Advances in Tabular Machine Learning (WS 2024/25) 1-19 Submitted 15.03.2025

Interpretable Neural Networks using EAGGA

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Abstract

- tabular data still difficult for NNs, where it's still outperformed by other ML model classes - research suggests NN performance benefits from heavy regularisation - using EAGGA, we regularise an NN and achieve both comparable performance as XGB on EAGGA as well as interpretability - for this, we propose a network architecture specifically suited for the EAGGA algorithm

Keywords: tabular data, multi-objective optimization, interpretability, deep learning

1 Introduction

Tabular Data - most common type of data - still difficult for neural networks - (Borisov et al., 2024, p. 7499) - recent research suggests that strong regularisation is beneficial to NN performance on tab data (Kadra et al., 2021, 8)

- we know regularisation from linear models can come with improvements in interpretabiltiy * e.g. LM-LASSO (L1) regularisation as feature selection -¿ reduces # features used in model by setting some coeffs to 0 (Tibshirani, 2018, p. 267) - other forms of regularisation improve performance * e.g. LM-Ridge (L2) on multi-collinear data (Hoerl and Kennard, 1970, p. 55) * e.g. NN dropout, reduces co-adaptation (Hinton et al., 2012, p. 1) * e.g. NN early stopping, reduces overfitting on training data (Finnoff et al., 1993, p. 778f)

- we want to explore if we can use NN regularisation to tackle both interpretability and improved performance (i.e. "comparable" to XGBoost) on tab data - using EAGGA framework, which proved it can improve performance while keeping (already high) performance of XGBoost on tab data -¿ see if interpretabiltiy improvements translate to NN + performance can also be on par

2 Background and Related Works

2.1 Interpretability

As there is no clear definition for interpretability, we will consider it as "the ability to provide *explanations* in *understandable terms* to a human", where *explanations* are logical decision rules and *understandable terms* relate to commonly used terms in the domain of the problem, as suggested by Zhang et al. (2021, chap. 1). Further, we use the term "explainability" in an exchangeable manner with "interpretability", as is commonly done.

Explainability of a model's reasoning is in many ways desirable. Zach (2019, pp. 3-4) gives a range of examples, amongst which are *gaining trust*, e.g. when doctors rely on medical diagnosis predictions, avoiding *subconcious biases* by making sure loan approvals are non-discriminatory, or *regulatory* reasons, most notably the EU's "Right to Explanation" warranted by the GDPR (Antamis et al., 2024, p. 1) or for approval of drugs discovered

using machine learning models (Zhang et al., 2021, 1B). It can further prove helpful for explaining unexpected drops in model performance, which could arise from optimising a model with respect to loss and then judging its performance on a different metric such as accuracy, a practice known as *model debugging* (Zhang et al., 2021, 1B) or for *scientific understanding* in domains where only models can make sense of increasingly complex data anymore and learnt knowledge encoded in a model needs to be made accessible to humans to be used reliably (Antamis et al., 2024, p. 1).

Commonly, methods for model interpretation are divided into intrinsic methods, where the search space only comprises models with a structure simple enough to be considered "explainable" (such as tree-based or simple linear models), and post-hoc methods, where interpretation methods are applied after model training. Amongst post-hoc techniques, we can further divide the space into model-specific (such as analysing GLM coefficients) and model-agnostic (e.g. partial depence plots, ALE) methods (Molnar, 2022, chap. 3.2).

Zhang et al. (2021, chap. 2) extend this distinction to a three-dimensional taxonomy, allowing for better categorisation of neural networks (NNs), a model class that in its fully-connected feedforwad form is inherently non-interpretable.
Passive vs Active Approaches, where *passive* are all post-hoc methods and *active* methods actively change either the architecture or training process to increase model interpretability.
Type of Explanations, distinguishing between *example* methods, providing concrete examples of what leads to a desired output, *attribution* methods that attribute the effect on the output for a specific feature, *hidden semantic* methods, which explain the types of inputs particular neurons or layers pick up on, and logical *rules*, such as if-then clauses or tree-induced rules.
Local vs Global Interpretability, ranging from *local* methods providing explanations based on individual samples, *semi-local* methods, explaining model behaviour for sets of samples grouped by some criterion, to *global* methods, which explain the network as a whole.

Given its unclear definition, evaluating interpretability can be challenging. Doshi-Velez and Kim (2017, 3) propose a taxonomy to categorise possible evaluation methods based on their rigorousness.
Application-grounded evaluation evaluates interpretations directly with respect to the task, by having human experts evaluate the outcome and is therefore the most expensive and time-consuming of the three approaches.
Human-grounded metrics is similar to application-grounded evaluation in that a human still evaluates the interpretations, but tries to simplify the task so that a layperson can do it. Human-grounded approaches are especially suitable if it's sufficient to validate the general concepts of a task. A typical evaluation set-up in this category is binary forced choice, where the human evaluator chooses, which of two generated explanations he prefers.
Functionally-grounded evaluation is the least rigorous, but easiest to implement of the three. It assess explanatory quality according to some formally defined proxy for interpretability and is particularly useful in ranking different models if their model-class is already identified (e.g. via human-grounded evaluation) to be interpretable. The main challenge for functionally-grounded evaluation is finding a good proxy.

2.2 Hyperparameter Optimization (HPO)

In contrast to model parameters, which are optimized during training, hyperparameters (HPs) are those describing the machine learning algorithm and are fixed before training. Because they usually have a significant impact on the trained model's performance, HPs are often optimized, too. Let $\mathcal{D} \subseteq \mathcal{X} \times \mathcal{Y}$ be a dataset consisting of n tuples drawn from the data-generating distribution, i.e. $(\boldsymbol{x}^{(i)}, y^{(i)}) \overset{i.i.d.}{\sim} \mathbb{P}_{\boldsymbol{x}y}, \forall i = 1, ..., n$. Furthermore, let $\mathcal{I} : (\mathbb{D} \times \boldsymbol{\Lambda}) \to \mathcal{H}, (\mathcal{D}, \boldsymbol{\lambda}) \mapsto \hat{f}$ be an algorithm that maps a given dataset $\mathcal{D}$ and HP configuration $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ to a model $\hat{f}$. Denote with $\mathcal{I}_{\boldsymbol{\lambda}}$ an algorithm with fixed HP configuration a chosen loss function with L. The goal of model training is, for fixed $\boldsymbol{\lambda}$, to have $\mathcal{I}_{\boldsymbol{\lambda}}$ find model $\hat{f}$ minimising the expected generalisation error $GE(\mathcal{I}_{\boldsymbol{\lambda}}, \mathcal{D}, L) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathbb{P}_{\boldsymbol{x}y}}[L(y, \mathcal{I}_{\boldsymbol{\lambda}}(\mathcal{D})(\boldsymbol{x}))]$ The goal of HPO, on the other hand, is to find $\boldsymbol{\lambda}$ minimising the expected generalisation error, i.e. $\arg\min_{\boldsymbol{\lambda}\in\boldsymbol{\Lambda}} GE(\mathcal{I}_{\boldsymbol{\lambda}}, \mathcal{D}, L)$. For this there is no analytical expression available, making HPO a blackbox optimization problem. (Karl et al., 2023, pp. 2f)

We will first outline model-free methods to approach blackbox optimization problems, before presenting a model-based variant.

The most basic model-free strategies for blackbox optimization are grid and random search. In the latter, the user defines a range of interest for each HP and then evaluating points along a grid within the cartesian product of those. This has the drawback of scaling extremely poorly in both number of HP dimensions and number of query points per range of interest. Random search, on the other hand, randomly samples a value for each HP until it runs out of budget. Its explorative nature, ease of use, and no assumptions about the model makes it a good baseline. It is also superior to grid search in cases were one or more HPs have little impact on model performance, as for a given budget B, each HP will likely be queried with B different values, whereas for grid search each HP will only be queried with $B^{1/N}$ different values for N HPs.

(evolutionary algorithms) - another model-free class of optimisation algorithms, inspired by naturally occuring evolution - based on a population, which iteratively (iteration = generation) generates λ offspring via 3 operators (all sub-bullets from Goldberg (1989, pp. 10-)) * **reproduction**: pick an individual to reproduce with prob proportional to its fitness * **crossover** - select 2 "parents" from pool of reproducing individuals - for a position k in their HP configs, with certain prob, swap their values after position k, yielding 2 new children * **mutation**: with certain prob, change values of an individual, e.g. by adding Gaussian noise (Gaussian mutation) to real values, or flipping bit for binary values - selection at end of each genertion: keep μ best individuals (based on some fitness function), either from only offspring ("(μ, λ)-selection") or (more commonly) from population + offspring ("$(\mu + \lambda)$-selection", guaranteed to keep best individual) - pro: conceptually simple + can handle even complex parameter spaces (continuous, discrete, hierarchical, etc.) given appropriate implementation of operators all above starting at HPO from (Feurer and Hutter, 2019, chap. 1.3) - prominent examples * CMA-ES - "Covariance Matrix Adapation Evolution Strategy" - offspring generation exclusively via multivariate normal (Hansen, 2023, p. 8) * mean = weighted average of previous generation * covariance = weighted covariance of previous generation, with weighting as for mean - weighing scheme done to sample in a way as to reproduce previously successful (i.e. selected) steps (Hansen, 2023, p. 11) * differential evolution (Storn and Price, 1997, -) - init population randomly so that entire param

space is covered * D-dim vectors $\boldsymbol{x}_{i,G}$ with $i = 1, 2, ..., n$ for gen G - mutation * for each $\boldsymbol{x}_{i,G}$, generate **mutant vector** $\boldsymbol{v}_{i,G+1} = \boldsymbol{x}_{r_1,G} + F \cdot (\boldsymbol{x}_{r_2,G} - \boldsymbol{x}_{r_3,G})$ * $r_1, r_2, r_3 \in \{1, 2, ..., n\}$ mutually different random idx + different from i * constant $F \in [0, 2]$ - crossover * **trial vector** $\boldsymbol{u}_{i,G+1} = (u_{i,G+1}^{(1)}, u_{i,G+1}^{(2)}, ..., u_{i,G+1}^{(D)})$ - chose random index $R \in \{1, 2, ..., D\}$ - sample $p \sim U[0, 1]$ - define crossover constant $\mathrm{CR} \in [0, 1]$ - $u_{i,G+1} = \begin{cases} v_{i,G+1}^{(j)} & \text{if } p \leq \mathrm{CR} \text{ or } j = R \\ x_{i,G}^{(j)} & \text{else} \end{cases}$ - selection: greedy, compare fitness of $\boldsymbol{u}_{i,G+1}$ with $\boldsymbol{x}_{i,G}$, pick better

[model based] - contrast to model free, fit a surrogate model on blackbox problem + optimise this (Bayesian optimisation) - iterative algo comprising of * surrogate model for black box problem, needs to be able to model mean + variance * acquisition function, to decide which point to query next - in each iteration * fit surrogate model on all data points (posterior distribution) * get highest utility point from acquisition function for newly fitted surrogate model -¿ add to data points -¿ hence Bayesian, get new query point given already previously fitted points * acquisition function trades off exploration + exploitation of surrogate * BO up to here from (Feurer and Hutter, 2019, chap. 1.3.2) + (Frazier, 2018, pp. 2-3) - no optimising of model directly, instead iteratively optimise acquisition function - common choices for surrogate models * **gaussian processes** - pros * fully specified by mean + covariance - covariance function (aka kernel) solely determines quality of GP - kernel as function of two points from search space, yields their covariance - usual property of kernels: the closer points are in search space, the more strongly their correlation (Frazier, 2018, p. 5) * well-calibrated uncertainty estimates * closed-form computability - con: neither scales well in # of data points nor in # of HP dimensions BUT workaround: sparse GPs, approx full GP with small subset of original dataset * **random forests** - can handle complex search spaces (high-dim, categorical, hierarchical), unlike GPs - computational complexity scales far better than GPs * GPs $O(n^3)$ fitting, $O(n^2)$ predicting * RFs $O(n \log n)$ fitting, $O(\log n)$ predicting - common choices for acquisition functions * **expected improvement** * **Thompson sampling** - all BO stuff if not specified differently comes from (Feurer and Hutter, 2019, chap. 1.3.2)

2.3 Neural Architecture Search (NAS)

- approaches specifically for NN HPO due to flexible structure of NNs and thus very large search space (each layer can have different # nodes, different activations, for CNN different pooling, etc. operations) - we don't employ NAS for our extension as research focusses on the NLP and image domains, whose datasets exhibit strong correlation amongst features (i.e. tokens or pixels, respectively), an effect that is much weaker for tabular data (Borisov et al., 2024, p. 7499) - at least want to give a little outline on most notable approaches * **cell search space** - modularise NN architecture into cells, NN as chain-structure of those - cell = basic building block, fixed component of an NN * e.g. linear layer with specific # of neurons in feedforward * or convolutional / pooling / etc layer for CNN - then optimise sequential placement of the cells as HPO problem * e.g. via random search or BO * Zoph and Le (2017, p. 3) + Zoph et al. (2018, pp. 2-4) use RNN to recursively optimise HPs of a cell given already determined previous cells (+ HPs of current cell), which is trained via RL with the different HPs the RNN predicts being the actions and performance on

held-out data being reward - (Elsken et al., 2019, chap. 3.2) * **one-shot model** - trains one overall "fabric" comprising all architectures of search space - visualisation as DAG, nodes are layers, edges in-between are operations on a layer's values - each path through DAG (from input to output node) represents one architecture of search space -¿ train entire DAG, then pick optimal path (architecture) - pro: very efficient training, individual architectures share operations along edges they share, training one-shot model trains all subsumed models (more expensive than training a single model but less expensive than trying out all configurations included in the fabric) - (Saxena and Verbeek, 2017, pp. 1-2, p.8)

2.4 Multi-Objective Optimization

- in most practical use cases one doesn't just want to optimise for performance but e.g. also for interpretability using some proxy metrics - formal definition * vector of objectives $c_1, c_2, ..., c_m = \boldsymbol{c} : \boldsymbol{\Lambda} \rightarrow \mathbb{R}^m$ * goal: minimise vector * (Karl et al., 2023, p. 11)

2.4.1 Pareto-optimality

- problem: usually conflicting objectives, i.e. minimisation of $\boldsymbol{c}$ not possible along all dimensions - thus aim to find trade-off solutions of non-dominated points - we say a "point dominates another" * if there is no other point strictly better in at least one dimension and better or equal in the remaining ones * formally: $\boldsymbol{\lambda}$ dominates $\boldsymbol{\lambda}'$ ($\boldsymbol{\lambda} \prec \boldsymbol{\lambda}'$) if and only if $\forall i \in \{1, ..., m\} : c_i(\boldsymbol{\lambda}) \leq c_i(\boldsymbol{\lambda}') \wedge \exists j \in \{1, ..., m\} : c_j(\boldsymbol{\lambda}) < c_j(\boldsymbol{\lambda}')$ * (Karl et al., 2023, pp. 7f) + (Goldberg, 1989, pp. 198f) - Pareto set: set of nondominated points $\mathcal{P} := \{\boldsymbol{\lambda} \in \boldsymbol{\Lambda} | \nexists \boldsymbol{\lambda}' \in \boldsymbol{\Lambda} \text{ s.t. } \boldsymbol{\lambda}' \prec \boldsymbol{\lambda}\}$ - Pareto front: image of nondominated points - goal: find set of nondominated points $\hat{\mathcal{P}}$ approximating true Pareto set $\mathcal{P}$ well (evaluation) - if knowledge over true Pareto-front, evaluating set of individuals can be done based on distance of estimated to true Pareto front - if no knowledge over true Pareto-front, volume-based approaches are popular, which measure volume between Pareto front estim and some chosen reference point (usually worst point in objective space), e.g. 0 for accuracy (optimum is 1) - (Karl et al., 2023, pp. 8-10)

2.4.2 A-priori

- requires specifying trade-off between objectives a-priori, will outline 2 popular approaches - e.g. different versions of **scalarization** * weighted sum of objective functions - $\arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} w_i c_i(\boldsymbol{\lambda})$ with $\sum_{i=1}^{k} w_i = 1$ and $w_i > 0, \forall i = 1, ..., k$ - drawbacks * solution sensitive to weights * different users might have different opinions on weights (Srinivas and Deb, 1994, chap. 3.1) - (Karl et al., 2023, p. 11) * ϵ-constraint - translate all but one objective into constraint, then optimise remaining objective subject to the constraints - w.l.o.g. $\arg\min_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} c_1(\boldsymbol{\lambda})$ s.t. $c_2(\boldsymbol{\lambda}) \leq \epsilon_2, ..., c_m(\boldsymbol{\lambda}) \leq \epsilon_m$ - conceptually similar to weighted sum: also sensitive to constraints, must be chosen sensibly - (Karl et al., 2023, p. 12) - **lexicographic method** * define priority of objectives * greedily optimise objectives in order of priority, constraint to the solutions of the already optimised (higher-priority) objectives * again very dependent on user-defined priorisation * (Riera et al., 2023, p. 13749)

2.4.3 A-posteriori

- problem a priori * either restrict search space to "enforce our will" (e.g. only use 50% of features), optimise only prediction performance + use this * or leave search space unrestricted but adjust loss function to incorporate multiple objectives + take optimum from there * in either case: no knowledge of interplay between HP config + performance on all objectives * in practical applications, it is oftentimes useful to make the decision of which point of the Pareto set to use a-posteriori, e.g. if only a slight decrease in one objective translates to a significant improvement in another that would have been missed if the problem was optimised using a-priori methods * a-posteriori evaluates configs just as a-priori, but keeps track of multiple "best" (non-dominated) solutions -¿ makes relationship between HP config + objectives visible - aside from usual baselines grid and random seach there are multi-objective BO adaptations, mainly using either of two approaches (1) fit single surrogate model on scalarised objectives, e.g. ParEGO, which employs the augemented Tchebycheff function as scalarisation to ensure the Pareto front is explored sufficiently (Karl et al., 2023, pp. 15f) + (Knowles, 2006, pp. 54-56) (2) fit one surrogate per objective, then - either one acquisition function per objective -¿ return set of promising next candidates - or one overall acquisition function aggregating surrogates, e.g. *EHI*, maximises expected improvement of hypervolume (Karl et al., 2023, p. 16) + (Emmerich et al., 2006, pp. 8f) - lastly, there is also multi-objective EA (MOEA) algorithms to explore Pareto front, one of which is NSGA-II (Nondominated Sorting Genetic Algorithm) * improves upon predecessor NSGA (Srinivas and Deb, 1994) by making it parameterless, ensuring elitism, and reducing computational complexity of ranking of individuals (Deb et al., 2002, p. 182) * uses all the regular operators, i.e. reproduction, mutation, crossover can be used from single-objective EA (SOEA) * difference to SOEA: ranking of individuals (SOEA uses scalar fitness, MOEA mutliple objectives) - multi-objective ranking mechanism based on 2 parts * non-dominated sorting, ensures elitism - iterative procedure to rank individuals in population by their fronts (1) determine pareto front, assign rank 0 (2) remove pareto front from population (3) if any individuals left, repeat from 1, increment rank # - (Goldberg, 1989, p. 201) + (Deb et al., 2002, pp. 183f) * crowding distance, ensures sufficient diversity, i.e. exploration of pareto front - assigns score depending on how crowded area around individual in objective space is - crowding distance of an individual = mean side length of cuboid spanned by its nearest neighbours as vertices in objective space - individuals without two neighbours in a dimension are assigned infinitely high distance value - (Deb et al., 2002, p. 185) -¿ the less the crowding distance, the more "crowded" an area is by other individuals -¿ rank individuals by nds front rank (ascending) + crowding distance (descending) as tie breaker * ranking used for selecting μ best individuals to keep for next generation + for reproduction: via binary tournament selection: select two random individuals, pick best w.r.t. nds + cd for offspring creation (i.e. mutation / crossover) * using nds for ranking / fitness makes intuitive sense, but why cd? - goal of MOO: not simply optimise HV, but approx true Pareto front well - only having individuals representing one area in objective space makes Pareto front estimate very "unstable": removing this area (i.e. solutions form that area) would "collapse" entire front - instead having multiple areas be represented makes the estimate "stable": removing one area wouldn't impact Pareto front estimate a lot - (Goldberg, 1989, p. 185, pp. 189-192)

3 EAGGA

- NSGA-II inspired evolutionary + genetic algorithm - uses AUC-ROC as performance metric and 3 interpretation metrics * NF: rel. # of features used in model * NI: rel. # of pairwise feature interaction effects * NNM: rel. # of non-monotone feature effects - aims to find high performing models (AUC) with low NF, NI, and NNM -¿ ensures better interpretability than simply optimising for performance but creates very large objective space $\check{\boldsymbol{\Lambda}}$ to be optimised over with tuples $(\boldsymbol{\lambda}, \boldsymbol{s}, \boldsymbol{I}_s, \boldsymbol{m}_{\boldsymbol{I}_s}) = \check{\boldsymbol{\lambda}} \in \check{\boldsymbol{\Lambda}}$ with * $\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ "regular" model HP config * $\boldsymbol{s} \in \{0,1\}^p$ vector denoting feature usage * $\boldsymbol{I}_s \in \{0,1\}^{p \times p}$ matrix denoting pairwise interactions * $\boldsymbol{m}_{\boldsymbol{I}_s} \in \{-1,0,1\}^p$ vector denoting monotonicity constraint of each feature (-1 decreasing, 0 none, 1 increasing) - thus would require to solve $\arg\min_{\check{\boldsymbol{\lambda}} \in \check{\boldsymbol{\Lambda}}}(GE(\mathcal{I}_{\check{\boldsymbol{\lambda}}}, \mathcal{D}), NF(\hat{f}_{\mathcal{D},\check{\boldsymbol{\lambda}}}), NI(\hat{f}_{\mathcal{D},\check{\boldsymbol{\lambda}}}), NNM(\hat{f}_{\mathcal{D},\check{\boldsymbol{\lambda}}}))$ - (Schneider et al., 2023, pp. 540f) - introduces equivalence relation R "allowed to interact" on features that significantly reduces search space for more efficient optimization - thus: augmented search space $\tilde{\boldsymbol{\Lambda}} = \boldsymbol{\Lambda} \times \mathcal{G}$ comprising model HP space and group structure space * each group structure $\boldsymbol{G} \in \mathcal{G}$ consists of g groups: - G_1 set of excluded features - $\forall k = 2, ..., g : G_k = (E_k, M_{E_k})$ tuple * E_k set of features allowed to interact with each other * M_{E_k} monotonicity constraint of entire group k - EA on model hyperparameters $\boldsymbol{\Lambda}$ - GGA on group structure space $\mathcal{G}$ with adapted mutation and crossover operators - (Schneider et al., 2023, pp. 541f) - futher introduces special initialisation of group structures to increase sample-efficiency of EAGGA algorithm compared to random init - (Schneider et al., 2023, pp. 542f)

4 Extension to neural networks

- original EAGGA applied to XGBoost model proved to vastly outperform union of competitor models w.r.t. dominated hypervolume and comparable or better than ParEGO on extended search space $\check{\boldsymbol{\Lambda}}$ (Schneider et al., 2023, pp. 543-545) - why extend it to NNs? * NNs notoriously uninterpretable due to complex transformation of the feature space * due to (lin alg) non-linear activation functions, interactions can be modelled * no monotonicity guarantees - our approach (general algorithm) * EAGGA algorithm implemented largely as described in the paper * HP init - NN total layers $\in \{3, ..., 10\}$, i.e. hidden layers $\in \{1, ..., 8\}$, init from trunc geom with prob=0.5 - NN nodes per hidden layer (for each group) $\in \{3, ..., 20\}$, init from trunc geom with prob=0.5 - NN dropout % $\in [0, 1]$, init from trunc gamma with shape=2, scale=0.15 * group structure init - feature detector * as described in paper * but instead of fitting 10 trees + taking rel. # of features used as prob for trunc geom, we simply use 0.5 (sklearn dectree examination not straightforward) * also in preliminary experiments we found the sampled # of features to be used occassionally to be ¿ # of non-0 values in normalised information gain filter (e.g. if former is = total # of features and one feature is indep. from target) in these edge cases we simply use all features with non-0 filter values - interaction detector * as described in paper * same as for feat detect: use prob=0.5 to sample # of interactions used instead of 10 dec trees * also for FAST algorithm don't use RSS (lin reg metric) but mean accuracy, as we fit log reg - monotonicity detector * as described in paper * use default HPs (max depth 30, minsplit = 20) of mlr3 classification tree implementation, as this is the library the paper uses -¿ both interaction + monotonicity detectors fit their models on 80% of train

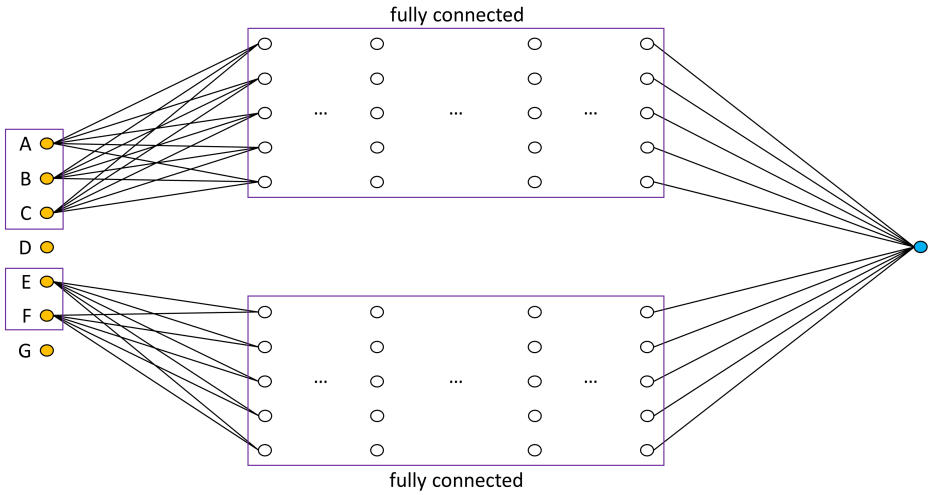

Figure 1: TODO: caption

split from holdout + eval on remaining 20% (implementation details) * group structures + datasets - group structures implemented as described in the paper with additional list encoding sign of monotonicity of the individual features as detected by the monotonicity detector - included features are passed to dataset, dataset outputs included features, multiplied by the features' individual monotonicity (-1 / 1), so that group monotonicity can be encoded with only $\{0, 1\}$, as proposed in paper - entire group structure is passed to NN, where architecture is built accordingly * neural network - "instead of XGB as in the original paper, we apply the method to NNs to examine whether this type of regularisation can achieve interpretability on NNs while outperforming EAGGA on XGB (original paper), ..., this requires special architecture, etc. pp." - NN * comprises of "sub-NNs", one for each equivalence relation -¿ basically non-fully connected NN * hidden layers use ReLU activation and dropout afterwards, then a shared output layer with concatenated sub-NNs' outputs as input and sigmoid activation * optimizer is AdamW with default params, loss is binary cross entropy loss (sigmoid thus implicit in the loss function for better numerical stability, NN itself outputs "logits", which refers to pre-activation output in pytorch) - feature sparsity thus achieved by only training on included feature groups -¿ goes somewhat against notion of deep learning where model is supposed to decide itself, which feature to "use" / put importance on -¿ ELABORATE - feature interaction achieved by grouping, max-operation in ReLU induces interaction effect (different kind of interaction than e.g. in LM with multiplication) -¿ equation why the interacting features need to be grouped together when using ReLU, cf. photos * given layer input $\boldsymbol{x}$ and w.l.o.g. omitting bias * $\text{ReLU}(\boldsymbol{x}) = \max(0, \sum_{j=1}^{p} w_p x_p)$ * interaction not of the form $x_j \cdot x_{j'}$ as used to from LMs but of a form where the sum $w_j x_j + w_{j'} x_{j'}$ decides whether $x_j, x_{j'}$ pass through the activation or not * in other words: $\max(0, w_j x_j + w_{j'} x_{j'}) \neq \max(0, w_j x_j) + \max(w_{j'} x_{j'})$ and thus there

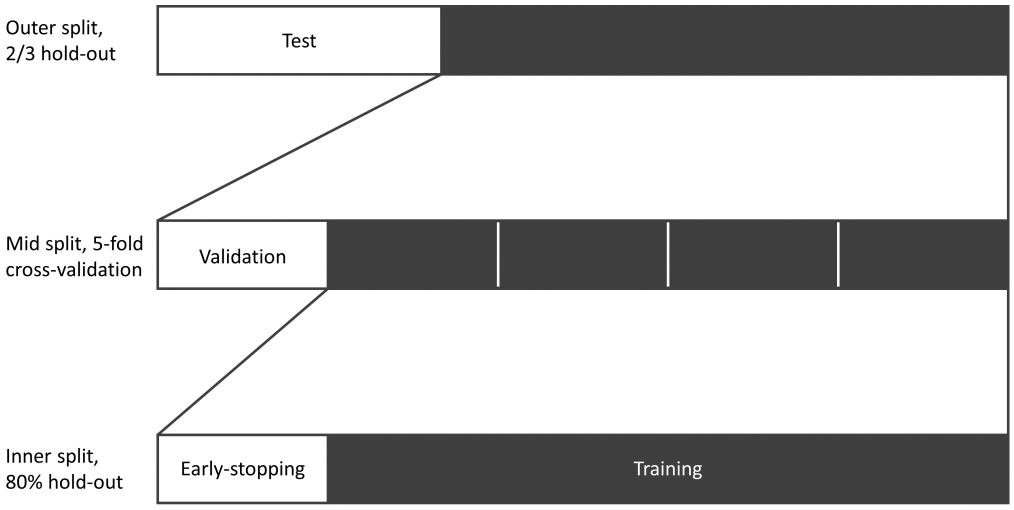

Figure 2: TODO: caption

is an interaction - monotonicty constraint achieved by clipping weights to [0, infty) after each epoch for restricted equivalence relations (monotonic decrease achieved via dataset object multiplying features with their individual signs), bias clipping not necessary (constant additive term) -¿ equation how monotonicity is enforced with this * consider vector form computation of hidden neuron $\boldsymbol{o}_{\text{in}}^{(l)} \in \mathbb{R}^{p^{(l)}}$ of layer l - $\boldsymbol{o}_{\text{in}}^{(l)} = \boldsymbol{W}\boldsymbol{o}_{\text{out}}^{(l-1)} + \boldsymbol{b}$ - where $\boldsymbol{o}_{\text{in}}^{(l)}$ refers to pre-activation values, $\boldsymbol{o}_{\text{out}}^{(l)}$ to value after applying ReLU - weight matrix $\boldsymbol{W} \in \mathbb{R}^{p^{(l)} \times p^{(l-1)}}$ - bias $\boldsymbol{b} \in \mathbb{R}^{p^{(l)}}$ * definition of monotonically increasing function f: for $x_1 \leq x_2$ it must hold that $f(x_1) \leq f(x_2)$ * $\boldsymbol{W}\boldsymbol{o}_{\text{out}}^{(l-1)} + \boldsymbol{b}$ clearly only monotonic if and only if $\boldsymbol{W} \in \mathbb{R}_{0+} p^{(l-1)} \times p^{(l)}$ - where $\mathbb{R}_{0+} = [0, \infty)$ - hence weight clipping necessary, bias clipping not because only constant additive term * $\boldsymbol{o}_{\text{out}}^{(l)} = ReLU(\boldsymbol{o}_{\text{in}}^{(l)}) = \max(0, \boldsymbol{o}_{\text{in}}^{(l)})$ monotonic * evaluation, holdout, cv, early stopping - evaluation via dominated hypervolume along AUC-ROC, NF, NI, NNM as defined in original paper * NF simply rel. # of included features * NI = sum of all possible pairwise interactions in each group over all possible pairwise interactions among all features = $\frac{\sum_g^G \binom{p_g}{2}}{\binom{p}{2}}$ * NNM = rel. # unconstrained features - outer holdout split: 2/3 train, 1/3 test (as in paper) * run EAGGA on holdout train split, i.e. train + select best $\mu = 100$ individuals based on non-dom-sorting (ascending) + crowding distance (descending) as tie breaker - inner CV split on outer train portion: 5-fold (as in paper) * in each fold fit model on 80% of CV-train portion, use remaining 20% of CV-train for early stopping - early stopping criterion * for each fold, always train for min 200 epochs, keep track of model with lowest loss * after that, use patience of 100: if current model's loss is ¿ mean of last 100 epochs' losses -¿ stop early * if no early stopping, train each fold for max 10 minutes * then stop training, return model with lowest loss -¿ refere Figure 2 - then evaluate on last re-

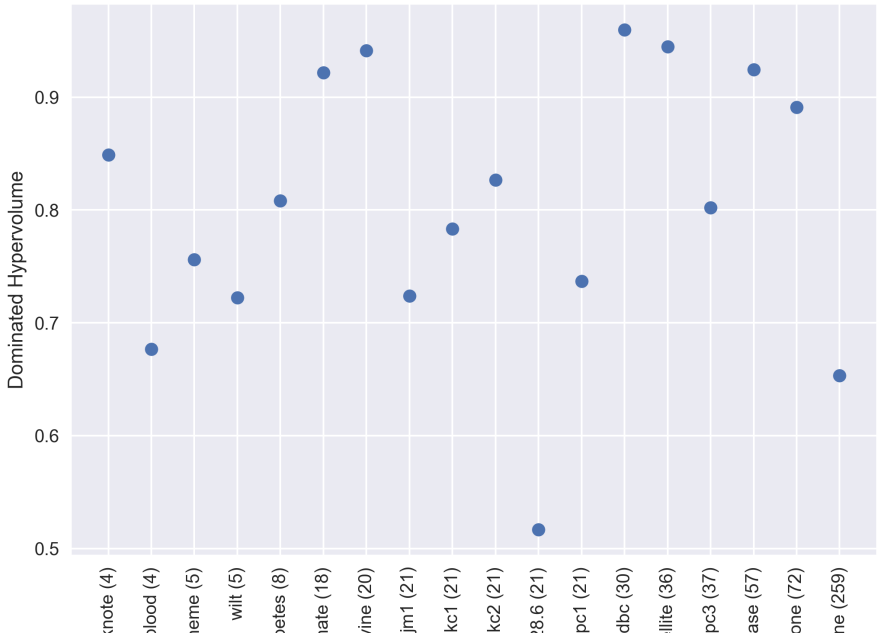

Figure 3: TODO: caption

maining from CV + keep best μ individuals + generate $\lambda = 10$ offspring for new generation + repeat - final evaluation of individuals of pareto set * for each individual, train model on training set of hold-out for max # of epochs taken during CV-training * decided on max # epochs instead of mean after looking at loss graphs in preliminary experiments, also refer Figure 4 * those show that there is no uptick in losses on the early stopping portion (disjunct from training portion) of the set, hence max is reasonable * hardware: training on Sagemaker Notebook instance - initial experiments on ml.g4dn.xlarge instance (2 vCPUs, 16GiB RAM, 1 NVIDIA T4, cf. https://aws.amazon.com/de/ec2/instance-types/g4/) using cuda not much faster than on ml.t3.medium (2 Intel Xeon 8000 vCPUs, 4GiB RAM, cf. https://aws.amazon.com/de/ec2/instance-types/t3/) - thus decided for more economic + ressourcen-schonend t3.medium * did not train on philippine and gina datasets (308, 970 features, respectively), as they ran out of memory when computing interaction detectors * known bugs - in rare cases (anecdotally once every 5-10 datasets), gga_mutate seems to be generating -1 as monotonicity attribute, despite np.random.randint(low=0, high=2, size=1) * loop crashes at group_structure creation, for these cases subtract previous runtime from 8hrs + load from last generation in output via load_population * so far only happened for madeline in after gen-8.json after 5hrs 45mins (at start of gen-9, which wasn't exported yet) -¿ loaded this and ran for another 2hrs 15mins

5 Experimental Results and Discussion

- preliminary * our implementation of feature + interaction detectors likely tend to include - more features + interactions for high p datasets - less for low p datasets - remember: original paper samples # of features included from truncated geometric distribution, what is not mentioned is probability of this distribution is determined from fitting 10 trees + looking at relative # of features used (cf. their github repo /R/TunerEAGGA.R function get_n_selected_rpart()) -¿ mlr3 default decision tree max depth 30 * i.e. datasets with p ¡ 30 might use all features, which translates to trunc geom prob = 1 * vice-versa for p ¿¿ 30 datasets relative # features ¡ 0.5 (our trunc geom prob) * similar reasoning for pairwise interactions * individuals not in Pareto sets occassionally exhibit AUC ¡ 0.5 - this is not by mistake, usually AUC on binary target can simply be inverted (simply predict the opposite class) - for us this cannot easily be inverted due to monotonicity constraints (weights cannot simply be multiplied by -1 if constraint) - could happen e.g. due to AdamW and weight clipping (employed to enforce monotonicity) * AdamW uses momentum * possible scenario: large momentum would yield negative weights, but after epoch they're clipped to [0,infty) + training stops due to early stopping * weight clipping very imperfect way of enforcing monotonicity, but currently in pytorch unfortunately only way to implement this - Figure 3 * suggests comparable performance to XGBoost EAGGA * did not compare to unrestricted NN, would not be sensible, as NF, NI, NNM would be 1, hence hypervolume = 0, as values along 3 dimensions would be at reference point * as XGBoost EAGGA, NN EAGGA consistently outperforms union of competitors as evident from (Schneider et al., 2023, Figure 2) * unfortunately due to time constraints no own union comparison with NN instead of XGBoost - overview over pareto sets can be accessed on our github repo at /code/export/*.csv * NN HPs - total layers mostly 3-4, most commonly 3, goes as high as 7 (Satellite (36), diabetes (8)) - nodes per hidden layer mostly 3-6, goes as high as 12 (diabetes (8)) - p dropout goes as high as 0.7 (climate (18), spambase (57)), but mostly in the 0.1 to 0.3 range * group structures - great diversity in NF across datasets * phoneme (5) up to 1 * blood (4) up to 1 * banknote (4) up to 0.75 * diabetes (8) up to 0.5 * climate (18) up to 0.67 -¿ low p datasets in the benchmark tend to have higher NF - possible consequence of shorter evaluation time - low p datasets have much higher # generations - group structure space much more likely to be exhausted, i.e. more exploration of NN hps - NI, NNM consequently (bounded by NF, can never be more than max # for respective # included features) rather low * dhv contributions - measures contribution of an individual to the hypervolume, i.e. difference between hypervolume of entire pareto front vs hypervolume of pareto front without individual $\boldsymbol{\lambda}$: $\text{CON}_{\mathcal{P}}(\boldsymbol{\lambda}) = \text{HYP}(\mathcal{P}) - \text{HYP}(\mathcal{P} \setminus \{\boldsymbol{\lambda}\})$, where $\text{HYP}(\mathcal{P})$ denotes the hypervolume induced by the pareto set $\mathcal{P}$ (Bringmann and Friedrich, 2010, p. 384) - predominately low for fitted models - mostly highest for featureless learner predicting majority class -¿ sign of good exploration of pareto front + stable estimate, refer Section 2.4.3 - loss graphs Figure 4 * suggests models could have benefitted from longer training on some datasets, as some loss curves haven't converged when stopping criterion hit * crit was likely triggered by short-term spike, thus could potentially be resolved by comparing average of last k losses against average of ¿patience¡ losses prior to that to not be as exposed to short-term spikes in loss * on other datasets, graphs suggest earlier stop would have been totally fine as the networks have long converged, but longer training likely not an issue as

loss graphs come from early stopping dataset portion, which is disjunct from training set - dhv over generations Figure 5 * compute on val set, i.e. had 5 folds per individual - NF, NI, NNM always the same for each fold - but 5 different AUCs -¿ hypervolume of (mean(AUC 1, AUC 2, ..., AUC 5), NF, NI, NNM) * artifacts / drops along y likely due to inconsistent computation of Pareto front by third-party library - preliminary experiments on dummy pareto fronts with 10x4 metrics: noticed nds function returning different rankings for same front - returned ranking switched back and forth between two only slightly different options (only 1 or 2 indices were swapped) - not sure what caused this, as made same observation using another library that was planned as alternative - thus unfortunately not fixable for me * all but 3 datasets (2 of which only trained for 1 generation, aynway) show improvement of dominated hypervolume over generations * BUT: absolute as well as relative improvement almost negligible -¿ no large final dhv decrease would we just have evaluated the models gotten from the detectors - this was also the reason we didn't run EAGGA on philippine and gina simply without the detectors (as that's where they crashed) -¿ evidence suggested that detectors are vital to initial performance - original paper supports this assumption (Schneider et al., 2023, Fig. 4, p. 545)

6 Conclusion and Future Outlook

(Conclusion) - tabular data still difficult discipline for neural networks - research suggests heavy regularisation to improve performance on tabular data - EAGGA proved to be successful in making XGBoost more interpretable while keeping performance on par with unregularised XGBoost - we extend EAGGA to neural networks to see if we can utilise the regularisation induced by it to make NNs both interpretable and performant on tabular data - as consequence propose new architecture allowing to model equivalence relations of EAGGA - ... conforming to Zhang et al. (2021, chap. 2) taxonomy it fits as ..., ..., ... - found overall performance comparable to that of XGBoost fitted using EAGGA, which is a plus, but no outperformance

(Future Outlook) - MO BO on group structure space possible, perhaps via restricted BO?

Appendix A. Software used

for implementation we used openml Vanschoren et al. (2014), Feurer et al. (2021), numpy Harris et al. (2020), pandas pandas development team (2023), Wes McKinney (2010), pytorch Ansel et al. (2024), scikit-learn Pedregosa et al. (2011), scipy Virtanen et al. (2020), pymoo Blank and Deb (2020), and tqdm da Costa-Luis et al. (2024)

Appendix B. Plots

Appendix C.

In this appendix we prove the following theorem from Section 6.2:
Theorem *Let u, v, w be discrete variables such that v, w do not co-occur with u (i.e., $u \neq 0 \Rightarrow v = w = 0$ in a given dataset $\mathcal{D}$). Let N_{v0}, N_{w0} be the number of data points for which $v = 0, w = 0$ respectively, and let I_{uv}, I_{uw} be the respective empirical mutual information values based on the sample $\mathcal{D}$. Then*

$$N_{v0} > N_{w0} \Rightarrow I_{uv} \leq I_{uw}$$

with equality only if u is identically 0. ■

Appendix D.

Proof. We use the notation:

$$P_v(i) = \frac{N_v^i}{N}, \quad i \neq 0; \quad P_{v0} \equiv P_v(0) = 1 - \sum_{i \neq 0} P_v(i).$$

These values represent the (empirical) probabilities of v taking value $i \neq 0$ and 0 respectively. Entropies will be denoted by H. We aim to show that $\frac{\partial I_{uv}}{\partial P_{v0}} < 0$....

Remainder omitted in this sample. See http://www.jmlr.org/papers/ for full paper.

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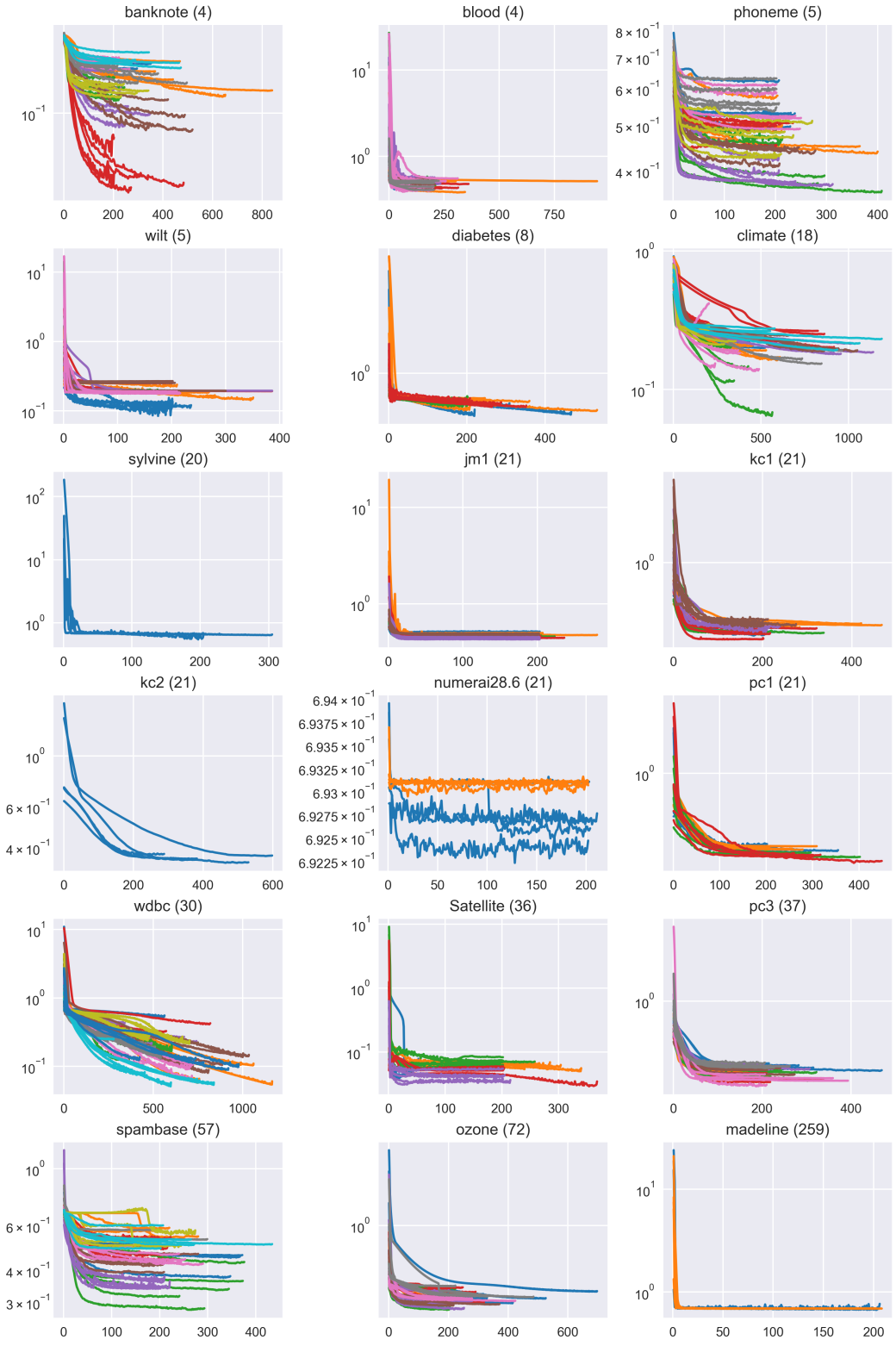

Figure 4: Pareto set loss of all datasets, evaluated on early stopping set. Same colours denote losses coming from folds of the same individual. x-axis portrait epochs, y-axis binary cross entropy loss.

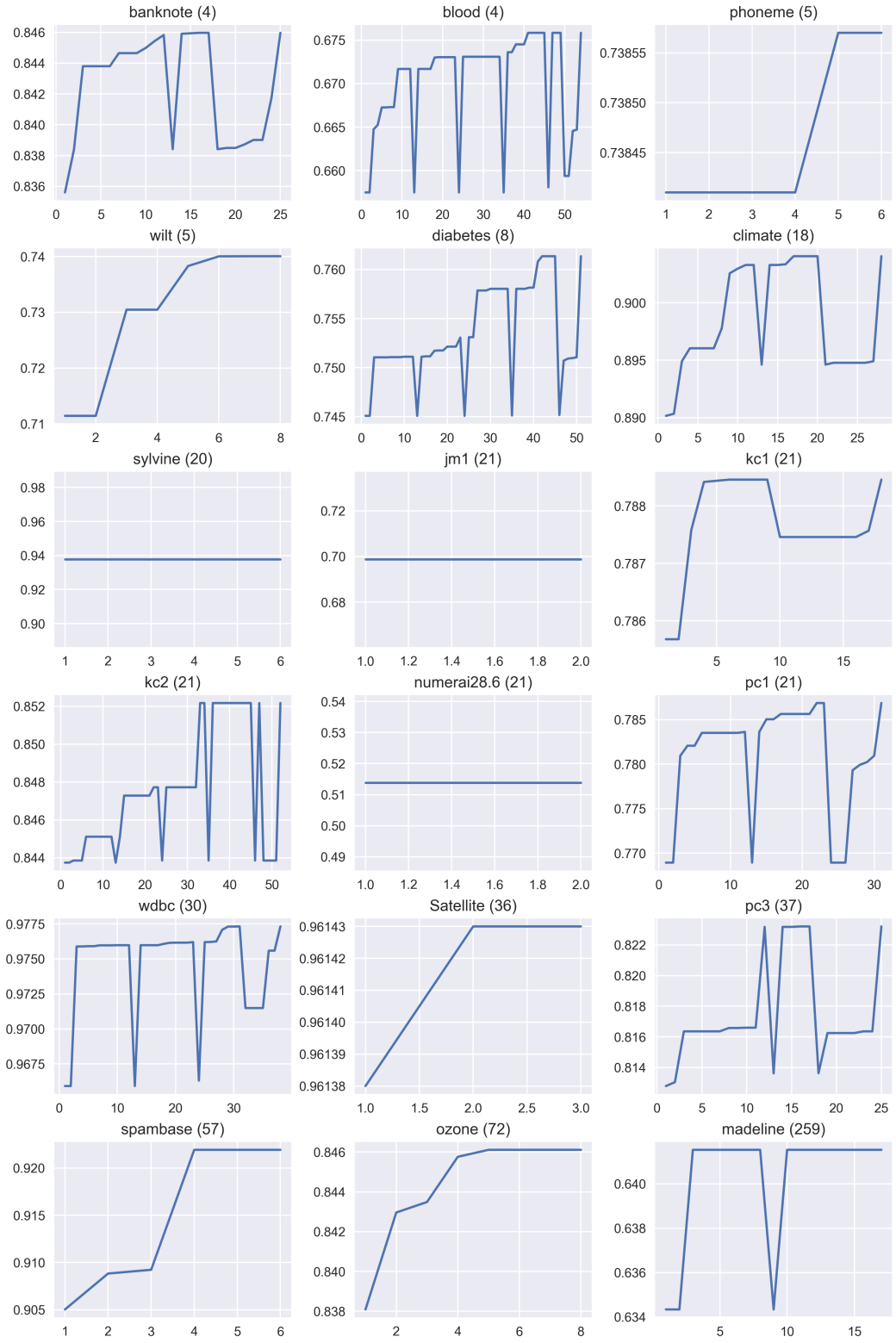

Figure 5: Dominated hypervolume over generations, evaluated on validation set. x-axis portrait generations, y-axis dominated hypervolume using mean AUC over folds.

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