2005, Introduction to machine learning by ethem alpaydin, mit press, 0-262-01211-1, 400 pp, *The Knowledge Engineering Review* **20**(4), 432–433.
- Pfannschmidt, L., Göpfert, C., Neumann, U., Heider, D. and Hammer, B.: 2019, Feature relevance intervals for interpretable and interactive data exploration, *2019 IEEE Conference on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB)*, IEEE, pp. 1–10.
- Reis, I., Baron, D. and Shahaf, S.: 2018, Probabilistic random forest: A machine learning algorithm for noisy data sets, *The Astronomical Journal* **157**(1), 16.
- Ribeiro, M. T., Singh, S. and Guestrin, C.: 2016, " why should i trust you?" explaining the predictions of any classifier, *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*, pp. 1135–1144.
- Royston, P., White, I. R. et al.: 2011, Multiple imputation by chained equations (mice): implementation in stata, *J Stat Softw* **45**(4), 1–20.
- Sato, A. S. and Yamada, K.: 1996, Generalized learning vector quantization, *Advances in Neural Information Processing Systems*, Vol. 8, pp. 423–429.
- Schneider, P.: 2010, *Advanced methods for prototype-based classification*, Atto Producties Europe.
- Schneider, P., Biehl, M. and Hammer, B.: 2007, Relevance matrices in learning vector quantization, in M. Verleysen (ed.), *Proc. of the 15th European Symposium on Artificial Neural Networks (ESANN)*, d-side publishing, Bruges, Belgium, pp. 37–43.
- Schneider, P., Biehl, M. and Hammer, B.: 2009, Adaptive relevance matrices in learning vector quantization, *Neural computation* **21**(12), 3532–3561.
- Schneider, P., Geweniger, T., Schleif, F.-M., Biehl, M. and Villmann, T.: 2011, Multivariate class labeling in robust soft lvq., *ESANN*.
- Schulz, A., Gisbrecht, A. and Hammer, B.: 2015, Using discriminative dimensionality reduction to visualize classifiers, *Neural Processing Letters* **42**(1), 27–54.
- Severson, K. A., Molaro, M. C. and Braatz, R. D.: 2017, Principal component analysis of process datasets with missing values, *Processes* **5**(3), 38.
- Shouman, M., Turner, T. and Stocker, R.: 2012, Applying k-nearest neighbour in diagnosing heart disease patients, *International Journal of Information and Education Technology* **2**(3), 220–223.

- Storbeck, K.-H., Schiffer, L., Baranowski, E. S., Chortis, V., Prete, A., Barnard, L., Gilligan, L. C., Taylor, A. E., Idkowiak, J., Arlt, W. et al.: 2019, Steroid metabolome analysis in disorders of adrenal steroid biosynthesis and metabolism, *Endocrine Reviews* **40**(6), 1605–1625.
- Tipping, M. E. and Bishop, C. M.: 1999, Mixtures of probabilistic principal component analyzers, *Neural computation* **11**(2), 443–482.
- van Veen, R.: 2016, *Analysis of missing data imputation applied to heart failure data*, Masters thesis, University of Groningen.
- Verma, S., Dickerson, J. and Hines, K.: 2020, Counterfactual explanations for machine learning: A review, *arXiv preprint arXiv:2010.10596* .
- Villmann, A., Kaden, M., Saralajew, S. and Villmann, T.: 2018, Probabilistic learning vector quantization with cross-entropy for probabilistic class assignments in classification learning, *International Conference on Artificial Intelligence and Soft Computing*, Springer, pp. 724–735.
- Wang, F., Kaushal, R. and Khullar, D.: 2020, Should health care demand interpretable artificial intelligence or accept black box medicine?
- Wilson, R. C., Hancock, E. R., Pekalska, E. and Duin, R. P. W.: 2014, Spherical and hyperbolic embeddings of data, *IEEE Trans. Pattern Anal. Mach. Intell.* **36**(11), 2255–2269.  
**URL:** <http://dx.doi.org/10.1109/TPAMI.2014.2316836>