Beyond Reason Codes A Blueprint for Human-Centered, Low-Risk AutoML

H2O.ai Machine Learning Interpretability Team

 $H_2O.ai$

February 11, 2019

Contents

Blueprint

EDA

Benchmark

Training

Post-Hoc Analysis

Human Review

Deployment

Human Appeal

Iterate

Open Questions

H₂O.ai

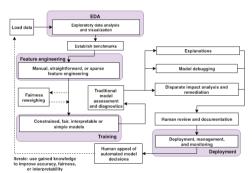
Blueprint

This mid-level technical document provides a basic blueprint for combining the best of AutoML, regulation-compliant predictive modeling, and machine learning research in the sub-disciplines of interpretable models, fairness, and post-hoc explanations to create a low-risk, human-centered machine learning framework.

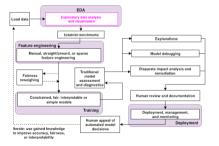
Look for compliance mode in Driverless AI soon.

Guidance from leading researchers and practitioners.

Blueprint

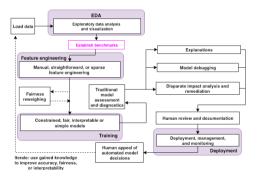


EDA and Data Visualization



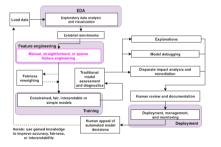
- Know thy data.
- Automation implemented in Driverless AI as AutoViz.
- OSS: H2O-3 Aggregator
- References: Visualizing Big Data Outliers through Distributed
 Aggregation; The Grammar of Graphics

Establish Benchmarks



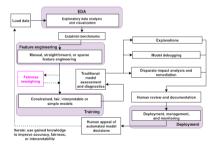
Establishing a benchmark from which to gauge improvements in accuracy, fairness, or interpretability is crucial for good ("data") science and compliance.

Manual, Straightforward, or Sparse Feature Engineering



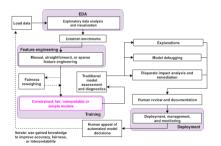
- Automation implemented in Driverless AI as high-interpretability transformers.
- OSS: Pandas Profiler, Feature Tools
- References: Deep Feature Synthesis: Towards Automating Data Science Endeavors; Label, Segment, Featurize: A Cross Domain Framework for Prediction Engineering

Fairness Reweighing



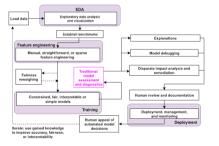
- OSS: IBM Al360
- References: Three Naïve Bayes
 Approaches for Discrimination-free
 Classification; Data Preprocessing
 Techniques for Classification Without
 Discrimination; Certifying and
 Removing Disparate Impact;
 Optimized Pre-processing for
 Discrimination Prevention
- Roadmap items for MLI-2.

Constrained, Fair, Interpretable or Simple Models



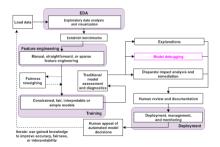
- Automation implemented in Driverless AI as GLM, RuleFit, Monotonic GBM
- References: Locally Interpretable
 Models and Effects Based on
 Supervised Partitioning (LIME-SUP);
 Explainable Neural Networks Based on
 Additive Index Models (XNN);
 Scalable Bayesian Rule Lists (SBRL)
- LIME-SUP, SBRL, XNN are roadmap items for MLI-2.

Traditional Model Assessment and Diagnostics



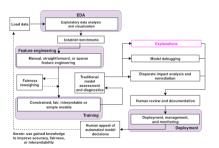
- Residual analysis, Q-Q plots, AUC and lift curves confirm model is accurate and meets assumption criteria.
- Implemented as model diagnostics in Driverless AI.
- Residual analysis is roadmap item for model diagnostics in Driverless Al.

Model Debugging



- Understanding and eliminating errors in model predictions by model testing: adversarial examples, "what-if" analysis, random attacks, explanation of residuals.
- OSS: cleverhans, pdpbox, what-if tool
- Adversarial examples, "what-if" analysis, explanation of residuals, measures of epistemic uncertainty are implemented and roadmap items in MLI-2.

Post-hoc Explanations



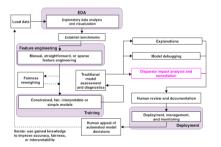
.0

- LIME and Tree SHAP implemented in Driverless AI.
- OSS: lime, shap
- References: Why Should I Trust You?: Explaining the Predictions of Any Classifier; A Unified Approach to Interpreting Model Predictions; Please Stop Explaining Black Box Models for High Stakes Decisions (criticism)
- Tree SHAP is roadmap item for H2O-3; Explanations for unstructured data are roadmap for MLI-2.

Interlude: The Time-Tested Shapley Value

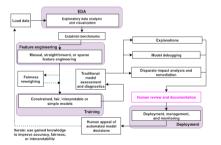
- 1. In the beginning: A Value for N-Person Games, 1953
- 2. **Nobel-worthy contributions**: The Shapley Value: Essays in Honor of Lloyd S. Shapley, 1988
- 3. Shapley regression: Analysis of Regression in Game Theory Approach, 2001
- 4. First reference in ML? Fair Attribution of Functional Contribution in Artificial and Biological Networks, 2004
- 5. Into the ML research mainstream, i.e. JMLR: An Efficient Explanation of Individual Classifications Using Game Theory, 2010
- 6. **Into the real-world data mining workflow** ... *finally*: Consistent Individualized Feature Attribution for Tree Ensembles, 2017
- 7. Unification: A Unified Approach to Interpreting Model Predictions, 2017

Post-hoc Disparate Impact Assessment and Remediation



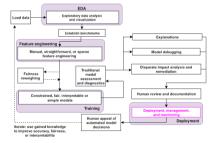
- Disparate impact analysis can be performed manually using Driverless AI or H2O-3.
- OSS: aequitas, IBM Al360, themis
- References: Equality of Opportunity in Supervised Learning; Certifying and Removing Disparate Impact
- Disparate impact analysis and remediation are roadmap items for MLI-2.

Human Review and Documentation



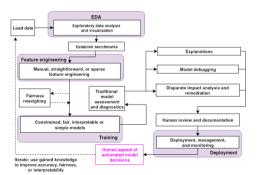
- Implemented as AutoDoc in Driverless Al.
- Various interpretability and fairness roadmap items to be added to AutoDoc.

Deployment, Management, and Monitoring



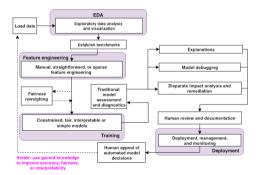
- Monitor models for accuracy and fairness in real-time, track model and data lineage.
- OSS: mlflow, modeldb
- Reference: Model DB: A System for Machine Learning Model Management
- Broader roadmap item for H2O.ai.

Human Appeal



Very important, may require custom implementation for each deployment environment?

Iterate: Use Gained Knowledge to Improve Accuracy, Fairness, or Interpretability



Improvements, KPIs should not be restricted to accuracy alone.

Open Conceptual Questions

- How much automation is appropriate, 100%?
- How to automate learning by iteration, reinforcement learning?
- How to implement human appeals, is it productizable?

This presentation:

https://github.com/jphal1663/h2oworld_sf_2019/blob/master/main.pdf

Driverless AI API Interpretability Technique Examples:

https://github.com/h2oai/driverlessai-tutorials

In-Depth Open Source Interpretability Technique Examples:

https://github.com/jphal1663/interpretable_machine_learning_with_python

"Awesome" Machine Learning Interpretability Resource List:

https://github.com/jphall663/awesome-machine-learning-interpretability

```
Calders, Toon and Sicco Verwer (2010). "Three Naïve Bayes Approaches for Discrimination-free Classification."
In: Data Mining and Knowledge Discovery 21.2. URL:
```

https://link.springer.com/content/pdf/10.1007/s10618-010-0190-x.pdf, pp. 277-292.

Calmon, Flavio et al. (2017). "Optimized Pre-processing for Discrimination Prevention." In: Advances in Neural Information Processing Systems. URL: http://papers.nips.cc/paper/6988-optimized-pre-processingfor-discrimination-prevention.pdf, pp. 3992-4001.

Feldman, Michael et al. (2015). "Certifying and Removing Disparate Impact." In: Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. URL:

https://arxiv.org/pdf/1412.3756.pdf. ACM, pp. 259-268.

Hardt, Moritz, Eric Price, Nati Srebro, et al. (2016). "Equality of Opportunity in Supervised Learning." In: Advances in neural information processing systems. URL:

http://papers.nips.cc/paper/6374-equality-of-opportunity-in-supervised-learning.pdf, pp. 3315-3323.

Hu, Linwei et al. (2018). "Locally Interpretable Models and Effects Based on Supervised Partitioning (LIME-SUP)." In: arXiv preprint arXiv:1806.00663. URL:

https://arxiv.org/ftp/arxiv/papers/1806/1806.00663.pdf

```
Kamiran, Faisal and Toon Calders (2012). "Data Preprocessing Techniques for Classification Without Discrimination." In: Knowledge and Information Systems 33.1. URL:
```

https://link.springer.com/content/pdf/10.1007/s10115-011-0463-8.pdf, pp. 1-33.

Kanter, James Max, Owen Gillespie, and Kalyan Veeramachaneni (2016). "Label, Segment, Featurize: A Cross Domain Framework for Prediction Engineering." In: Data Science and Advanced Analytics (DSAA), 2016 IEEE International Conference on. URL:

http://www.jmaxkanter.com/static/papers/DSAA_LSF_2016.pdf. IEEE, pp. 430-439.

Kanter, James Max and Kalyan Veeramachaneni (2015). "Deep Feature Synthesis: Towards Automating Data Science Endeavors." In: Data Science and Advanced Analytics (DSAA), 2015. 36678 2015. IEEE International Conference on. URL:

https://groups.csail.mit.edu/EVO-DesignOpt/groupWebSite/uploads/Site/DSAA_DSM_2015.pdf. IEEE, pp. 1-10.

Keinan, Alon et al. (2004). "Fair Attribution of Functional Contribution in Artificial and Biological Networks." In: Neural Computation 16.9. URL: https://www.researchgate.net/profile/Isaac_Meilijson/publication/2474580_Fair_Attribution_of_Functional_Contribution_in_Artificial_and_Biological_Networks/links/09e415146df8289373000000/Fair-Attribution-of-Functional-Contribution-in-Artificial-and-Biological-Networks.pdf, pp. 1887-1915.

- Kononenko, Igor et al. (2010). "An Efficient Explanation of Individual Classifications Using Game Theory." In: Journal of Machine Learning Research 11. Jan. URL:
- http://www.jmlr.org/papers/volume11/strumbelj10a/strumbelj10a.pdf, pp. 1-18.
- Lipovetsky, Stan and Michael Conklin (2001). "Analysis of Regression in Game Theory Approach." In: Applied Stochastic Models in Business and Industry 17.4, pp. 319–330.
- Lundberg, Scott M., Gabriel G. Erion, and Su-In Lee (2017). "Consistent Individualized Feature Attribution for Tree Ensembles." In: Proceedings of the 2017 ICML Workshop on Human Interpretability in Machine Learning (WHI 2017). Ed. by Been Kim et al. URL: https://openreview.net/pdf?id=ByTKSo-m-. ICML WHI 2017, pp. 15-21.
- Lundberg, Scott M and Su-In Lee (2017). "A Unified Approach to Interpreting Model Predictions." In: Advances in Neural Information Processing Systems 30. Ed. by I. Guyon et al. URL:
 - http://papers.nips.cc/paper/7062-a-unified-approach-to-interpreting-model-predictions.pdf. Curran Associates, Inc., pp. 4765-4774.
- Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin (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. URL:
 - http://www.kdd.org/kdd2016/papers/files/rfp0573-ribeiroA.pdf. ACM, pp. 1135-1144.

- Rudin, Cynthia (2018). "Please Stop Explaining Black Box Models for High Stakes Decisions." In: arXiv preprint arXiv:1811.10154. URL: https://arxiv.org/pdf/1811.10154.pdf.
- Shapley, Lloyd S (1953). "A Value for N-Person Games." In: Contributions to the Theory of Games 2.28. URL: http://www.library.fa.ru/files/Roth2.pdf#page=39, pp. 307-317.
- Shapley, Lloyd S, Alvin E Roth, et al. (1988). *The Shapley Value: Essays in Honor of Lloyd S. Shapley*. URL: http://www.library.fa.ru/files/Roth2.pdf. Cambridge University Press.
- Vartak, Manasi et al. (2016). "Model DB: A System for Machine Learning Model Management." In: Proceedings of the Workshop on Human-In-the-Loop Data Analytics. URL:
 - https://www-cs.stanford.edu/~matei/papers/2016/hilda_modeldb.pdf. ACM, p. 14.
- Vaughan, Joel et al. (2018). "Explainable Neural Networks Based on Additive Index Models." In: arXiv preprint arXiv:1806.01933. URL: https://arxiv.org/pdf/1806.01933.pdf.
- Wilkinson, Leland (2006). The Grammar of Graphics.
- (2018). "Visualizing Big Data Outliers through Distributed Aggregation." In: IEEE Transactions on Visualization & Computer Graphics 1. URL:
 - https://www.cs.uic.edu/~wilkinson/Publications/outliers.pdf, pp. 1-1.
- Yang, Hongyu, Cynthia Rudin, and Margo Seltzer (2017). "Scalable Bayesian Rule Lists." In: Proceedings of the 34th International Conference on Machine Learning (ICML). URL:
 - https://arxiv.org/pdf/1602.08610.pdf.