Muddling Label Regularization: Deep Learning for Tabular Datasets

Karim Lounici  
CMAP, Ecole Polytechnique  
Route de Saclay  
91128 PALAISEAU Cedex  
FRANCE  
karim.lounici@polytechnique.edu

Katia Meziani  
CEREMADE - Université Paris Dauphine-PSL  
Place du Maréchal De Lattre De Tassigny  
75775 PARIS CEDEX 16  
FRANCE  
meziani@ceremade.dauphine.fr

Benjamin Riu  
CMAP, Ecole Polytechnique  
Route de Saclay  
91128 PALAISEAU Cedex  
FRANCE  
benjamin.riu@polytechnique.edu

June 30, 2021

Abstract

Deep Learning (DL) is considered the state-of-the-art in computer vision, speech recognition and natural language processing. Until recently, it was also widely accepted that DL is irrelevant for learning tasks on tabular data, especially in the small sample regime where ensemble methods are acknowledged as the gold standard. We present a new end-to-end differentiable method to train a standard FFNN. Our method, Muddling labels for Regularization (MLR), penalizes memorization through the generation of uninformative labels and the application of a differentiable close-form regularization scheme on the last hidden layer during training. MLR outperforms classical NN and the gold standard (GBDT, RF) for regression and classification tasks on several datasets from the UCI database and
Kaggle covering a large range of sample sizes and feature to sample ratios. Researchers and practitioners can use MLR on its own as an off-the-shelf DL solution or integrate it into the most advanced ML pipelines.

1 Introduction

Over the last decade, we have witnessed the spectacular performance of Deep Learning (DL) in the fields of computer vision [10], audio [85] and natural language processing [20]. Until recently, it was also widely believed that DL is irrelevant for tabular data [59]. While the need to handle tabular data arises in many fields (e.g. material science [23], medicine [60], online advertising [76, 30], finance [10]), DL for tabular data remains understudied and underused. It may seem strange considering that tabular data appears at first more straightforward to handle than image or textual data.

Most experiments seem to indicate that tree based ensemble methods [19, 24, 48, 69] are the most reliable option on tabular data and often work well even without any parameter tuning [24, 69]. By contrast, training DL models usually requires extensive trial and error, expertise and time to properly tune the hyperparameters [65]. This comparison is even worse in the small data regime (n < 10^3 or even n < 300). In many fields including material sciences [23], medicine [54, 60], environmental studies [11], small datasets are not rare occurrences since collecting samples and assembling large datasets may be costly, or even impossible by the nature of the task at hand [1].

Deep learning mostly relies on transfer learning schemes to tackle small datasets [53], which are almost never an option for tabular datasets [65]. This is due to the lack of transferable domain knowledge between tabular features. Another important line of work focuses on the preprocessing of categorical features which was an historical limitation of DL [57, 31, 70, 15, 17, 74]. In that regard, entity embeddings [30], which try to capture relationships between categories, have become standard in DL libraries (tensorflow, PyTorch, etc.). Meanwhile, tree based ensemble methods and Gradient Boosting Decision Trees (GBDT) are still considered the best option to handle categorical data [56, 1, 34].

Developing a DL solution for tabular data is desirable as it can leverage the particular strengths of DL, in particular its ability to perform automatic feature engineering and end-to-end training via gradient descent. The recent PyTorch Tabular project [39] and the growing number of articles on tabular data in recent years show the increasing interest of the DL community in this topic [72, 2, 77, 49, 22, 42, 52, 8, 40, 44, 63, 32, 55, 21].

Regularization. Two classical DL regularization strategies, dropout [67] and weight decay [33], have been compared by [75] on tabular data. They found dropout to be better, however dropout may still fail in some tabular data tasks [32]. Moreover [66, 75, 58, 31] seem to indicate that dropout parameters are data and model dependent.

\[1\] e.g. decision making on a limited amount of cases during a pandemic.
**Interpretability.** The "black-box" aspect of DL remains a major obstacle to its wider use in AI is an important concern. Recently, a line of research focuses on the development of novel network architectures with interpretable features. **DNDT** [72] is a specific neural network architecture which can be trained via end-to-end gradient descent. In addition, it can also be rendered as a decision tree for the sake of interpretation. However, DNDT is not scalable w.r.t. the number of features and does not outperform Random Forests (RF) or standard NN on the UCI database. **Attention-Mechanism (AM)** has boosted DL performance on a range of NLP tasks ([4, 20]). It turns out that AM can also be used for interpretability purpose. Recently [2] exploited AM to develop TabNet, an interpretable DL method for tabular data, and claimed it outperforms the gold standard on a limited number of data sets of size \( \gtrsim 10^K \). A limitation of this approach is the complicated data dependent fine-tuning of the hyperparameters.

**Hybrid architecture.** Several recent works propose to combine decision trees with DL. In that regard, [77, 49, 22] proposed to stack layers of RF or GBDT. However, these architectures cannot be trained end-to-end, which may result in potentially inferior performance. **TabNN** [42] is a hybrid machine learning algorithm using GBDT and Deep Neural Networks (DNN). TabNN outperforms standard Feed-Forward Neural Networks (FFNN) but the improvement over GBDT seems marginal in their experiments on 6 data sets ranging in size from 15K up to 7.9M training samples. More recently, **NODE** [55], a new DNN architecture consisting of differentiable oblivious decision trees, can be trained end-to-end via backpropagation. NODE marginally outperforms ensemble methods (CatBoost [56], XGBoost [14]) on 4 out of 6 large size tabular data sets and requires careful hyperparameter optimization.

**New loss functions.** Our contribution falls in this line of research. It consists in replacing the usual loss used to train DNN by specific losses with interesting properties. In that regard, **Regularization Learning Networks (RLN)** [63] is a new family of neural networks trained with a new loss, named counterfactual loss, together with stochastic gradient descent. RLN performs significantly better than standard NN but could not beat GBDT.

**Other approaches.** We can also cite Neural Tangent Kernel (NTK) [3], Net-DNF [40] and Self-Normalized Neural Networks (SNN) [44]. Table [1] summarizes their properties. We provide more details about these methods in the Appendix.

**Contributions.** We propose a pure deep learning solution to train a standard FFNN for tabular data. Our method, **Muddling labels for Regularization (MLR)**, penalizes memorization over permuted labels and structured noise through the application of a differentiable close-form regularization scheme on the last hidden layer during training. More specifically:
Our method outperforms usual methods (Ensemble, SVM, Boosting, Linear Regression, etc.) including the gold standards RF and GBDT for the usual statistics (Mean $R^2$, Friedman rank, P90, P95, P98, PMA) on a diverse collection of regression datasets. Our method also comes in a close second for classification tasks.

The MLR method only requires the most basic standardization, one-hot-encoding and standard imputation of missing data. MLR is fully compatible with all feature engineering schemes (e.g. embeddings, Nyström [71] and RBF [61] kernels, tree leaves). All the popular DL schemes can also be leveraged including learning rate schedulers [64], optimizers, weight decay, batch-normalization, drop-out, residual layers and leaky activations [65].

The performances of MLR-NN are not tied with any of the well-known class of methods. Thus they should be a great addition to the stack of models aggregated by meta-learners. Researchers and practitioners can use MLR on its own as an off-the-shelf DL solution or integrate it into the most advanced ML pipelines.

The implementation of our method in torch is available as a stand-alone which follows the scikit-learn API (i.e. it can be directly encapsulated into parameter search routines, bagging meta models, etc.). For the sake of replicability, the code to run the benchmarks, the ablation study and the preprocessing applied to each dataset is also provided.

The rest of the paper is organized as follows. We describe our approach in Section 2. In Section 3, we carry out a detailed ablation study of our method and evaluate its performances on real data.

2 The MLR-FFNN

2.1 The (MLR) method for Regression

Let $D_{train} = (x, Y) = \{(x_i, Y_i)\}_{i=1}^{n}$ be the train-set with $x_i \in \mathbb{R}^d$ where $d$ denotes the number of features and $Y_i \in \mathbb{R}$. We consider a simple FFNN with $L$ layers, $J$ nodes on each hidden layer and the ReLu activation function between each hidden layer. For $n$ observations $x$, we set $A^0 = x \in \mathbb{R}^{n \times d}$ and $A^1 = \text{ReLU}(A^0 W^1 + B^1), \ W^1 \in \mathbb{R}^{d \times J}$

$$A^L = A^{L-1} W^L, \ W^L \in \mathbb{R}^{J \times 1}, \ (1)$$

where $\forall \ell \in [1, L - 1]$, $B^\ell = \mathbb{1}_n \otimes b^\ell, \ b^\ell \in \mathbb{R}^J$ are the bias terms.

The 3 essential ingredients of the MLR method are Ridge regularization, structured dithering and random permutations as they promote generalization when we train this FFNN.

We introduce first the Ridge regularization. For $\lambda > 0$, we set

$$P = P(\theta, \lambda, x) = [(A^{L-1})^\top A^{L-1} + \lambda \mathbb{I}_J]^{-1} (A^{L-1})^\top \in \mathbb{R}^{J \times n} \ (2)$$

$$H = H(\theta, \lambda, x) = A^{L-1} P \in \mathbb{R}^{n \times n} \ (3)$$
where the last hidden layer is $A^{L-1} := A^{L-1}(\theta, x)$ and $I_{:}$ denotes the identity matrix. Note that $H$ is differentiable w.r.t. $\theta = \{(W^t, b^t)\}_{t=0}^L$ and $\lambda$. We apply Ridge regularization\footnote{Ridge model : $f(\theta, \lambda, x) = x^\top \beta_A(x, Y) := x (x^\top x + \lambda I)^{-1} x^\top Y$} to the last hidden layer $A^{L-1}$ instead of input $x$:

$$f(\theta, \lambda, x) := A^{L-1} W^L = A^{L-1} P(\theta, \lambda, x) Y = H(\theta, \lambda, x) Y.$$

Next we introduce the permutations. For a permutation $\pi$ of $n$ elements, we define the corresponding label permutation operator $\pi$ of $Y = (Y_1, \cdots, Y_n)$ as $\pi(Y) = (Y_{\pi(1)}, \cdots, Y_{\pi(n)})$. Fix $T \geq 1$ and draw $T$ label permutation operators uniformly at random in the set of all possible label permutations : $(\pi^t(Y))_{t=1}^T$. This operation can be seen as a form of data-augmentation on the labels.

**Definition 1** (MLR regression loss). Set $H = H(\theta, \lambda, x)$. We draw i.i.d. random vectors $\xi$ and $(\xi_i)_{i=1}^T$ distributed as $N(0_n, I_n)$. Let $(\pi^t(Y))_{t=1}^T$ be $T$ independently drawn permutations of $Y$. We set $\overline{Y} = \text{mean}(Y)$ and define the MLR loss as

$$\text{MLR}(\theta, \lambda) = \text{RMSE} (Y + (I_n - H) \xi ; H \overline{Y}) + \frac{1}{T} \sum_{t=1}^T \left| \text{RMSE}(Y ; \overline{Y} I_n) - \text{RMSE} (\pi^t(Y) + (I_n - H) \xi_t ; H \pi^t(Y)) \right|.$$

The MLR loss contains two antagonistic terms and was first introduced in the linear regression setting \cite{PMLR}. The first term is the usual RMSE while the second term quantifies the amount of memorization of a model by comparing its RMSE on uninformative labels to the baseline $\text{RMSE}(Y ; \overline{Y} I_n)$, i.e. the performance achieved without fitting the data. Using the RMSE instead of the MSE in the comparison slightly improves the generalization performances. We explain below the role of $(I_n - H) \xi$ and $(I_n - H) \xi_t$.

**The benefit of close-form regularization.** The replacement of the output layer with Ridge regularizes the network in two ways: (i) the weights on the output layer are a direct function of the last hidden layer $A^{L-1}$. This effect is much stronger than adding a constraint or a penalty directly on $W^L$ the weights of the $L$-th layer in \cite{PMLR}; (ii) the close-form we choose is the Ridge instead of the OLS, which implicitly subjects the weights to a steerable $L_2$ regularization.

**The generalization effect of random permutations.** Our work is loosely related to \cite{PMLR} where label permutations are used after the model has been trained as a qualitative observational method to exhibit the overfitting capacity of Neural networks. In our approach, we go further as we use random permutations during the training phase to define a quantitative measure of the amount of overfitting of a model. More precisely, label permutation is used to produce a control set $(x, \pi(Y))$ that can only be fitted through memorization. MLR focuses on patterns that appear only in $(x, Y)$ and not in uncorrelated pairs $(x, \pi(Y))$. 
Structured Dithering. We describe an additional scheme to prevent memorization. We apply a dithering scheme which adapts to the spectral structure of $H$, the "regularized projector" based on $A^{L-1}$ (the output of the last hidden layer). More specifically, we muddle the target using $(I_n - H)\xi$ which introduces noise of higher variance along the weakly informative eigendirections of $H$.

Computational point of view. The permutations are drawn once before the training and are not updated or changed thereafter. Once the FFNN is trained, these permutations have no further use and are thus discarded. In practice we take $T = 16$ for all the datasets in our benchmark. Therefore, $T$ does not require hyperparameter tuning. Moreover, note that the choice of the seed used to generate the permutations has no impact on the values of the MLR loss. The additional computational cost of using MLR is marginal. We only need to compute a matrix inverse on the output of the last hidden layer $A^{L-1}$. This operation is differentiable and inexpensive as parallelization schemes provide linear complexity on GPU when some memory constraints are met [50, 51, 16].

2.2 Model: MLR-NN and training protocol

The MLR-NN Architecture. We consider the FFNN described in (1) with $L$ layers and all the hidden layers of constant width $J$. In our experiments, we always take $J$ as large as possible (our machine with 11GVRAM allowed for $J = 2^{10}$) and $L \in \mathcal{G}_L := \{1, 2, 3, 4\}$.

The MLR neural net (MLR-NN) is

$$\text{MLR-NN}(\hat{\theta}, \hat{\lambda}, \cdot) = A^{L-1}(\hat{\theta}, \cdot) P(\hat{\theta}, \hat{\lambda}, x) Y$$

with $P(\cdot, \cdot, x)$ as defined in (2). The initialization of $\theta$ is as in [29].

Initialization of the Ridge parameter. The initialization of $\lambda$ is both crucial and non trivial. Choosing $\lambda$ close to 0 will hinder regularization. Furthermore, a very small value of $\lambda$ will cause numerical instability during the matrix inversion. Conversely, choosing $\lambda$ too big will prevent any learning. Indeed, the gradient with respect to $\lambda$ will vanish in both cases. From our initial calibration, we discovered that there exists no universal value to initialize $\lambda$. The appropriate initial value depends on many factors such as data size, network architecture, difficulty of the task, etc. However, we found a very efficient heuristic to pick an appropriate initial value. We want to start training from the point where fitting the data will lead to generalization as much as possible instead of memorization. In this region, the variation of MLR with respect to $\lambda$ is maximum. In practice, we pick $\lambda_{\text{init}}$ by running a grid-search on the finite difference approximation for the derivative of MLR in (5) on the grid $\mathcal{G}_\lambda = \{\lambda^{(k)} = 10^{-1} \times 10^{5\times k/11} : k = 0, \cdots, 11\}$:

$$\lambda_{\text{init}} = \sqrt{\lambda^{(\hat{k})}} \lambda^{(\hat{k}+1)} \text{ where } \hat{k} = \arg \max \left\{ \left(\text{MLR}(\theta, \lambda^{(k)}) - \text{MLR}(\theta, \lambda^{(k+1)})\right), \lambda^{(k)} \in \mathcal{G}_\lambda \right\}. \quad (5)$$
From a computational point of view, the overcost of this step is marginal because we only compute $A^{L-1}$ once, and we do not compute the derivation graph of the 11 matrix inversions or of the unique forward pass. The Ridge parameter $\lambda$ is not an hyperparameter of our method; it is trained alongside the weights of the Neural Net architecture.

**Dither [62].** We do not apply the MLR loss on $Y$ and the permuted labels $(\pi^t(Y))_{t=1}^T$ but rather on noisy versions of them. We draw $T+1$ i.i.d. $\mathcal{N}(0_n, \tilde{\sigma}^2 I_n)$ noise vectors that are added to $Y$ and $\pi^t(Y)$, $1 \leq t \leq T$. Here again, $\tilde{\sigma}$ is not an hyperparameter as we use the same value $\tilde{\sigma} = 0.03$ for all the data sets in our benchmark.

**Training protocol.** Using wider architecture ($J = 2^{10}$) and bigger batch size ($b_s = \min(J, n)$) is always better. To train our FFNN, we use Adam [43] with default parameters except for the learning rate $\ell_r$ (which depends on the number of layers $L$). See Table 2 and we select a validation-set of size $n_{val} = 20\% n$.

Choice of maxIter and early stopping. We fix the budget ($\text{FixB} = 5 \text{ min}$) and denote by $n_{iter}$ the possible number of iterations during the alloted time $\text{FixB}$. We fix the maximum number of iterations maxIter (depending on the value of $L$). Then, $\text{Iter} = \min(\text{maxIter}, n_{iter})$ is the number of iterations that will actually be performed. We read the $R^2$-score for each iteration on the validation-set and take the iteration with the best $R^2$-score: $\text{Iter}^* := \arg\max\{R_k^2, k = 1, \ldots, \text{Iter}\}$. Finally, $(\hat{\theta}, \hat{\lambda})$ will take its value at iteration $\text{Iter}^*$.

The generic values ($\tilde{\sigma} = 0.03$ and $T = 16$) for the dither and the number of permutations hyperparameters yield consistently good results overall. The dither parameter admits an optimal value which seems to correspond to the standard deviation of the target noise. As soon as $T = 16$, the choice of permutations has little impact on the value and the MLR loss. In addition, when $T = 16$, GPU parallelization is still preserved. Recall that the Ridge parameter $\lambda$ is trained alongside the weights of the FFNN architecture and the initial value $\lambda_{\text{init}}$ is fixed by the heuristic choice [14]. Our investigations reveals that this choice is close to the optimal oracle choice on the test set. We can also see that the runtime overhead cost of replacing a matrix multiplication with a matrix inversion depends only linearly on the width $J$ and the batch size $b_s$, which are fixed in our method. As a pure DL method, MLR method is scalable. Its complexity is the same as training a standard NN [50]. We refer to the Appendix for a detailed description of the training protocol.

**Our final models.** We propose several models with varying depth based on FFNN trained with the MLR loss. We also create ensemble models combining architectures of different depth. Our models are:

- **MLR-L**: a simple FFNN of depth $L$ ($1 \leq L \leq 4$).
- **Bag-MLR-L**: a bagging of 10 FFNN of depth $L$ ($L = 1$ or $L = 2$).
- **Ens-MLR**: an ensemble of 20 FFNN (the aggregation of Bag-MLR1 and Bag-MLR2 of depth 1 and 2 respectively).
• **Best-MLR**: the best prediction among 20 MLR-NN in terms of the validation score.
• **Top5-MLR**: the aggregation of the top 5 among 20 MLR-NN in terms of the validation score.

For the methods based on bagging [7], the final prediction is the mean of each MLR-NN prediction.

### 2.3 Classification tasks with the BCE-MLR loss

The adaptation of the MLR method to classification tasks is relatively simple. The FFNN architecture and the training protocol are essentially unchanged. The usual loss for binary classification task is the **BCE** loss that combines a Sigmoid and the Cross Entropy (CE) loss. Set \( \text{Sig} (\cdot) = \text{Sigmoid} (\cdot) \), then

\[
\text{BCE}(Y, f(\theta, x)) = -\frac{1}{n} \left[ Y^T \log(\text{Sig}(f(\theta, x))) + (1_n - Y)^T \log(1_n - \text{Sig}(f(\theta, x))) \right].
\]

**Definition 2 (BCE-MLR loss).** Let \( \xi \) and \( (\xi_t)_{t=1}^T \) be i.i.d. \( \mathcal{N}(0_n, I) \) vectors. Set \( Y^* = 2Y - 1 \). We define the **BCE-MLR** loss as

\[
\text{BCE-MLR}(\theta, \lambda) = \text{BCE}(Y; Y^* + (1_n - H)\xi + HY^*)
\]

\[
+ \frac{1}{T} \sum_{t=1}^T \left| \text{BCE}(Y; \text{Y}_{1:n}) - \text{BCE}(\pi'(Y^*); \pi'(Y^*) + (1_n - H)\xi_t + H \pi'(Y^*)) \right|.
\]

The quantity \( \text{BCE}(Y; \text{Y}_{1:n}) \) is our baseline. The structured dithering is applied to the prediction rather than the target \( Y \) because the BCE is only defined for binary target \( Y \in \{0, 1\}^n \).

The **BCE-MLR** neural net (BCE-MLR-NN) is

\[
\text{BCE-MLR-NN}(\hat{\theta}, \hat{\lambda}, \cdot) = \text{Hardmax}(A_{L-1}(\hat{\theta}, \cdot) P(\hat{\theta}, \hat{\lambda}, x)) Y \in \{0, 1\}^{obs.}
\]

with \( (\hat{\theta}, \hat{\lambda}) = \arg \min_{\theta, \lambda} \text{BCE-MLR}(\theta, \lambda) \),

with \( P(\cdot, \cdot, x) \) defined as in [2]. We refer to the Appendix for a detailed discussion on this specific adaptation.

### 3 Experiments

We provide both the code to download raw files and apply each steps, and the resulting data matrices. All results are fully reproducible as both random seeds and random states were manually set and saved at every step of our experiments.

See the supplementary material for the the github repository, the detailed description of our experimental setting and the exhaustive list of compared methods with their performances.
3.1 Setting.

**Benchmark description.** To produce this benchmark we aggregated 32 tabular datasets (16 in regression and 16 in classification), from the UCI repository and Kaggle. For computational reasons, we have chosen to restrict the number of datasets but we performed more train/test splitting in order to reduce the variance of our results. We curated the UCI repository and Kaggle through a set of rules detailed in the appendix (e.g. discard empty or duplicate datasets, times series, missing target, non i.i.d. samples, text format, etc.).

**Preprocessing.** To avoid biasing the benchmark towards specific methods and to get a result as general as possible, we only applied as little preprocessing as we could, without using any feature augmentation scheme. The goal is not to get the best possible performance on a given dataset but to compare the methods on equal ground. We first removed features with constant values such as sample index. Categorical features with more than 12 modalities were discarded as learning embeddings is out of the scope of this benchmark. We also removed samples with missing target. Next, all missing values are imputed with the mean and the mode for numerical and categorical features respectively. We applied one-hot-encoding for categorical values and standardization for numerical features and target.

We repeated our experiments 10 times using a different 80 : 20 train/test split of the data and no stratification scheme.

**Compared methods.** We ran the benchmark with all the methods available in the scikit-learn library for classification and regression (including RF and XGB) as well as the GBDT methods. In the rest of the paper, we only display the main classes of methods in Table 3.

| Class of Methods | Methods |
|------------------|---------|
| MLR (this paper) | MLR-L, Bag-MLR-L, Ens-MLR, Best-MLR, Top5-MLR |
| GBDT             | XGB [8, 26, 27], CatBoost [69], XGBoost [14], LightGBM [41] |
| RF               | RF and LSF [49] |
| SVM              | Lin-SVR, SVM, ν-SVR [12] |
| NN               | Fast.ai [38], MLP [66] |
| GLM              | OLS, Elastic-Net [28], Ridge [37], Lasso [65], Logistic regression [18] |
| MARS             | MARS [28] |
| TREE             | CART, XCART [6, 28, 44] |
| Baseline         | Reg: Intercept | Classif: Class probabilities |

Table 3: Main classes of methods.
3.2 Ablation Analysis.

| Step                        | Mean $R^2$           | Bagging $R^2$ |
|-----------------------------|----------------------|---------------|
| FFNN                        | $-0.081 \pm 0.173$   | $-0.046 \pm 0.169$ |
| + Ridge                     | $0.321 \pm 0.081$    | $0.394 \pm 0.082$ |
| + Ridge + Struct. Dithering | $0.323 \pm 0.075$    | $0.400 \pm 0.048$ |
| + Ridge + Permut.           | $0.364 \pm 0.060$    | $0.432 \pm 0.035$ |
| MLR                         | $0.371 \pm 0.024$    | $0.333 \pm 0.000$ |

Table 4: Ablation Study in Regression.

We ran our ablation study (Table 4) in the regression setting on 3 datasets with different sample sizes and feature to sample ratios. We repeated each experiment over 100 random train/test splits. All the results presented here correspond to the architecture and hyperparameters of MLR-2 and Bag-MLR2.

A standard FFNN of 2 layers with a wide architecture ($J = 1024$) cannot be trained efficiently on such small datasets as the FFNN instantly memorizes the entire dataset. This cannot be alleviated through bagging at all. Note also its lower overall performance on the complete benchmark (Table 5). Applying Ridge on the last hidden layer allows an extremely overparametrized FFNN to learn but its generalization performance is still far behind the gold standard RF. However, when using bagging with ten such models, we reach very competitive results, underlying the potential of the MLR approach.

The random permutations component gives a larger improvement than Structured Dithering. However, when using both ingredients together, a single MLR-NN can reach or even outperform the gold-standard methods on most datasets. Furthermore, the improvement yielded by using bagging (0.062) is still of the same order of magnitude as the one we got when we applied permutations on top of Ridge to the FFNN (0.043). This means these two ingredients (permutations and struct. dithering) are not just simple variance reduction techniques but actually generate more sophisticated models.
### 3.3 Overall Performance comparisons.

Table 5: Performances of the best method in each class of methods for the regression task on our benchmark. P90, P95, P98: the number of datasets a model achieves 90%, 95%, 98% or more of the maximum test $R^2$-score respectively, divided by the total number of datasets. PMA: average percentage of the maximum test $R^2$-score.

| Class of Methods | F. Rank | Mean $R^2$-score | P90   | P95   | P98   | PMA     |
|------------------|---------|------------------|-------|-------|-------|---------|
| MLR              | 2.525 ± 1.355 | 0.744 ± 0.022  | 0.963 | 0.856 | 0.719 | 0.946 ± 0.089 |
| GBDT             | 2.719 ± 1.850 | 0.726 ± 0.093  | 0.863 | 0.756 | 0.650 | 0.898 ± 0.237 |
| RF               | 3.538 ± 1.896 | 0.724 ± 0.070  | 0.825 | 0.681 | 0.481 | 0.914 ± 0.159 |
| SVM              | 4.281 ± 1.534 | 0.711 ± 0.068  | 0.831 | 0.594 | 0.362 | 0.882 ± 0.172 |
| NN               | 4.331 ± 2.206 | Averaging value | 0.725 | 0.606 | 0.475 | Averaging value |
| MARS             | 5.644 ± 1.623 | 0.677 ± 0.060  | 0.573 | 0.350 | 0.163 | 0.861 ± 0.167 |
| LM               | 5.938 ± 1.804 | 0.658 ± 0.094  | 0.531 | 0.294 | 0.156 | 0.837 ± 0.179 |
| TREE             | 7.125 ± 1.613 | 0.512 ± 0.237  | 0.338 | 0.188 | 0.119 | 0.578 ± 0.570 |
| Baseline         | 8.900 ± 0.375 | −0.023 ± 0.211 | 0.000 | 0.000 | 0.000 | −0.031 ± 0.075 |

The MLR method clearly outperforms all the compared methods for the regression task. Ens-MLR with a P98 of 0.719 on the whole benchmark and Friedman Rank of 2.525 is above GBDT, with a P98 of 0.65 and Friedman Rank 2.719 in Table 5. As revealed by its PMA statistics at 0.946, Ens-MLR is far ahead of the other methods. This means that MLR produces reliable results at a rate that is even above methods like RF which are often deemed the safest pick. Standard NN with equivalent architecture and MSE loss performs poorly with a Friedman rank of 4.331. Noticeably, Ens-MLR was most often the best method among all the MLR methods.

Table 6: Performances of the best method in each class of methods for the classification task with the accuracy score.

| Class of Methods | F. Rank | Mean Acc. | P90   | P95   | P98   | PMA     |
|------------------|---------|-----------|-------|-------|-------|---------|
| GBDT             | 1.769 ± 0.998 | 0.889 ± 0.038 | 0.963 | 0.881 | 0.819 | 0.971 ± 0.054 |
| MLR              | 2.913 ± 1.403 | 0.882 ± 0.031 | 0.963 | 0.869 | 0.800 | 0.956 ± 0.070 |
| RF               | 3.056 ± 1.415 | 0.882 ± 0.038 | 0.912 | 0.819 | 0.656 | 0.958 ± 0.063 |
| GLM              | 3.756 ± 1.561 | 0.862 ± 0.060 | 0.806 | 0.631 | 0.463 | 0.940 ± 0.062 |
| TREE             | 4.763 ± 1.195 | 0.836 ± 0.062 | 0.731 | 0.381 | 0.237 | 0.908 ± 0.084 |
| QDA              | 5.675 ± 1.688 | 0.723 ± 0.160 | 0.338 | 0.194 | 0.169 | 0.796 ± 0.159 |
| Baseline         | 6.856 ± 1.574 | 0.593 ± 0.168 | 0.069 | 0.025 | 0.025 | 0.661 ± 0.133 |
| NN               | 7.213 ± 0.980 | 0.565 ± 0.152 | 0.025 | 0.013 | 0.013 | 0.625 ± 0.136 |
### Table 7: Performances of the best in each class of methods for the classification task with AUC score.

| Class of Methods | F. Rank | Mean AUC | P90 | P95 | P98 | PMA |
|------------------|---------|----------|-----|-----|-----|-----|
| GBDT             | 1.738 ± 1.190 | 0.918 ± 0.048 | 0.938 | 0.912 | 0.875 | 0.963 ± 0.108 |
| MLR              | 2.900 ± 1.304 | 0.908 ± 0.012 | 0.912 | 0.844 | 0.694 | 0.952 ± 0.106 |
| RF               | 2.938 ± 1.390 | 0.912 ± 0.047 | 0.931 | 0.887 | 0.706 | 0.956 ± 0.095 |
| LM               | 3.881 ± 1.572 | 0.889 ± 0.060 | 0.775 | 0.662 | 0.475 | 0.935 ± 0.094 |
| NN               | 4.856 ± 1.545 | 0.843 ± 0.154 | 0.706 | 0.506 | 0.412 | 0.896 ± 0.155 |
| TREE             | 5.975 ± 1.160 | 0.813 ± 0.091 | 0.394 | 0.212 | 0.212 | 0.852 ± 0.119 |
| QDA              | 6.631 ± 1.371 | 0.772 ± 0.149 | 0.394 | 0.256 | 0.150 | 0.818 ± 0.152 |
| Baseline         | 7.681 ± 1.084 | 0.499 ± 0.151 | 0.006 | 0.000 | 0.000 | 0.537 ± 0.072 |

For binary classification task with the usual accuracy score, MLR is a close second behind GBDT both in terms of Accuracy and AUC scores.

### 4 Conclusion

All these findings reveal MLR as a remarkably reliable method for tabular datasets, one which consistently produces either state-of-the-art or very competitive results, for a large range of sample sizes, feature to sample ratios, types of features and difficulty across very diverse areas of applications. Furthermore, MLR can achieve these steady performances without any intensive tuning. Nonetheless, higher performances can be achieved with the MLR approach by data-dependent tuning of the hyperparameters in Table 2 and/or leveraging usual DL schemes.

By replacing the standard losses by the MLR loss to train a simple FFNN, we were able to break down the tabular data deadlock and outperform the gold standard. However, nothing in our method is constrained to this setting. The MLR approach is perfectly applicable on CNN for classification tasks in the low sample regime with robustness issues.

### References

[1] Andreea Anghel, Nikolaos Papandreou, Thomas P. Parnell, Alessandro De Palma, and Haralampos Pozidis. Benchmarking and optimization of gradient boosted decision tree algorithms. CoRR, abs/1809.04559, 2018.

[2] Sercan O. Arik and Tomas Pfister. Tabnet: Attentive interpretable tabular learning, 2020.

[3] Sanjeev Arora, Simon S. Du, Zhiyuan Li, Ruslan Salakhutdinov, Ruosong Wang, and Dingli Yu. Harnessing the power of infinitely wide deep nets on small-data tasks. In International Conference on Learning Representations, 2020.
[4] Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. arXiv, 2014.

[5] Iñigo Barandiaran. The random subspace method for constructing decision forests. IEEE transactions on pattern analysis and machine intelligence, 1998.

[6] L. Breiman, J. Friedman, R. Olshen, and C. Stone. Classification and Regression Trees. Wadsworth and Brooks, Monterey, CA, 1984. new edition.

[7] Leo Breiman. Bagging predictors. Mach. Learn., 24(2):123–140, August 1996.

[8] Leo Breiman. Arcing the edge. Technical report, 1997.

[9] Leo Breiman. Random forests. Machine Learning, 45(1):5–32, 2001.

[10] Hans Buehler, Lukas Gonon, Josef Teichmann, Ben Wood, Baranidharan Mohan, and Jonathan Kochems. Deep Hedging: Hedging Derivatives Under Generic Market Frictions Using Reinforcement Learning. SSRN Scholarly Paper ID 3355706, Social Science Research Network, Rochester, NY, March 2019.

[11] M. Cassotti, D. Ballabio, R. Todeschini, and V. Consonni. A similarity-based qsar model for predicting acute toxicity towards the fathead minnow (pimephales promelas). SAR and QSAR in Environmental Research, 26(3):217–243, 2015. PMID: 25780951.

[12] Chih-Chung Chang and Chih-Jen Lin. Libsvm: A library for support vector machines. ACM Trans. Intell. Syst. Technol., 2(3), May 2011.

[13] Jianbo Chen, Le Song, Martin J. Wainwright, and Michael I. Jordan. Learning to explain: An information-theoretic perspective on model interpretation, 2018.

[14] Tianqi Chen and Carlos Guestrin. Xgboost: A scalable tree boosting system. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD ’16, page 785–794, New York, NY, USA, 2016. Association for Computing Machinery.

[15] Heng-Tze Cheng, Levent Koc, Jeremiah Harmsen, Tal Shaked, Tushar Chandra, Srini Aradhye, Glen Anderson, Greg Corrado, Wei Chai, Mustafa Ispir, Rohan Anil, Zakaria Haque, Lichan Hong, Vihaan Jain, Xiaobing Liu, and Hemal Shah. Wide & Deep Learning for Recommender Systems. In Proceedings of the 1st Workshop on Deep Learning for Recommender Systems, pages 7–10, Boston MA USA, September 2016. ACM.
[16] Andrzej Chrzeszczyk and Jakub Chrzeszczyk. Matrix computations on the GPU, CUBLAS and MAGMA by example. developer.nvidia.com, 01 2013.

[17] Paul Covington, Jay Adams, and Emre Sargin. Deep Neural Networks for YouTube Recommendations. In Proceedings of the 10th ACM Conference on Recommender Systems, pages 191–198, Boston Massachusetts USA, September 2016. ACM.

[18] David R Cox. The regression analysis of binary sequences. Journal of the Royal Statistical Society: Series B (Methodological), 20(2):215–232, 1958.

[19] Misha Denil, David Matheson, and Nando De Freitas. Narrowing the gap: Random forests in theory and in practice. In Eric P. Xing and Tony Jebara, editors, Proceedings of the 31st International Conference on Machine Learning, volume 32 of Proceedings of Machine Learning Research, pages 665–673, Beijing, China, 22–24 Jun 2014. PMLR.

[20] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), pages 4171–4186, Minneapolis, Minnesota, June 2019. Association for Computational Linguistics.

[21] Simon Du and Wei Hu. Width provably matters in optimization for deep linear neural networks. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, Proceedings of the 36th International Conference on Machine Learning, volume 97 of Proceedings of Machine Learning Research, pages 1655–1664. PMLR, 09–15 Jun 2019.

[22] Ji Feng, Yang Yu, and Zhi-Hua Zhou. Multi-layered gradient boosting decision trees. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

[23] Shuo Feng, Huiyu Zhou, and Hongbiao Dong. Using deep neural network with small dataset to predict material defects. Materials & Design, 162:300–310, 2019.

[24] Manuel Fernández-Delgado, Eva Cernadas, Senén Barro, and Dinani Amorim. Do we need hundreds of classifiers to solve real world classification problems? Journal of Machine Learning Research, 15(90):3133–3181, 2014.

[25] Jerome H. Friedman. Multivariate Adaptive Regression Splines. The Annals of Statistics, 19(1):1 – 67, 1991.

[26] Jerome H. Friedman. Greedy function approximation: A gradient boostingmachine. The Annals of Statistics, 29(5):1189 – 1232, 2001.
[27] Jerome H. Friedman. Stochastic gradient boosting. Comput. Stat. Data Anal., 38(4):367–378, February 2002.

[28] Servane Gey and Elodie Nedelec. Model selection for CART regression trees. IEEE Transactions on Information Theory, 51(2):658–670, 2005.

[29] Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In Yee Whye Teh and Mike Titterington, editors, Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, volume 9 of Proceedings of Machine Learning Research, pages 249–256, Chia Laguna Resort, Sardinia, Italy, 13–15 May 2010. PMLR.

[30] Cheng Guo and Felix Berkhahn. Entity Embeddings of Categorical Variables. arXiv e-prints, page arXiv:1604.06737, April 2016.

[31] Huifeng Guo, Ruiming Tang, Yunning Ye, Zhenguo Li, and Xiuqiang He. DeepFM: A Factorization-Machine based Neural Network for CTR Prediction. In Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, pages 1725–1731, Melbourne, Australia, August 2017. International Joint Conferences on Artificial Intelligence Organization.

[32] Malay Haldar, Mustafa Abdool, Prashant Ramanathan, Tao Xu, Shulin Yang, Huizhong Duan, Qing Zhang, Nick Barrow-Williams, Bradley C. Turnbull, Brendan M. Collins, and Thomas Legrand. Applying deep learning to airbnb search. In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, KDD ’19, page 1927–1935, New York, NY, USA, 2019. Association for Computing Machinery.

[33] Stephen Hanson and Lorien Pratt. Comparing biases for minimal network construction with back-propagation. pages 177–185, 01 1988.

[34] Vasyl Harasymiv. Lessons from 2 million machine learning models on kaggle, 2015.

[35] Geoffrey Hinton, Li Deng, Dong Yu, George E. Dahl, Abdel-rahman Mohamed, Navdeep Jaitly, Andrew Senior, Vincent Vanhoucke, Patrick Nguyen, Tara N. Sainath, and Brian Kingsbury. Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups. IEEE Signal Processing Magazine, 29(6):82–97, 2012.

[36] Geoffrey E. Hinton. Connectionist learning procedures, 1989.

[37] A. E. Hoerl and R. W. Kennard. Ridge regression: Biased estimation for nonorthogonal problems. Technometrics, 12:55–67, 1970.

[38] Jeremy Howard and Sylvain Gugger. Fastai: A layered API for deep learning. Inf., 11(2):108, 2020.
[39] Manu Joseph. Pytorch tabular: A framework for deep learning with tabular data, 2021.

[40] Liran Katzir, Gal Eldan, and Ran El-Yaniv. Net-{dnf}: Effective deep modeling of tabular data. In International Conference on Learning Representations, 2021.

[41] Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. Lightgbm: A highly efficient gradient boosting decision tree. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.

[42] Guolin Ke, Jia Zhang, Zhenhui Xu, Jiang Bian, and Tie-Yan Liu. TabNN: A universal neural network solution for tabular data, 2019.

[43] Diederik P Kingma and Jimmy Ba. Adam (2014), a method for stochastic optimization. In Proceedings of the 3rd International Conference on Learning Representations (ICLR), arXiv preprint arXiv, volume 1412, 2014.

[44] Günter Klambauer, Thomas Unterthiner, Andreas Mayr, and Sepp Hochreiter. Self-normalizing neural networks. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.

[45] Jason Klusowski. Sparse learning with cart. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, Advances in Neural Information Processing Systems, volume 33, pages 11612–11622. Curran Associates, Inc., 2020.

[46] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. Imagenet classification with deep convolutional neural networks. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 25, pages 1097–1105. Curran Associates, Inc., 2012.

[47] Karim Lounici, Katia Meziani, and Benjamin Riu. Muddling labels for regularization, a novel approach to generalization, 2021.

[48] Lucas Menth and Siyu Zhou. Randomization as regularization: A degrees of freedom explanation for random forest success. Journal of Machine Learning Research, 21(171):1–36, 2020.

[49] Kevin Miller, Chris Hettinger, Jeffrey Humpherys, Tyler Jarvis, and David Kartchner. Forward thinking: Building deep random forests. CoRR, abs/1705.07366, 2017.
[50] Varalakshmi Murugesan, Amit Kesarkar, and Daphne Lopez. Embarrassingly parallel gpu based matrix inversion algorithm for big climate data assimilation. International Journal of Grid and High Performance Computing, 10:71–92, 01 2018.

[51] Rajib Nath, Stanimire Tomov, and Jack Dongarra. Accelerating gpu kernels for dense linear algebra. In Proceedings of the 2009 International Meeting on High Performance Computing for Computational Science, VECPAR10, Berkeley, CA, June 22-25 2010. Springer.

[52] Matthew Olson, Abraham Wyner, and Richard Berk. Modern neural networks generalize on small data sets. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

[53] Maxime Oquab, Leon Bottou, Ivan Laptev, and Josef Sivic. Learning and transferring mid-level image representations using convolutional neural networks. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR), June 2014.

[54] Antonello Pasini. Artificial neural networks for small dataset analysis. Journal of Thoracic Disease, 7(5), 2015.

[55] Sergei Popov, Stanislav Morozov, and Artem Babenko. Neural oblivious decision ensembles for deep learning on tabular data. In International Conference on Learning Representations, 2020.

[56] Liudmila Prokhorenkova, Gleb Gusev, Aleksandr Vorobev, Anna Veronika Dorogush, and Andrey Gulin. Catboost: unbiased boosting with categorical features. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

[57] Yanru Qu, Han Cai, Kan Ren, Weinan Zhang, Yong Yu, Ying Wen, and Jun Wang. Product-Based Neural Networks for User Response Prediction. In 2016 IEEE 16th International Conference on Data Mining (ICDM), pages 1149–1154, Barcelona, Spain, December 2016. IEEE.

[58] Yanru Qu, Bohui Fang, Weinan Zhang, Ruiming Tang, Minzhe Niu, Huifeng Guo, Yong Yu, and Xiuqiang He. Product-based neural networks for user response prediction over multi-field categorical data. ACM Trans. Inf. Syst., 37(1), October 2018.

[59] Bhiksha Raj. Carnegie mellon university deep learning , representation learning, 2018. S18 Lecture 15: Representation Learning.

[60] Alvin Rajkomar, E. Oren, K. Chen, Andrew M. Dai, Nissan Hajasj, Michaela Hardt, Peter J. Liu, X. Liu, Jake Marcus, M. Sun, Patrik Sundberg, H. Yee, Kun Zhang, Y. Zhang, Gerardo Flores, Gavin E Duggan,
Jamie Irvine, Quoc V. Le, Kurt Litsch, Alexander Mossin, Justin Tansuwan, D. Wang, James Wexler, J. Wilson, Dana Ludwig, S. Volchenboum, Katherine Chou, Michael Pearson, Srinivasan Madabushi, N. Shah, A. Butte, M. Howell, Claire Cui, Greg Corrado, and Jeffrey Dean. Scalable and accurate deep learning with electronic health records. NPJ Digital Medicine, 1, 2018.

[61] Carl Edward Rasmussen and Christopher K. I. Williams. Gaussian processes for machine learning. Adaptive computation and machine learning. MIT Press, 2006.

[62] L. Schuchman. Dither signals and their effect on quantization noise. IEEE Transactions on Communication Technology, 12(4):162–165, 1964.

[63] Ira Shavitt and Eran Segal. Regularization learning networks: Deep learning for tabular datasets. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 31. Curran Associates, Inc., 2018.

[64] Leslie N. Smith. Cyclical learning rates for training neural networks, 2015. cite arxiv:1506.01186Comment: Presented at WACV 2017; see https://github.com/bckenstler/CLR for instructions to implement CLR in Keras.

[65] Leslie N Smith. A disciplined approach to neural network hyper-parameters: Part 1–learning rate, batch size, momentum, and weight decay. arXiv preprint arXiv:1803.09820, 2018.

[66] Weiping Song, Chence Shi, Zhiping Xiao, Zhijian Duan, Yewen Xu, Ming Zhang, and Jian Tang. Autoint: Automatic feature interaction learning via self-attentive neural networks. In CIKM, pages 1161–1170, 2019.

[67] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: A simple way to prevent neural networks from overfitting. Journal of Machine Learning Research, 15(56):1929–1958, 2014.

[68] R. Tibshirani. Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society (Series B), 58:267–288, 1996.

[69] Michael Wainberg, Babak Alipanahi, and Brendan J. Frey. Are random forests truly the best classifiers? J. Mach. Learn. Res., 17(1):3837–3841, January 2016.

[70] Hao Wang, Naiyan Wang, and Dit-Yan Yeung. Collaborative Deep Learning for Recommender Systems. In Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1235–1244, Sydney NSW Australia, August 2015. ACM.

18
Christopher K. I. Williams and Matthias Seeger. Using the Nyström method to speed up kernel machines. In T.K. Leen, T.G. Dietterich, and V. Tresp, editors, Advances in Neural Information Processing Systems 13 (NIPS 2000), pages 682–688. MIT Press, 2001.

Yongxin Yang, Irene Garcia Morillo, and Timothy M. Hospedales. Deep Neural Decision Trees. arXiv e-prints, page arXiv:1806.06988, June 2018.

Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. arXiv preprint arXiv:1611.03530, 2016.

Shuai Zhang, Lina Yao, Aixin Sun, and Yi Tay. Deep Learning Based Recommender System: A Survey and New Perspectives. ACM Computing Surveys, 52(1):1–38, February 2019.

Weinan Zhang, Tianming Du, and Jun Wang. Deep learning over multi-field categorical data: A case study on user response prediction. Corr, abs/1601.02376, 2016.

Guorui Zhou, Xiaojiang Zhu, Chenru Song, Ying Fan, Han Zhu, Xiao Ma, Yanghui Yan, Junqi Jin, Han Li, and Kun Gai. Deep interest network for click-through rate prediction. In Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, KDD '18, page 1059–1068, New York, NY, USA, 2018. Association for Computing Machinery.

Zhi-Hua Zhou and Ji Feng. Deep forest: Towards an alternative to deep neural networks. In Proceedings of the Twenty-Sixth International Joint Conference on Artificial Intelligence, IJCAI-17, pages 3553–3559, 2017.

Hui Zou and Trevor Hastie. Regularization and variable selection via the elastic net. Journal of the Royal Statistical Society, Series B, 67:301–320, 2005.

Supplementary Material

Replicability

Our Python code is released as an open source package for replication: github/anonymousNeurIPS2021submission5254/.

Configuration machine

We ran our experiments using several setups and GPU’s:

- Google Cloud Platform: NVIDIA Tesla P100,
- Google Colab: NVIDIA Tesla TESLA K80 and NVIDIA Tesla TESLA T4,
5 State of the Art

We complete here the review of the existing literature on deep learning on tabular data.

An interesting line of research proposes to transpose the "leverage weak learners" idea underlying ensemble methods into neural networks. [52] proposes an interpretation of fitted FFNN as ensembles of relatively weakly correlated, low-bias sub-networks. Thus this paper provides some insight on the generalization ability of overparametrized FFNN on small datasets. Their experiments concerns binary classification on the UCI dataset but they did not attempt to outperform ensemble methods as it was not the goal of this work.

The paper [3] carried out a study of Neural Tangent Kernel (NTK) induced by infinitely wide neural networks on small classification tasks. NTK slightly outperforms RF implemented as in [24] on small UCI data sets ($n \leq 5000$). NTK performs well on small size ($n \leq 640$) subsets of the CIFAR-10 benchmark but is inferior to ResNet-34 for larger size. However their architecture does not cover the regression task. Moreover, the super-quadratic running time of NTK limits its use in large scale learning tasks.

Net-DNF [40] is an end-to-end DL model to handle tabular data. Its architecture is designed to emulate Boolean formulas in decision making. However, XGBoost outperforms Net-DNF in their experiments.

[44] proposes Self-Normalized Neural Networks (SNN) based on the SELU activation function to train very deep feed-forward neural networks more efficiently. SNN architecture is motivated as it makes SGD more stable. However SNN requires careful tuning of hyperparameters and does not outperform SVM or RF on the UCI database.

6 The MLR-FFNN

6.1 The MLR loss

Recall

$$H = H(\theta, \lambda, \mathbf{x}) = A^{L-1} [(A^{L-1})^T A^{L-1} + \lambda I]^{-1} (A^{L-1})^T \in \mathbb{R}^{n \times n},$$

Where $A^{L-1}$ denotes the last hidden layer.

Definition 3 (MLR regression loss). Set $H = H(\theta, \lambda, \mathbf{x})$. We draw i.i.d. random vectors $\xi$ and $(\xi_i)_{i=1}^{T}$ distributed as $\mathcal{N}(0_n, I_n)$. Let $(\pi^t(Y))_{i=1}^{T}$ be $T$ independently drawn permutations of $Y$. We set $\bar{Y} = \text{mean}(Y)$ and define the MLR loss as
\[ \text{MLR}(\theta, \lambda) = \text{RMSE}(Y + (\mathbb{1}_n - H)\xi; HY) + \frac{1}{T} \sum_{t=1}^{T} \left| \text{RMSE}(Y; \mathbb{Y}\mathbb{1}_n) - \text{RMSE}(\pi_t(Y) + (\mathbb{1}_n - H)\xi_t; H\pi_t(Y)) \right|. \]

**The benefit of close-form regularization.** The replacement of the output layer with Ridge regularizes the network in two ways: (i) the weights on the output layer are a direct function of the last hidden layer \( A^{L-1} \). This effect is much stronger than adding a constraint or a penalty directly on \( W^L \) the weights of the \( L \)-th layer of the FFNN; (ii) the close-form we choose is the ridge instead of the OLS, which implicitly subjects the weights to a steerable \( L_2 \) regularization.

**The generalization effect of random permutations.** Our work is loosely related to [73] where label permutations are used after the model has been trained as a qualitative observational method to exhibit the overfitting capacity of Neural networks. In our approach, we go further as we use random permutations during the training phase to define a quantitative measure of the amount of overfitting of a model. This measure is actively used to penalize overfitting during the training phase. This is the underlying mechanism behind the MLR loss.

First, when we take a permuted label vector we obtain a new label vector with two properties. First both \( Y \) and \( \pi(Y) \) admit the same marginal distributions. This new vector can be seen as a "realistic" data-augmented new sample for the training set. Second the expected number of fixed points \( (\pi(i) = i) \) in a permutation drawn uniformly at random is equal to 1 (See Chapter 5 in [?]); i.e. the proportion of fixed points in a random permutation of \( n \) elements is insignificant. Thus the label permutation breaks the dependence relationship between \( Y_{\pi(i)} \) and \( x_i \). Therefore, \( x_i \) provides no information on the possible value of \( Y_{\pi(i)} \) and predicting \( Y_{\pi(i)} \) using \( x_i \) can only result in overfitting. In other words, label permutation is used to produce a control set \( (x, \pi(Y)) \) that can only be fitted through memorization. MLR focuses on patterns that appear only in \( (x, Y) \) and not in uncorrelated pairs \( (x, \pi(Y)) \).

**Structured Dithering.** We describe an additional scheme to prevent memorization. We apply a dithering scheme which adapts to the spectral structure of \( H \), the "regularized projector" based on \( A^{L-1} \) (the output of the last hidden layer). More specifically, we muddle the target using \( (\mathbb{1}_n - H)\xi \) which introduces noise of higher variance along the weakly informative eigendirections of \( H \).

### 6.2 Cross-Entropy loss

In the classification task, the FFNN architecture is essentially unchanged. The usual loss for binary classification task is the BCE loss that combines a Sigmoid
and the Cross Entropy (CE) loss. (namely \texttt{torch.nn.BCEWithLogitsLoss} in PyTorch and referred to as BCE in this paper). Set \( \text{Sig}() = \text{Sigmoid}() \), then

\[
\text{BCE}(Y, f(\theta, x)) = -\frac{1}{n} [Y^T \log(\text{Sig}(f(\theta, x)) + (1_n - Y)^T \log(1_n - \text{Sig}(f(\theta, x)))]
\]

**Definition 4 (BCE-MLR loss).** Let \( \xi \) and \((\xi_t)_{t=1}^T\) be i.i.d. \( N(0, I) \) vectors. Set \( Y^* = \frac{2}{n} Y - 1 \). We define the BCE-MLR loss as

\[
\text{BCE-MLR}(\theta, \lambda) = \text{BCE}(Y; (1_n - H)\xi + HY^*) + \frac{1}{T} \sum_{t=1}^T \left| \text{BCE}(Y; Y^*_{1:n}) - \text{BCE}(\pi^t(Y^*); \pi^t(Y^*) + (1_n - H)\xi + H \pi^t(Y^*)) \right|
\]

The quantity \( \text{BCE}(Y; Y^*_{1:n}) \) is our baseline. Note that \( Y^* \) with values in \( \{-1, 1\} \) is the symmetrized version of \( Y \). Next, the Structured dithering is applied to the prediction rather than the target \( Y \) because the BCE is only defined for binary target \( Y \in \{0; 1\}^n \).

**Definition 5 (BCE-MLR-NN).** Our BCE-MLR neural net (BCE-MLR-NN) is

\[
\text{BCE-MLR-NN}(\hat{\theta}, \hat{\lambda} ; \cdot) = \text{Hardmax}(A^{L-1}(\hat{\theta} ; \cdot) P(\hat{\theta}, \hat{\lambda}; x)) Y \in \{0, 1\}^{obs.}
\]

with \((\hat{\theta}, \hat{\lambda}) = \arg\min_{\theta, \lambda} \text{BCE-MLR}(\theta, \lambda),\)

and \( P(\cdot, \cdot, x) \) s.t. \( P = P(\theta, \lambda, x) = [(A^{L-1})^T A^{L-1} + \lambda I]^{-1} (A^{L-1})^T \in \mathbb{R}^{J \times n} \).

### 7 Training a FFNN with MLR

**The MLR-NN Architecture.** We consider FFNN with \( L \) layers, \( L \in \mathcal{G}_L := \{1, 2, 3, 4\} \), and with all the hidden layers of constant width \( J \). In our experiments, we always take \( J \) as large as possible (our machine with 11GVRAM allowed for \( J = 2^{10} \)).

| Architecture | \( L \) | \( t_r \) | maxiter | FixB | \( J \) | \( b_n \) | \( T \) | \( \sigma \) |
|-------------|------|------|-------|------|-----|-----|-----|------|
| MLR-1       | 1    | \( 10^{-2} \) | 200   | 10   | 2^{10} | \text{Reg.:} 0.03 | | |
| MLR-2       | 2    | \( 10^{-3} \) | 200   | \text{id.} | \text{id.} | \text{id.} | | |
| MLR-3       | 3    | \( 10^{-3.5} \) | 400   | \text{id.} | \text{id.} | \text{id.} | | |
| MLR-4       | 4    | \( 10^{-4} \) | 400   | \text{id.} | \text{id.} | \text{id.} | | |

Table 8: Benchmarked architectures.
Dither \cite{62}. This step is distinct from the Structured dithering that we introduced in the MLR method. In the regression setting, we do not apply the MLR loss on $Y$ but rather on a noisy version of $Y$ as is usually done in practice. Let $\epsilon, (\epsilon^t)_{t \leq d} \sim N(0, \tilde{\sigma}^2 I)$. We set $Y_\epsilon = Y + \epsilon$ and $\pi^t_\epsilon(Y) = \pi^t(Y) + \epsilon^t$. In our experiments, we use the MLR loss on $\left( Y_\epsilon, (\pi^t_\epsilon(Y))_{t=1}^T \right)$ instead of $\left( Y, (\pi^t(Y))_{t=1}^T \right)$.

$$\text{MLR}(\theta, \lambda) = \text{RMSE} \left( Y_\epsilon + (\mathbb{I}_n - H) \xi; HY \right) + \frac{1}{T} \sum_{t=1}^T \left| \text{RMSE} \left( Y; \mathbb{Y}_{n} \right) - \text{RMSE} \left( \pi^t_\epsilon(Y) + (\mathbb{I}_n - H) \xi_t; H \pi^t_\epsilon(Y) \right) \right|.$$

Here again, $\tilde{\sigma}$ is not an hyperparameter as we use the same value $\tilde{\sigma} = 0.03$ for all the datasets in our benchmark. Moreover, in our approach the batch size $b_s$ is not a hyperparameter as we fix it as in the table above.

Note that we do not apply this dither step in the classification setting.

Initialization of $\theta$. The initialization of $\theta$ is as in \cite{29}.

Recall $|\text{input}| = d$ and $|\text{out}| = 1$

\begin{itemize}
  \item $\forall \ell \in [1, L - 1], b^f = 0$. The entries of $W^f$ are generated independently from the uniform distribution on the interval $\mathcal{I}_\ell$:
    \begin{itemize}
      \item $\mathcal{I}_1 = \left( -\sqrt{\frac{6}{(d+J)}, \sqrt{\frac{6}{(d+J)}}} \right)$ and $\mathcal{I}_L = \left( -\sqrt{\frac{6}{(d+1)}, \sqrt{\frac{6}{(d+1)}}} \right)$
      \item $\mathcal{I}_\ell = \left( -\sqrt{\frac{6}{(d+J)}, \sqrt{\frac{6}{(d+J)}}} \right), \forall \ell \in [2, L - 1]$
    \end{itemize}
\end{itemize}

Efficient heuristic to initialize the Ridge parameter. In our experiments, we pick $\lambda_{init}$ by running a grid-search on the finite difference approximation for the derivative of MLR on the grid $\mathcal{G}_\lambda = \{ \lambda^{(k)} = 10^{-1} \times 10^{5 \times k/11} : k = 0, \ldots, 11 \}$:

$$\lambda_{init} = \sqrt[\hat{k}]{\lambda^{(\hat{k})}} \lambda^{(k+1)}$$ where $\hat{k} = \arg \max \left\{ \left( \text{MLR}(\theta, \lambda^{(k+1)}) - \text{MLR}(\theta, \lambda^{(k)}) \right) : \lambda^{(k)} \in \mathcal{G}_\lambda \right\}$.

The Ridge parameter $\lambda$ is not an hyperparameter of our method; it is trained alongside the weights of the Neural Net architecture.

Choice of the number of iterations during the train.

- We fix the maximum number of iterations $\max_{\text{Iter}}$ (depending on the value of $L$).
- We fix the budget ($\text{FixB} = 5$ min) and denote by $n_{\text{Iter}}$ the possible number of iterations during the allotted time $\text{FixB}$. 

23
• We denote by \( \text{Iter} \) the number of iterations that will actually be performed, \( i.e. \)
\[
\text{Iter} = \min(\max(\text{Iter}, n_{\text{Iter}}))
\]

**Training MLR-NN.** We train the FFNN with \( b_s = \min(J, n) \) and we use Adam [43] with default parameters except for the learning rate \( \ell_r \) which depends on the number of layers \( L \) (Table 2).

| Training |
| --- |
| **Initialization** |
| set \( \theta \) |
| set \( \lambda \) |
| **Optimization** |
| while \( e < \text{Iter} \) do: |
| | \( A^0 \rightarrow x \in \mathbb{R}^{b_s \times d} \) |
| | for \( \ell = 1 \ldots L - 1 \) : |
| | \( A^\ell \rightarrow \text{ReLU}(A^{\ell-1}W^\ell + B^\ell) \) |
| | \( H(\theta, \lambda) \rightarrow A^{L-1}[(A^{L-1})^\top A^{L-1} + \lambda I_J]^{-1} A^{L-1\top} \) |
| | Compute MLR(\( \theta, \lambda \)) or BCE-MLR(\( \theta, \lambda \)) |
| | Backpropagate \( (\theta, \lambda) \) through MLR(\( \theta, \lambda \)) or BCE-MLR(\( \theta, \lambda \)) |
| | \( e \rightarrow e + 1 \) |

We select a validation-set of size \( n_{\text{val}} = 20\% n \). We read the \( R^2 \)-score for each iteration on the validation-set and take the iteration with the best \( R^2 \)-score:
\[
\text{Iter}^* := \arg \max \{ R_k^2, k = 1, \ldots, \text{Iter} \}.
\]

Finally, \((\hat{\theta}, \hat{\lambda})\) will take its value at iteration \( \text{Iter}^* \)

**Our final models.** We propose several models with varying depth based on FFNN trained with the MLR loss. We also create ensemble models combining architectures of different depth. Our models are:

- **MLR-L:** a simple FFNN of depth \( L \) (\( 1 \leq L \leq 4 \)).
- **Bag-MLR-L:** a bagging of 10 FFNN of depth \( L \) (\( L = 1 \) or \( L = 2 \)).
- **Ens-MLR:** an ensemble of 20 FFNN (the aggregation of Bag-MLR1 and Bag-MLR2 of depth 1 and 2 respectively).
- **Best-MLR:** the best prediction among 20 MLR-NN in terms of the validation score.
- **Top5-MLR:** the aggregation of the top 5 among 20 MLR-NN in terms of the validation score.

For the methods based on bagging [44], the final prediction is the mean of each MLR-NN prediction.
8 Construction of the Benchmark

To produce this benchmark (Table 9), we aggregated 32 tabular datasets (16 in regression and 16 in classification), from the UCI repository and Kaggle. For computational reasons, we have chosen to restrict the number of datasets but we performed more train/test splitting in order to reduce the variance of our results. We curated the UCI repository and Kaggle through a set of rules (e.g. discard empty or duplicate datasets, times series, missing target, non i.i.d. samples, text format, etc.).

| Description                                      | Task | n   | d   | # Num. | # Cat. |
|--------------------------------------------------|------|-----|-----|--------|--------|
| Concrete Slump Test -2                          | Reg  | 103 | 8   | 8      | 0      |
| Concrete Slump Test -3                          | Reg  | 103 | 8   | 8      | 0      |
| Concrete Slump Test -1                          | Reg  | 103 | 8   | 8      | 0      |
| Servo                                            | Reg  | 168 | 24  | 2      | 4      |
| Computer Hardware                                | Reg  | 210 | 7   | 7      | 0      |
| Yacht Hydrodynamics                              | Reg  | 308 | 33  | 5      | 3      |
| QSAR aquatic toxicity                            | Reg  | 546 | 34  | 8      | 3      |
| QSAR Biocentration classes                       | Reg  | 779 | 25  | 8      | 4      |
| QSAR fish toxicity                               | Reg  | 909 | 18  | 6      | 2      |
| insurance                                        | Reg  | 1338| 15  | 3      | 4      |
| Communities and Crime                            | Reg  | 1994| 108 | 99     | 2      |
| Abalone R                                        | Reg  | 4178| 11  | 7      | 1      |
| Squark automotive CLV training                   | Reg  | 8099| 77  | 7      | 16     |
| Seoul Bike Sharing Demand                        | Reg  | 8760| 15  | 9      | 3      |
| Electrical Grid Stability Simu                   | Reg  | 10000|12   | 12     | 0      |
| bir real estate prices                           | Reg  | 13320|2   | 2      | 0      |
| Cervical Cancer Behavior Risk                    | Classif | 72 | 149 | 19   | 14     |
| Post-Operative Patient                           | Classif | 91 | 32  | 0     | 8      |
| Breast Cancer Coimbra                            | Classif | 116 | 9   | 9      | 0      |
| Heart failure clinical records                   | Classif | 259 | 12  | 7      | 5      |
| Ionosphere                                        | Classif | 352 | 34  | 32     | 2      |
| Congressional Voting Records                     | Classif | 436 | 64  | 0      | 16     |
| Cylinder Bands                                   | Classif | 541 | 111 | 1     | 19     |
| Credit Approval                                  | Classif | 691 | 42  | 4      | 8      |
| Tic-Tac-Toe Endgame                              | Classif | 959 | 36  | 0      | 9      |
| QSAR biodegradation                              | Classif | 1056| 141 | 41     | 15     |
| Chess (King-Rook vs. King-Pawn)                  | Classif | 3196| 102 | 0     | 36     |
| Mushroom                                         | Classif | 8125| 125 | 0      | 21     |
| Electrical Grid Stability Simu                   | Classif | 10000|12  | 12     | 0      |
| MAGIC Gamma Telescope                            | Classif | 19021|10  | 10     | 0      |
| Adult                                            | Classif | 32561|34  | 6      | 5      |
| Internet Firewall Data                           | Classif | 65532|11  | 11     | 0      |

Table 9: Benchmark datasets. # Num. and # Cat. denote the initial number of numerical and categorical features respectively. We denote by d the number of features after the pre-processing and one-hot encoding.

8.1 Pre-processing

To avoid biasing the benchmark towards specific methods and to get a result as general as possible, we only applied as little preprocessing as we could, without
using any feature augmentation scheme. The goal is not to get the best possible performance on a given dataset but to compare the methods on equal ground. We first removed uninformative features such as sample index. Categorical features with more than 12 modalities were discarded as learning embeddings is out of the scope of this benchmark. We also removed samples with missing target.

**Target treatment.** The target is centered and standardized via the function \( \text{function-T}(\cdot) \). We remove the observation when the value is missing.

\[
\text{function-T}(Y) = Y - \text{float32}(Y) \\
\text{for } i = 1 : n \\
\quad \text{if } Y_i == \text{NAN} \\
\quad \quad \text{remove}(x_i, Y_i) \\
Y - \frac{Y - Y}{\sigma(Y)}
\]

**Features treatment.** The imputation treatment is done during processing. For categorical features, \text{NAN} Data may be considered as a new class. For numerical features, we replace missing values by the mean. Set \( n_j = \#\text{set}(X_j) \) the number of distinct values taken by the feature \( X_j \). We proceed as follows:

- When \( n_j = 1 \), the feature \( X_j \) is irrelevant, we remove it.
- When \( n_j = 2 \) (including potentially \text{NAN} class), we perform numerical encoding of binary categorical features.
- Numerical features with less than 12 distinct values are also treated as categorical features (\( 2 < n_j \leq 12 \)). We apply one-hot-encoding.
- Finally, categorical features with \( n_j > 12 \) are removed.

### 8.2 Compared methods

We ran the benchmark with all the methods (see Table \ref{tab:methods}) available in the scikit-learn library for classification and regression (including RF and XGB) as well as the GBDT methods. All methods were ran with the default hyperparameters.
9 MLR Parameters Analysis

In this section we study the behavior of the MLR method and the impact of its key components through extensive evaluation on three datasets, Concrete Slump Test−3, QSAR aquatic toxicity and Seoul Bike Sharing Demand, for which \((n, d)\) are equal to \((103, 8)\), \((546, 34)\) and \((8760, 15)\) respectively. We repeated each experiment over 100 random train/test splits.

### 9.1 Impact of the MLR components.

In this section, we study the impact of the different components in the MLR approach on the \(R^2\)-score on the test and validation sets, computation time, the convergence of the method (Iter) and the initialization of the Ridge parameter \(\lambda_{\text{init}}\). To study the impact of each specific parameter, we set the other ones equal to their default values in Table 2. Note that for the following study, we chose a batch size \(b_s = \min(n, 2^{14})\), unlike in our main experiments where we took \(b_s = \min(n, 2^{10})\) due to time constraints.

Note also that due to access failure to Cloud Computing, computation time was sometimes obtained on a less powerful configuration in Tables 11, 12, 13 and 15. We marked by an asterisk * any computation time obtained on the NVIDIA RTX 2080 MaxQ configuration.

**Structured Dithering.** Recall that we added Structured noise \((I_n - H)\xi\) to the target \(Y\) with \(\xi \sim \mathcal{N}(0, \sigma^2 I)\). Table 11 reveals the impact of the structured dithering parameter \(\sigma\). Default value \((\sigma = 1)\) yields consistently good generalization performance. Of course, it is always possible to tune this hyperparameter around value 1 for potential improvement of the generalization performances. Higher values of \(\sigma\) lead to a significant degradation of \(R^2\)-score as it caused the method to diverge. In our experiments, \(\sigma\) was not an hyperparameter as it was always set equal to 1. Moreover, adding structured dithering has no impact on the value of \(\lambda_{\text{init}}\) or computational time.

### Table 10: Main classes of methods.

| Class of Methods | Methods |
|------------------|---------|
| MLR (this paper) | MLR-L, Bag-MLR-L, Ens-MLR, Best-MLR, Top5-MLR |
| GBDT             | XGB [8, 26, 27], CatBoost [50], XGBoost [14], LightGBM [41] |
| RF               | RF and XRF [9, 10] |
| SVM              | Lin-SVM, SVM, ν-SVM [12] |
| NN               | Fast.ai [38], MLP [9] |
| GLM              | OLS, Elastic-Net [78], Ridge [37], Lasso [68], Logistic regression [18] |
| MARS             | MARS [25] |
| TREE             | CART, XCART [6, 28, 45] |
| Baseline         | Reg: Intercept | Classif: Class probabilities |
Permutations. We studied the impact of the randomness aspect of the MLR loss. We compared different sets of permutations drawn at random. The choice of the seed has little impact on the value of the MLR loss as soon as $T \geq 2^2$. Table 12 reveals a significant jump in $R^2$-score on the test going from $T = 0$ to $T = 1$ permutation. Then, increasing the value of $T > 1$ may sometimes slightly improve $R^2$-score. Meanwhile, a larger number of permutations has a direct negative impact on runtime per iteration and VRAM footprint. Past a certain threshold $2^8$, GPU parallelization no longer prevents the linear dependency on $T$. We escape any trade-off by picking $T = 2^4$ permutations in all our experiments. This value is large enough for the MLR loss to converge (with regards to $T$), yet still leveraging GPU parallelization.

| Concrete Slump Test−3 | $\sigma$ | $R^2$ | Time | Iter | $R^2_{val}$ | $\lambda_{init}$ |
|------------------------|---------|-------|-------|------|------------|----------------|
|                        | 0       | 0.321 | 30.356| 60.650| 0.479      | 219.345        |
|                        | 0.2     | 0.338 | 30.424| 79.830| 0.496      | 219.345        |
|                        | 1       | 0.357 | 30.423| 99.570| 0.515      | 219.345        |
|                        | 2       | 0.089 | 1.312 | 0.250 | 0.137      | 219.345        |
|                        | 3       | 0.068 | 1.257 | 0.000 | 0.116      | 219.345        |
| QSAR aquatic toxicity  | $\sigma$| $R^2$ | Time | Iter | $R^2_{val}$ | $\lambda_{init}$ |
|                        | 0       | 0.463 | 32.250| 11.200| 0.511      | 774.264        |
|                        | 0.2     | 0.463 | 32.408| 14.550| 0.514      | 774.264        |
|                        | 1       | 0.460 | 32.281| 46.750| 0.525      | 774.264        |
|                        | 2       | 0.220 | 1.276 | 0.020 | 0.226      | 774.264        |
|                        | 3       | 0.216 | 1.288 | 0.000 | 0.223      | 774.264        |
| Seoul Bike Sharing Demand | $\sigma$| $R^2$ | Time | Iter | $R^2_{val}$ | $\lambda_{init}$ |
|                        | 0       | 0.863 | 89.425| 181.300| 0.864      | 10000.001      |
|                        | 0.2     | 0.863 | 90.206| 188.520| 0.864      | 10000.001      |
|                        | 1       | 0.855 | 89.968| 191.920| 0.857      | 10000.001      |
|                        | 2       | 0.364 | 1.876 | 0.000 | 0.363      | 10000.001      |
|                        | 3       | 0.364 | 1.891 | 0.000 | 0.363      | 10000.001      |

Table 11: Structured dithering dependence.
### Table 12: Permutation dependence. \( * \): computation time was obtained with a NVIDIA RTX 2080 MaxQ.

**Initialization of Ridge parameter** \( \lambda_{\text{init}} \). Recall that Ridge regularization is the essential component of the MLR method as it provides a closed form representation of the last hidden layer on which we can conveniently apply the follow-up steps: structured dithering and random permutations. Contrary to \( T \) and the dither parameter \( \sigma \), the choice of the appropriate initial value of \( \lambda \) is very impactful and depends on both network architecture and dataset characteristics as shown in Table 13.

When we compare the value \( \lambda_{\text{init}} \) given by our heuristic (in bold) with the other values chosen in Table 13, we observe that our heuristic is quite effective, as in average on the 3 datasets, it is always within 3\% of the best value in the grid of Table 13 in term of \( R^2 \)-score on the **test**. As we can see for the QSAR aquatic toxicity dataset, the optimal value was not within the bounds of the grid \( G_\lambda \) we chose. Using a larger grid with a bigger granularity would improve the results.

Despite access failure to Cloud Computing for one specific value of \( \lambda_{\text{init}} \), our main experiments reveal a small runtime overcost for the initialization step.

| Dataset                          | \( T \) | \( R^2 \) | Time   | Iter | \( R^2_{\text{val}} \) | \( \lambda_{\text{init}} \) |
|----------------------------------|--------|----------|--------|------|--------------------------|---------------------------|
| Concrete Slump Test - 3          | 0      | 0.252    | 3.184  | 61.050 | 0.401                    | 31.831                    |
|                                  | 1      | 0.331    | 3.357  | 110.040 | 0.459                    | 285.238                   |
|                                  | 2      | 0.338    | 3.359  | 109.960 | 0.468                    | 215.370                   |
|                                  | \( 2^4 \) | 0.343   | 3.358  | 109.370 | 0.473                    | 219.345                   |
|                                  | \( 2^4 \) | 0.347   | 4.012  | 116.190 | 0.484                    | 216.235                   |
|                                  | \( 2^8 \) | 0.351   | 3.371  | 117.160 | 0.494                    | 219.345                   |
|                                  | \( 2^{10} \) | 0.349  | 3.433  | 117.650 | 0.495                    | 219.345                   |

| Dataset                          | \( T \) | \( R^2 \) | Time   | Iter | \( R^2_{\text{val}} \) | \( \lambda_{\text{init}} \) |
|----------------------------------|--------|----------|--------|------|--------------------------|---------------------------|
| QSAR aquatic toxicity            | 0      | 0.460    | 3.253  | 46.770 | 0.509                    | 774.264                   |
|                                  | 1      | 0.461    | 3.452  | 62.020 | 0.518                    | 774.264                   |
|                                  | 2      | 0.466    | 3.461  | 60.040 | 0.518                    | 774.264                   |
|                                  | \( 2^4 \) | 0.469   | 3.462  | 60.720 | 0.521                    | 774.264                   |
|                                  | \( 2^4 \) | 0.473   | 6.172  | 72.800 | 0.527                    | 774.264                   |
|                                  | \( 2^{10} \) | 0.477  | 3.496  | 81.900 | 0.532                    | 774.264                   |

| Dataset                          | \( T \) | \( R^2 \) | Time   | Iter | \( R^2_{\text{val}} \) | \( \lambda_{\text{init}} \) |
|----------------------------------|--------|----------|--------|------|--------------------------|---------------------------|
| Seoul Bike Sharing Demand        | 0      | 0.817    | 8.251  | 197.830 | 0.817                    | 10000.001                 |
|                                  | 1      | 0.813    | 8.606  | 197.860 | 0.813                    | 10000.001                 |
|                                  | 2      | 0.813    | 8.654  | 197.400 | 0.814                    | 10000.001                 |
|                                  | \( 2^4 \) | 0.813   | 8.645  | 197.780 | 0.814                    | 10000.001                 |
|                                  | \( 2^4 \) | 0.814   | 30.654 | 197.100 | 0.814                    | 10000.001                 |
|                                  | \( 2^{10} \) | 0.813  | 10.391 | 197.230 | 0.814                    | 10000.001                 |
|                                  | \( 2^{10} \) | 0.814  | 17.330 | 197.070 | 0.814                    | 10000.001                 |
mostly because all steps including the matrix inversion need to be performed only once and do not require computing the derivation graph. We favored a small simple grid $G_\lambda = \{ \lambda^{(k)} = 10^{-1} \times 10^{5 \times k/11} \ : \ k = 0, \ldots, 11 \}$ to select $\lambda_{\text{init}}$. This grid was designed to work well on small size datasets. Of course, it is possible to refine this grid with respect to the dataset size and architecture at hand to achieve even higher generalization performance. Another possible approach could be to tune $\lambda_{\text{init}}$ on the validation set. Indeed, we observe in Table 13 that the optimal value of $\lambda_{\text{init}}$ on the test seems to be close to that obtained on the validation set.

| Concrete Slump Test–3 | $\lambda_{\text{init}}$ | $R^2$ | Time | Iter | $R^2_{\text{val}}$ |
|------------------------|-------------------------|-------|------|------|------------------|
| 0                      | -0.110                  | 0.180 | 7.790| -0.020|
| $10^{-3}$              | -0.444                  | 2.078 | 90.270| 0.265|
| $10^{-1}$              | 0.097                   | 2.083 | 70.310| 0.254|
| 10                     | 0.320                   | 2.070 | 116.630| 0.466|
| 216.235                | 0.347                   | 2.902*| 116.190| 0.484|
| $10^3$                 | 0.359                   | 2.087 | 125.020| 0.480|
| $10^5$                 | 0.334                   | 2.103 | 152.460| 0.428|
| $10^7$                 | 0.263                   | 2.104 | 188.630| 0.339|
| $10^9$                 | -0.050                  | 2.089 | 197.890| -0.009|

| QSAR aquatic toxicity  | $\lambda_{\text{init}}$ | $R^2$ | Time | Iter | $R^2_{\text{val}}$ |
|------------------------|-------------------------|-------|------|------|------------------|
| 0                      | -0.276                  | 0.014 | 0.010| -0.244|
| $10^{-3}$              | -33.053                 | 0.133 | 2.510| -9.371|
| $10^{-1}$              | -3.768                  | 2.137 | 36.770| -0.151|
| 10                     | 0.422                   | 2.086 | 9.530| 0.477|
| 774.263                | 0.473                   | 3.426 | 72.800| 0.527|
| $10^3$                 | 0.477                   | 2.094 | 73.530| 0.529|
| $10^5$                 | 0.486                   | 2.088 | 132.420| 0.522|
| $10^7$                 | 0.477                   | 2.088 | 191.320| 0.488|
| $10^9$                 | 0.273                   | 2.086 | 200.000| 0.287|

| Seoul Bike Sharing Demand| $\lambda_{\text{init}}$ | $R^2$ | Time | Iter | $R^2_{\text{val}}$ |
|--------------------------|-------------------------|-------|------|------|------------------|
| 0.0                      | -0.091                  | 0.052 | 0.010| -0.088|
| $10^{-3}$                | 0.761                   | 5.042 | 97.970| 0.775|
| $10^{-1}$                | 0.795                   | 5.009 | 66.370| 0.807|
| 10                       | 0.844                   | 4.989 | 161.160| 0.847|
| 774.263                  | 0.843                   | 4.974 | 194.550| 0.844|
| $10^3$                   | 0.814                   | 19.208*| 197.100| 0.814|
| $10^5$                   | 0.774                   | 4.966 | 197.510| 0.775|
| $10^7$                   | 0.711                   | 4.956 | 198.600| 0.710|
| $10^9$                   | 0.614                   | 4.942 | 198.830| 0.613|

Table 13: Dependence on $\lambda_{\text{init}}$. *: computation time was obtained with a NVIDIA RTX 2080 MaxQ.
Ablation study. We ran our ablation study (Table 4) in the regression setting on the same 3 datasets (Concrete Slump Test, QSAR aquatic toxicity, Seoul Bike Sharing Demand). We repeated each experiment over 100 random train/test splits. All the results presented here correspond to the architecture of MLR-2 and Bag-MLR2 with hyperparameters fixed as in Table 2.

A standard NN2 (FFNN with 2 wide layers $J = 2^{10}$) cannot be trained efficiently on small datasets as the FFNN instantly memorizes the entire dataset. This cannot be alleviated through bagging at all. Note also its lower overall performance on the complete benchmark.

Applying Ridge on the last hidden layer allows an extremely overparametrized FFNN to learn but its generalization performance is still far behind the gold standard RF. However, when using bagging with ten such models, we reach very competitive results, underlying the potential of the MLR approach.

The random permutations component gives a larger improvement than Structured Dithering. However, when using both ingredients together, a single MLR-NN can reach or even outperform the gold-standard methods on most datasets. Furthermore, the improvement yielded by using bagging (0.062) is still of the same order of magnitude as the one we got when we applied permutations on top of Ridge to the FFNN (0.043). This means these two ingredients (permutations and Structure Dithering) are not just simple variance reduction techniques but actually generate more sophisticated models.

| Step                              | Mean $R^2$  | Bagging $R^2$ |
|-----------------------------------|-------------|---------------|
| NN2                               | $-0.081 \pm 0.173$ | $-0.046 \pm 0.169$ |
| FFNN + Ridge                      | $0.321 \pm 0.081$   | $0.394 \pm 0.052$   |
| FFNN + Ridge + Struct. Dithering | $0.323 \pm 0.075$   | $0.400 \pm 0.048$   |
| FFNN + Ridge + Permut.            | $0.364 \pm 0.050$   | $0.432 \pm 0.035$   |
| MLR                               | $0.371 \pm 0.024$   | $0.433 \pm 0.000$   |

Table 14: Ablation Study in Regression.

9.2 Other hyperparameters.

The impact of the other hyperparameters on the MLR method is discussed below.

Dither. At each iteration, we draw and add i.i.d. gaussian noise $\mathcal{N}(0, \hat{\sigma}^2 I)$ on the target $Y$ in the regression setting. In Table 15 we see that adding a small amount of noise improves performances. We performed our main experiments with $\hat{\sigma} = 0.03$ as this value works well with standard FFNN. But here again, we may improve generalization performance by considering $\hat{\sigma}$ as an hyperparameter to be tuned. Rather unsurprisingly, applying dithering has no impact on runtime per iteration or on the value of $\lambda_{init}$. 
Width. Most notably, Table 15 reveals that wide architectures (large $J$) usually provide better generalization performance. We recall that for standard NN trained without MLR, wider architectures are more prone to overfitting. Table 16 also reveals that larger architectures work better for bigger datasets like Seoul Bike Sharing Demand. For small datasets, $J = 2^{10}$ provides good generalization performance for smaller runtime. When the width parameter exceeds GPU memory, parallelization is lost and we observe a dramatic increase in computational time.
Table 16: Width dependence.

**Batch size.** We added the *Beijing PM2.5 Data* of size \((n, d) = (43824, 33)\) in this experiment in order to measure the impact of batch-size on a larger dataset but this dataset was not included in the benchmark.

In view of Table 17 our recommendation is very simple: "**As big as possible!**". For small datasets this means using the entire train-set at each iteration, while GPU memory constraints rule out going beyond \(2^{14}\) for large datasets.

| Concrete Slump Test−3 | \(J\) | \(R^2\) | Time | Iter | \(R^2_{\text{var}}\) | \(\lambda_{\text{init}}\) |
|-----------------------|------|--------|------|------|----------------|---------------------|
| \(2^4\)              | 0.184 | 0.705  | 162.120 | 0.284 | 210.307       |
| \(2^6\)              | 0.276 | 0.751  | 160.030 | 0.364 | 211.555       |
| \(2^8\)              | 0.325 | 0.905  | 135.400 | 0.431 | 205.351       |
| \(2^{10}\)           | 0.344 | 2.201  | 113.610 | 0.484 | 222.455       |
| \(2^{12}\)           | 0.322 | 15.796 | 94.180  | 0.503 | 220.900       |

| QSAR aquatic toxicity | \(J\) | \(R^2\) | Time | Iter | \(R^2_{\text{var}}\) | \(\lambda_{\text{init}}\) |
|----------------------|------|--------|------|------|----------------|---------------------|
| \(2^4\)              | 0.367 | 0.724  | 184.540 | 0.379 | 678.097       |
| \(2^6\)              | 0.442 | 0.743  | 157.840 | 0.471 | 628.464       |
| \(2^8\)              | 0.467 | 0.907  | 115.510 | 0.512 | 774.264       |
| \(2^{10}\)           | 0.470 | 2.188  | 71.790  | 0.527 | 774.264       |
| \(2^{12}\)           | 0.460 | 16.987 | 37.210  | 0.524 | 774.264       |

| Seoul Bike Sharing Demand | \(J\) | \(R^2\) | Time | Iter | \(R^2_{\text{var}}\) | \(\lambda_{\text{init}}\) |
|--------------------------|------|--------|------|------|----------------|---------------------|
| \(2^4\)                 | 0.622 | 1.008  | 200.000 | 0.620 | 9350.431      |
| \(2^6\)                 | 0.714 | 1.134  | 200.000 | 0.713 | 9927.827      |
| \(2^8\)                 | 0.773 | 1.955  | 199.880 | 0.773 | 10000.001     |
| \(2^{10}\)              | 0.825 | 7.062  | 198.240 | 0.825 | 10000.001     |
| \(2^{12}\)              | 0.856 | 54.121 | 193.270 | 0.857 | 10000.001     |
Concrete Slump Test–3 & $b$ & $R^2$ & Time & Iter & $R^2_{\text{val}}$ & $A_{\text{max}}$ \\
1 & $-0.122$ & 4.875 & 62.996 & 0.014 & 38.452 \\
3 & 0.334 & 5.194 & 129.674 & 0.523 & 82.567 \\
6 & 0.449 & 5.194 & 107.269 & 0.547 & 110.214 \\
15 & 0.393 & 5.352 & 115.115 & 0.500 & 246.689 \\
\text{min}(n, 2^{15}) = 103 & 0.401 & 5.228 & 114.385 & 0.499 & 237.899 \\

Table 17: Batch size dependence

| Depth. | As we can see in Table 18 the optimal choice of the depth parameter seems to be data-dependent and significantly impacts the $R^2$-score. This motivated the introduction of the bagging MLR models that we described in the main paper. We consider only architectures of depth $L \in \mathcal{G}_L = \{1, 2, 3, 4\}$ which reached state of the art results nonetheless. Going deeper is outside of the scope we set for this study, since it would probably require more careful and manual tuning of the hyperparameters on each dataset. |
width, depth, batch-size and number of permutations which are either fix or bounded (for batch-size).

| Dataset                        | n  | d  | MLR-1 | MLR-2 | MLR-3 | MLR-4 |
|-------------------------------|----|----|-------|-------|-------|-------|
| Concrete Stump Test -1        | 103| 8  | 0.940 ± 0.020 | 0.954 ± 0.018 | 0.964 ± 0.025 | 0.986 ± 0.032 |
| Concrete Stump Test -3        | 103| 8  | 0.899 ± 0.132 | 0.913 ± 0.171 | 0.929 ± 0.210 | 0.946 ± 0.149 |
| Concrete Stump Test -2        | 103| 8  | 0.926 ± 0.135 | 0.935 ± 0.159 | 0.946 ± 0.171 | 0.965 ± 0.245 |
| Servo                        | 168| 24 | 0.856 ± 0.031 | 0.839 ± 0.046 | 0.854 ± 0.043 | 0.843 ± 0.049 |
| Computer Hardware             | 210| 7  | 0.984 ± 0.008 | 0.984 ± 0.008 | 0.985 ± 0.008 | 0.985 ± 0.007 |
| Yacht Hydrodynamics           | 306| 33 | 0.952 ± 0.021 | 0.962 ± 0.030 | 0.965 ± 0.020 | 0.965 ± 0.021 |
| QSAR aquatic toxicity         | 546| 34 | 0.448 ± 0.081 | 0.459 ± 0.071 | 0.458 ± 0.070 | 0.470 ± 0.087 |
| QSAR Bioconcentration classes | 772| 25 | 0.617 ± 0.042 | 0.616 ± 0.032 | 0.616 ± 0.041 | 0.616 ± 0.042 |
| QSAR Fish toxicity            | 999| 18 | 0.590 ± 0.014 | 0.586 ± 0.017 | 0.582 ± 0.014 | 0.579 ± 0.016 |
| Yonkers                      | 1385| 15 | 0.839 ± 0.021 | 0.839 ± 0.026 | 0.834 ± 0.031 | 0.832 ± 0.029 |
| Communities and Crime         | 1994| 108| 0.679 ± 0.031 | 0.677 ± 0.029 | 0.680 ± 0.030 | 0.680 ± 0.027 |
| Abalone R                     | 4178| 11 | 0.566 ± 0.028 | 0.543 ± 0.018 | 0.523 ± 0.016 | 0.518 ± 0.018 |
| squark automotive CLV training | 9999| 77 | 0.901 ± 0.006 | 0.900 ± 0.006 | 0.900 ± 0.006 | 0.901 ± 0.006 |
| Seoul Bike Sharing Demand     | 8760| 15 | 0.850 ± 0.009 | 0.878 ± 0.008 | 0.901 ± 0.008 | 0.893 ± 0.008 |
| Electrical Grid Stability Simu | 10000| 12 | 0.917 ± 0.001 | 0.958 ± 0.002 | 0.963 ± 0.002 | 0.955 ± 0.002 |
| All real estate prices        | 3530| 2  | 0.514 ± 0.012 | 0.522 ± 0.012 | 0.522 ± 0.013 | 0.521 ± 0.013 |

Table 18: Depth dependence. Mean and standard deviation of R²-score over 100 seeds.

**Learning rate.** We used ADAM with default parameters except for the learning rate. Indeed, since the width and batch size we picked were outside of the usual ranges, we had to adjust the learning rate accordingly (Table 2). We did not attempt to use another optimizer as ADAM worked well.

**Scalability.** The main limitation is the size of the GPU VRAM with a current maximum of 32G on the best available configuration. We conducted these experiments on devices with either 8 or 11G–VRAM.

Recall that the cost for the inversion of a $J \times J$ matrix is linear on a GPU thanks to parallelization whereas it is quadratic on a CPU.

The runtime per iteration is almost constant since it depends mostly on width, depth, batch-size and number of permutations which are either fix or bounded (for batch-size).
Table 1: State-of-the-art: Deep Learning for supervised tasks on tabular data.
* uses the UCI database which has some well-known flaws [3, 44, 69].

| Method         | End-to-end | Differentiable | Works without | Task | Benchmark datasets | Range n | Consistently outperforms |
|----------------|------------|----------------|---------------|------|--------------------|---------|-------------------------|
| TabNet [14]    | ✓          | no             | no            | Reg/Classif | 6                  | 500K-11M | no                      |
| Tablet [4]     | self-supervised | no           | no            | Reg/Classif | 4                  | 10K-11M  | ✓                      |
| BNMT [5]       | ✓          | ✓              | ✓             | Classif | 14                 | 100K-1.1M | no                      |
| FPS [23]       | ✓          | ✓              | no            | Classif | 90*                | 10-180K  | no                      |
| TabNet [18]    | ✓          | no             | no            | Reg/Classif | 122*               | 16-180K  | no                      |
| Net-ResNet [25] | ✓    | ✓              | ✓             | Reg     | 9                  | 7.6K      | no                      |
| NLR (this work)| ✓          | ✓              | ✓             | Reg/Classif | 32                 | 72-65K   | Reg ✓                   |

* uses the UCI database which has some well-known flaws [3, 44, 69].

Table 2: Benchmarked architectures.

| Architecture | L     | $t_r$ | maxState | FixB | $J$      | $b_p$ | $T$  | $\sigma$ |
|--------------|-------|-------|----------|------|----------|-------|------|----------|
| MLR-1        | 1     | $10^{-2}$ | 200    | 10^7 | $2^{10}$ | min(n, J) | 16  | Reg.: 0.03  |
| MLR-2        | 2     | $10^{-3}$ | 200    | id.  | id.      | id.   | id.  | id.      |
| MLR-3        | 3     | $10^{-3.5}$ | 400    | id.  | id.      | id.   | id.  | id.      |
| MLR-4        | 4     | $10^{-4}$ | 400    | id.  | id.      | id.   | id.  | id.      |

Table 2: Benchmark architectures.