Muddling Labels for Regularization, a novel approach to generalization

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Abstract

Generalization is a central problem in Machine Learning. Indeed most prediction methods require careful calibration of hyperparameters usually carried out on a hold-out validation dataset to achieve generalization. The main goal of this paper is to introduce a novel approach to achieve generalization without any data splitting, which is based on a new risk measure which directly quantifies a model’s tendency to overfit. To fully understand the intuition and advantages of this new approach, we illustrate it in the simple linear regression model ($Y = X\beta + \xi$) where we develop a new criterion. We highlight how this criterion is a good proxy for the true generalization risk. Next, we derive different procedures which tackle several structures simultaneously (correlation, sparsity,...). Noticeably, these procedures concomitantly train the model and calibrate the hyperparameters. In addition, these procedures can be implemented via classical gradient descent methods when the criteria is differentiable w.r.t. the hyperparameters. Our numerical experiments reveal that our procedures are computationally feasible and compare favorably to the popular approach (Ridge, LASSO and Elastic-Net combined with grid-search cross-validation) in term of generalization. They also outperform the baseline on two additional tasks: estimation and support recovery of $\beta$. Moreover, our procedures do not require any expertise for the calibration of the initial parameters which remain the same for all the datasets we experimented on.

Introduction

Generalization is a central problem in machine learning. Regularized or constrained Empirical Risk Minimization (ERM) is a popular approach to achieve generalization [Kukac\v{c}ka et al., 2017]. Ridge [Hoerl and Kennard 1970], LASSO [Tibshirani 1996] and Elastic-net [Zou and Hastie 2005] belong to this category. The regularization term or the constraint is added in order to achieve generalization and to enforce some specific structures on the constructed model (sparsity, low-rank, coefficient positivity,...). This usually involves introducing hyperparameters which require calibration. The most common approach is data-splitting. Available data is partitioned into a training/validation-set. The validation-set is used to evaluate the generalization error of a model built using only the training-set.

Several hyperparameter tuning strategies were designed to perform hyperparameter calibration: Grid-search, Random search [Bergstra and Bengio 2012] or more advanced hyperparameter optimization techniques [Bergstra et al., 2011] Bengio, 2000, Schmidhuber, 1987. For instance, BlackBox optimization [Brochu et al., 2010] is used when the evaluation function is not available [Lacoste et al., 2014]. It includes in particular Bayesian hyperparametric optimization such as Thompson sampling [M\v{c}kus, 1975 Snoek et al., 2012, Thompson, 1933]. These techniques either scale exponentially with the dimension of the hyperparameter space, or requires a smooth convex optimization space [Shahriari et al., 2015]. Highly non-convex optimization problems on a high dimensionnal space can be tackled by Population based methods (Genetic Algorithms[Chen et al., 2018, Real et al., 2017, Olson et al., 2016], Particle Swarm [Lorenzo et al., 2017, Lin et al., 2008]) but at a high computational cost. Another family of advanced methods, called gradient-based techniques, take advantage of gradient optimization techniques [Domke, 2012] like our method. They fall into two categories, Gradient Iteration and Gradient approximation. Gradient Iteration directly computes the gradient w.r.t. hyperparameters on the training/evaluation graph. This means differentiating a potentially lengthy optimization process which is known to be a major bottleneck [Pedregosa, 2016]. Gradient approximation is used to circumvent this difficulty, through implicit differentiation [Larsen et al., 1996, Bertrand et al., 2020]. However, all these advanced methods require data-splitting to evaluate the trained model on a hold-out validation-set, unlike our approach.

Another approach is based on unbiased estimation of the generalization error of a model (SURE [Stein, 1981], AIC [Akaike, 1974], $C_p$-Mallows [Mallows, 2000]) on the training-set. Meanwhile, other methods improve generalization during the training phase without using a hold-out validation-set. For instance, Stochastic Gradient Descent
and the related batch learning techniques [Bottou 1998] achieve generalization by splitting the training data into a large number of subsets and compute the Empirical Risk (ER) on a different subset at each step of the gradient descent. This strategy converges to a good estimation of the generalization risk provided a large number of observations is available. Bear in mind this method and the availability of massive datasets played a crucial role in the success of Deep neural networks. Although batch size has a positive impact on generalization [He et al. 2019], it cannot maximize generalization on its own.

Model aggregation is another popular approach to achieve generalization. It concerns for instance Random Forest [Ho 1995, Breiman 2001], MARS [Friedman 1991] and Boosting [Freund and Schapire 1995]. This approach aggregates weak learners previously built using bootstrapped subsets of the training-set. The training time of these models is considerably lengthened when a large number of weak learners is considered, which is a requirement for improved generalization. Recall XGBOOST [Chen and Guestrin 2016] combines a version of batch learning and model aggregation to train weak learners. MARS, Random Forest, XGBOOST and Deep learning have obtained excellent results in Kaggle competitions and other machine learning benchmarks [Fernández-Delgado et al., 2014, Escalera and Herbrich 2018]. However these methods still require regularization and/or constraints in order to generalize. This implies the introduction of numerous hyperparameters which require calibration on a hold-out validation-set for instance via Grid-search. Tuning these hyperparameters requires expensive human expertise and/or computational resources.

We approach generalization from a different point of view. The underlying intuition is the following. We no longer see generalization as the ability of a model to perform well on unseen data, but rather as the ability to avoid finding pattern where none exist. Using this approach, we derive a novel criterion and several procedures which do not require data splitting to achieve generalization.

This paper is intended to be an introduction to this novel approach. Therefore, for the sake of clarity, we consider here the linear regression setting but our approach can be extended to more general settings like deep learning.

Let us consider the linear regression model:

\[ \mathbf{Y} = \mathbf{X} \beta^\star + \xi, \]

where \( \mathbf{X} = (X_1, \ldots, X_n) \) is the \( n \times p \) design matrix and the \( n \)-dimensional vectors \( \mathbf{Y} = (Y_1, \ldots, Y_n)^T \) and \( \xi = (\xi_1, \ldots, \xi_n)^T \) are respectively the response and the noise variables. Throughout this paper, the noise level \( \sigma > 0 \) is unknown. Set \( ||\mathbf{v}||_N = (\frac{n}{2} \sum_{i=1}^{n} v_i^2)^{1/2} \) for any \( \mathbf{v} = (v_1, \ldots, v_n)^T \in \mathbb{R}^n \).

In practice, the correlation between \( X_i \) and \( Y_i \) is unknown and may actually be very weak. In this case, \( X_i \) provides very little information about \( Y_i \) and we expect from a good procedure to avoid building a spurious connection between \( X_i \) and \( Y_i \). Therefore, by understanding generalization as “do not fit the data in non-informative cases”, we suggest creating an artificial dataset which preserves the marginal distributions while the link between \( X_i \) and \( Y_i \) has been completely removed. A simple way to do so is to construct an artificial set \( \mathcal{D} = (X, Y) \) by applying permutations \( \pi \in \mathcal{S}_n \) (the set of permutations of \( n \) points) on the components of \( Y \) of the initial dataset \( \mathcal{D} \) where for any \( y \in \mathbb{R}^n \), we set \( \pi(y) = (y_{\pi(1)}, \ldots, y_{\pi(n)})^T \).

The rest of the paper is organized as follows. In Section I we introduce our novel criterion and highlight its generalization performance. In Section II, this new approach is applied to several specific data structures in order to design adapted procedures which are compatible with gradient-based optimization methods. We also point out several advantageous points about this new framework in an extensive numerical study. Finally we discuss possible directions for future work in Section III.

1. **Label muddling criterion**

In model (1), we want to recover \( \beta^\star \) from \( \mathcal{D} = (X, Y) \). Most often, the \( n \) observations are partitioned into two parts of respective sizes \( n_{\text{train}} \) and \( n_{\text{val}} \), which we denote the train-set \( (X_{\text{train}}, Y_{\text{train}}) \) and the validation-set \( (X_{\text{val}}, Y_{\text{val}}) \) respectively. The train-set is used to build a family of estimators \{\( \beta(\theta, X_{\text{train}}, Y_{\text{train}}) \)\} \( \theta \) which depends on a hyperparameter \( \theta \). Next, in order to achieve generalization, we use the validation-set to calibrate \( \theta \). This is carried out by minimizing the following empirical criterion w.r.t. \( \theta \):

\[ \|Y_{\text{val}} - X_{\text{val}} \beta(\theta, X_{\text{train}}, Y_{\text{train}})\|_{n_{\text{val}}}. \]

In our approach, we use the complete dataset \( \mathcal{D} \) to build the family of estimators and to calibrate the hyperparameter \( \theta \).

**Definition 1.** Fix \( T \in \mathbb{N}^+ \). Let \( \{n_i^{(T)}\}_{i=1}^{T} \) be \( T \) permutations in \( \mathcal{S}_n \). Let \( \{\beta(\theta, \cdot, \cdot)\}_{\theta} \) be a family of estimator.
The **MLR criterion** is defined as:

\[
MLR(\theta) = \|Y - X\beta(\theta, X, Y)\|_n
- \frac{1}{T} \sum_{t=1}^{T}\|\pi^t(Y) - X\beta(\theta, X, \pi^t(Y))\|_n.
\]  

The MLR criterion performs a trade-off between two antagonistic terms. The first term fits the data while the second term prevents overfitting. Since the MLR criterion is evaluated directly on the whole sample without any hold-out validation-set, this approach is particularly useful for small sample sizes where data-splitting approaches can produce strongly biased performance estimates [Varoquaux et al., 2018]. We highlight in the following numerical experiment the remarkable generalization performance of the MLR criterion.

**Numerical Experiments.**

We consider two families

\[
F(\theta) = \{\beta(\theta, X_{train}, Y_{train})\}_{\theta}
\]

of estimators constructed on a *train*-dataset and indexed by \(\theta\): Ridge and LASSO. We are interested in the problem of calibration of the hyperparameter \(\theta\) on a grid \(\Theta\). We compare two criteria \(C(\theta)\) to calibrate \(\theta\): the MLR criterion and cross-validation (implemented as Ridge, Lasso in Scikit-learn [Pedregosa et al., 2011]). For each criterion \(C(\theta)\), the final estimator \(\beta_{train} = \beta(\hat{\theta}, X_{train}, Y_{train})\) is s.t.

\[
\hat{\theta} = \arg\min_{\theta \in \Theta} C(\theta).
\]

**R²-score.** For each family, the generalization performance of each criterion is evaluated using the hold-out *test*-dataset \(D_{test} = (X_{test}, Y_{test})\) by computing the following R²-scores:

\[
R^2(\beta_{train}) = 1 - \frac{\|Y_{test} - X_{test}\beta_{train}\|_2}{\|Y_{test} - \bar{Y}_{test}\|_2} (\leq 1),
\]

where \(\bar{Y}_{test}\) is the empirical mean of \(Y_{test}\). For the sake of simplicity, we set \(R^2(\hat{\theta}) = R^2(\beta_{train})\). The oracle we aim to match is

\[
\theta^* = \arg\min_{\theta \in \Theta} R^2(\theta).
\]

Our first numerical experiments concern synthetic data.

**Synthetic data.** For \(p = 80\), we generate observations \((X, Y) \in \mathbb{R}^p \times \mathbb{R}, \text{s.t. } Y = X^T \beta^* + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma), \sigma = 10 \text{ or } 50\). We consider three different scenarios. **Scenario A** (correlated features) corresponds to the case where the LASSO is prone to fail and Ridge should perform better. **Scenario B** (sparse setting) corresponds to a case known as favorable to LASSO. **Scenario C** combines sparsity and correlated features. For each scenario we sample a *train*-dataset of size \(n_{train} = 100\) and a *test*-dataset of size \(n_{test} = 1000\). For each scenario, we perform \(M = 100\) repetitions of the data generation process to produce \(M\) pairs of *train/Test* datasets. Details on the data generation process can be found in the Appendix.

**Performances evaluation.** For each family \(F(\theta)\) and each criterion \(C(\theta)\), we construct on every *train*-dataset, the corresponding model \(\hat{\beta}_{train}\). Next, using the corresponding hold-out *test*-dataset \(D_{test} = (X_{test}, Y_{test})\), we compute their R²-scores.

**Impact of \(T\).** In Figure 1 we study the impact of the number of permutations \(T\) on the generalization performance of the criterion measured via the R²-score in (3). The most striking finding is the sharp increase in the generalization performance from the first added permutation in Scenarios A and C. Adding more permutations does not impact the generalization but actually improves the running time and stability of the novel procedures which we will introduce in the next section. In a pure sparsity setting (Scenario B with LASSO), adding permutations marginally increases the generalization.

**Comparison of generalization performance.** For Scenario A with the Ridge family, we compute the difference \(R^2(\hat{\theta}^C(\theta)) - R^2(\hat{\theta}^M(\theta))\), for the two criteria \(C(\theta)\) (MLR and CV). For Scenarios B and C, we consider the LASSO family and compute the same difference. Boxplots in Figure 1 summarize our findings over 100 repetitions of the synthetic data. The empirical mean is depicted by a green triangle on each boxplot. Moreover, to check for statistically significant margin in R²-scores between different procedures, we use the Mann-Whitney test (as detailed in
![Image] (Kruskal [1957] and implemented in scipy [Virtanen et al., 2020]). The boxplots highlighted in yellow correspond to the best procedures according to the Mann-Whitney (MW) test. As we observed, the MLR criterion performs better than CV for the calibration of the Ridge and LASSO hyperparameters in Scenarios A and C in the presence of correlation in the design matrix.

**Plot of the generalization performance.** In order to plot the different criteria together, we use the following rescaling. Let $F : \Theta \rightarrow \mathbb{R}$, we set

$$\hat{\theta} = \arg \min_{\theta \in \Theta} F(\theta) \quad \text{and} \quad \bar{\theta} = \arg \max_{\theta \in \Theta} F(\theta).$$

For any $\theta \in \Theta$, we define

$$\Lambda_F(\theta) = \frac{F(\hat{\theta}) - F(\theta)}{F(\bar{\theta}) - F(\hat{\theta})}.$$

Figure 3 contains the rescaled versions of the R$^2$-score on the test set and the MLR and CV criteria computed on the train-dataset. The vertical lines correspond to the selected values of the hyperparameter in the grid $\Theta$ by the MLR and CV criteria as well as the optimal hyperparameter $\theta^*$ for the R$^2$-score on the test set. The MLR criterion is a good proxy for the generalization performance (R$^2$-score on the test-dataset) on the whole grid $\Theta$ for the Ridge in Scenario A. In Scenario C with the LASSO, the MLR criterion is a smooth function with steep variations in a neighborhood of its global optimum. This is an ideal configuration for the implementation of gradient descent schemes.

the MLR criterion performs better than CV on correlated data for grid-search calibration of the LASSO and Ridge hyperparameters. However CV works better in the pure sparsity scenario. This motivated the introduction of novel procedures based on the MLR principle which can handle the sparse setting better.

**2. Novel procedures**

In Section 4 we used 2 to perform grid-search calibration of the hyperparameter. However, if $\{\beta(\theta)\}_{\theta}$ is a family of models differentiable w.r.t. $\theta$, we can minimize 2 w.r.t. $\theta$ via standard gradient-based methods. This motivated the introduction of new procedures based on the MLR criterion.

**Definition 2.** Consider $\{\beta(\theta)\}_{\theta}$ a family of models differentiable w.r.t. $\theta$. Let $\{\pi^T\}_{T=1}^T$ be $T$ derangements in $\mathcal{S}_n$. The $\beta$-MLR procedure is

$$\hat{\beta} = \beta(\hat{\theta}) \quad \text{with} \quad \hat{\theta} = \arg \min_{\theta} \text{MLR}_\beta(\theta). \tag{4}$$

where $\text{MLR}_\beta$ is defined in 2.

Moreover, using our approach, we can also enforce several additional structures simultaneously (sparsity, correlation, group sparsity, low-rank,...) by constructing appropriate families of models. In this regard, let us consider the 3 following procedures which do not require a hold-out validation-set.

**R–MLR procedure for correlated designs.** The Ridge family of estimators $\{\beta^R(\lambda, \mathbf{X}, \mathbf{Y})\}_{\lambda > 0}$ is defined as follows:

$$\beta^R(\lambda, \mathbf{X}, \mathbf{Y}) = (\mathbf{X}^T \mathbf{X} + \lambda I_p)^{-1} \mathbf{X}^T \mathbf{Y}, \quad \lambda > 0. \tag{5}$$

Applying Definition 2 with the Ridge family, we obtain the $R$–MLR procedure $\hat{\beta}^R = \beta^R(\hat{\lambda})$ where $\hat{\lambda} = \arg \min_{\lambda > 0} \text{MLR}_{\beta^R}(\lambda)$. This new optimisation problem can be solved by gradient descent, contrarily to the previous section where we performed a grid-search calibration of $\lambda$.

**S–MLR for sparse models.** We design in Definition 3 below a novel differentiable family of models to enforce sparsity in the trained model. Applying Definition 2 to this family, we can derive the $S$–MLR procedure: $\hat{\beta}^S = \beta^S(\hat{\theta})$ where $\hat{\theta} = \arg \min_{\theta} \text{MLR}_{\beta^S}(\theta)$.

![Image] (Figure 2. Generalization performance for MLRand CV for Ridge and LASSO Hyperparameter calibration)

![Image] (Figure 3. Criterion landscape for grid-search calibration with MLR (Up) and CV (down)).
Definition 3. Let \( \{ \beta^S(\lambda, \kappa, \gamma, X, Y) \}_{(\lambda, \kappa, \gamma) \in \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R}_+} \) be a family closed-form estimators defined as follows:
\[
\beta^S(\lambda, \kappa, \gamma, X, Y) = S(\kappa, \gamma) \beta^R(\lambda, X S(\kappa, \gamma), Y), \quad (6)
\]
where \( \beta^R \) is defined in \([5]\), the quasi-sparsifying function \( S: \mathbb{R}_+^* \times \mathbb{R}_+^p \rightarrow [0, 1]^{p \times p} \) is s.t.
\[
S(\kappa, \gamma) = \text{diag}(S_1(\kappa, \gamma), \ldots, S_p(\kappa, \gamma)),
\]
where for any \( j = 1, \ldots, p \),
\[
S_j(\kappa, \gamma) = \left( 1 + e^{-\kappa \times (\sigma_j^2 + 10^{-2})(\gamma_j - \tau)} \right)^{-1}
\]
with \( \tau = \frac{1}{p} \sum_{i=1}^p \gamma_i \) and \( \sigma_j^2 = \sum_{i=1}^p (\gamma_i - \tau)^2 \).

The new family \([\mathcal{S}]\) enforces sparsity on the regression vector but also directly onto the design matrix. Hence it can be seen as a combination of data-preprocessing (performing feature selection) and model training (using the ridge estimator).

Noticeably, the “quasi-sparsifying” trick transforms feature selection (a discrete optimization problem) into a continuous optimization problem which is solvable via classical gradient-based methods. The function \( S \) produces diagonal matrices with diagonal coefficients in \([0, 1]\). Although the sigmoid function \( S_j \) cannot take values 0 or 1, for very small or large values of \( \gamma_j \), the value of the corresponding diagonal coefficient of \( S(\kappa, \gamma) \) is extremely close to 0 or 1. In those cases, the resulting model is weakly sparse in our numerical experiments. Thresholding can then be used to perform feature selection.

**A-MLR for correlated designs and sparsity.** Aggregation is a statistical technique which combines several estimators in order to attain higher generalization performance \([\text{Tsybakov, 2003}]\). We propose in Definition 4 a new aggregation procedure to combine the estimators \([\mathcal{S}]\) and \([\mathcal{R}]\). This essentially consists in an interpolation between \( \beta^R \) and \( \beta^S \) models, where the coefficient of interpolation is quantified via the introduction of a new regularization parameter \( \mu \in \mathbb{R} \).

Definition 4. We consider the family of models
\[
\{ \beta^A(\lambda, \kappa, \gamma, \mu, X, Y) \}_{(\lambda, \kappa, \gamma, \mu) \in \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R}_+} \ni
\]
\[
\beta^A(\theta, X, Y) = S(\mu) \times \beta^R(\lambda, X, Y) + (1 - S(\mu)) \times \beta^S(\lambda, \kappa, \gamma, X, Y), \quad (7)
\]
where \( \beta^R(\lambda, Y) \) and \( \beta^S(\lambda, \kappa, \gamma, X, Y) \) are defined in \([5]\) and \([6]\) respectively and \( S \) is the sigmoid \( \text{diag}(S_1(\kappa, \gamma), \ldots, S_p(\kappa, \gamma)) \).

Applying Definition 2 to this family, we can derive the A-MLR procedure: \( \hat{\beta}^A = \beta^A(\hat{\theta}) \) where \( \hat{\theta} = \arg \min_{\theta} \text{MLR}_A(\theta) \).

This procedure is designed to handle both correlation and sparsity.

Figure 4. Distribution of the value of \( S(\hat{\mu}) \) over 100 repetitions on synthetic data.

**Algorithmic complexity.** Using the MLR criterion, we develop fully automatic procedures to tune regularization parameters while simultaneously training the model in a single run of the gradient descent algorithm without a holdout validation set. The computational complexity of our methods is \( O(n(p + r)K) \) where \( n, p, r, K \) denote respectively the number of observations, features, regularization parameters and iterations of the gradient descent algorithm. The computational complexity of our method grows only arithmetically w.r.t. the number of regularization parameters.

**NUMERICAL EXPERIMENTS.** We performed numerical experiments on the synthetic data from Section I and also on real datasets described below.

**Real data.** We test our methods on several commonly used real datasets (UCI \([\text{Asuncion and Newman, 2007}]\) and Svmlib \([\text{Chang and Lin, 2011}]\) repositories). See Appendix for more details. Each selected UCI dataset is split into a 80% train-dataset and a 20% test-dataset. We repeat this operation \( M = 100 \) times to produce \( M \) pairs of \((\text{train}, \text{test})\)-datasets.

In order to test our procedures in the setting \( n \leq p \), we selected, from Svmlib, the news20 dataset which contains a train and a test dataset. We fixed the number of features \( p \) and we sample six new 20news train-datasets of different sizes \( n \) from the initial news20 train-dataset. For each
size $n$ of dataset, we perform $M = 100$ repetitions of the sampling process to produce $M$ train-datasets. We kept the initial test-set for the evaluation of the generalization performances.

**Number of iterations.** We choose to solve (4) using ADAM but other GD methods could be used. Figure 5 contains the boxplots of the number of ADAM iterations for the MLR procedures on the synthetic and real datasets over the $M = 100$ repetitions. Although $MLR_{\beta S}$ and $MLR_{\beta A}$ are highly non-convex, the number of iterations required for convergence is always about a few several dozen in our experiments. This was already observed in other non-convex settings [Kingma and Ba, 2014].

![Figure 5. Synthetic, UCI and 20news data: Number of iterations](image)

**Running time.** Our procedures were coded in Pytorch to underline how they can be parallelized on a GPU. A comparison of the running time with the benchmark procedures is not pertinent as they are implemented on cpu by Scikit-learn. The main point of our experiments was rather to show how the MLR procedures can be successfully parallelized. This opens promising prospects for the MLR approach in deep learning frameworks.

From a computational point of view, the matrix inversion in (5) is not expensive in our setting as long as the covariance matrix can fully fit on the GPU. Figure 6 and 7 confirm the running time is linear in $n, p$ for the MLR procedures. This confirms the MLR procedures are scalable.

![Figure 6. UCI data: running time as a function of $n$](image)

![Figure 7. 20news data: running time as a function of $p$](image)

Consequently, our procedures run in reasonable time as illustrated in Figures 8 and 9.

![Figure 8. Synthetic data: running times in seconds.](image)

![Figure 9. UCI data (left) and 20news data (right): running times.](image)

**Initial parameters.** Strikingly, the initial values of the parameters (see Table 1) used to implement our MLR procedures could remain the same for all the datasets we considered while still yielding consistently good prediction performances. These initial values were calibrated only once in the standard setting ($n \geq p$) on the Boston dataset [Harrison Jr and Rubinfeld, 1978, Belsley et al., 2005] which we did not include in our benchmark when we evaluated the performance of our procedures. We emphasize again we used these values without any modification on all the synthetic and real datasets. The synthetic and UCI datasets fall into the standard setting. Meanwhile, the 20news datasets correspond to the high-dimensional setting ($p \gg n$). As such, it might be possible to improve the generalization performance by using a different set of initial parameters better adapted to the high-dimensional setting. This will be investigated in future work.

However, in this paper, we did not intend to improve the generalization performance by trying to tune the initial parameters for each specific dataset. This was not the point of this project. We rather wanted to highlight our gradient-based methods compare favorably in terms of generalization with benchmark procedures just by using the default initial values in Table 1.

We also studied the impact of parameter $T$ on the performances of the MLR procedures on the synthetic data. In Figure 10, the generalization performance ($R^2$-score) increases significantly from the first added permutation ($T = 1$). Starting from $T \approx 10$, the $R^2$-score has converged to

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Inversion of a $p \times p$ matrix has a $p^3$ complexity on CPU, but parallelization schemes provide linear complexity on GPU when some memory constraints are met [Murugesan et al., 2018, Nath et al., 2010, Chrzeszczyk and Chrzeszczyk, 2013].
its maximum value. An even more striking phenomenon is the gain observed in the running time when we add $T$ permutations (for $T$ in the range from 1 to approximately 100) when compared with the usual empirical risk ($T = 0$). Larger values of $T$ are neither judicious nor needed in this approach. In addition, the needed number of iterations for ADAM to converge is divided by 3 starting from the first added permutation. Furthermore, this number of iterations remained stable (below 20) starting from $T = 1$. Based on these observations, the hyperparameter $T$ does not require calibration. We fixed $T = 30$ in our experiments even though $T = 10$ might have been sufficient.

| Optimization parameters | Parameter initialization |
|-------------------------|--------------------------|
| Tolerance               | $10^{-3}$                |
| Max. iter.              | $10^3$                   |
| Learning rate           | 0.5                      |
| Adam $\beta_1$         | 0.5                      |
| Adam $\beta_2$         | 0.9                      |

Table 1. Parameters for the MLR procedures.

Performance comparisons. We compare our MLR procedures against cross-validated Ridge, LASSO and Elastic-net (implemented as RidgeCV, LassoCV and ElasticnetCV in Scikit-learn [Pedregosa et al., 2011]) on simulated and real datasets. Our procedures are implemented in PyTorch [Paszke et al., 2019] on the centered and rescaled response $Y$. Complete details and results can be found in the Appendix. In our approach $\theta$ can always be tuned directly on the train set whereas for benchmark procedures like LASSO, Ridge, Elastic net, $\theta$ is typically calibrated on a hold-out validation-set using grid-search CV for instance.

Generalisation performance. Figures 11 and 12 show the MLR procedures consistently attain the highest $R^2$-scores for the synthetic and UCI data according to the Mann-Whitney test over the $M = 100$ repetitions. Regarding, the 20news datasets, the MLR procedures are always within 0.05 of the best (E-net).

Figure 10. Synthetic data: impact of $T$ on the MLR procedures.

Figure 11. Synthetic data: $R^2$-score

Figure 12. UCI data (left) and 20news data (right): $R^2$-score

Estimation of $\beta^*$ and support recovery accuracy. For the synthetic data, we also consider the estimation of the regression vector $\beta^*$. We use the $l_2$-norm estimation error $\| \hat{\beta} - \beta^* \|_2$ to compare the procedures. As we can see in Figure 13, the MLR procedures perform better than the benchmark procedures.

Figure 13. $\beta^*$ estimation (best in yellow according to MW)

We finally study the support recovery accuracy in the sparse setting (Scenario B). We want to recover the support $J(\beta^*) = \{ j : \beta^*_j \neq 0 \}$. For our procedures, we build the following estimator $\hat{J}(\hat{\beta}) = \{ j : |\hat{\beta}_j| > \hat{\tau} \}$ where the threshold $\hat{\tau}$ corresponds to the first sharp decline of the coefficients $|\hat{\beta}_j|$. Denote by $\# J$ the cardinality of set $J$. The support recovery accuracy is measured as follows:

$$\text{Acc}(\beta) := \frac{\# (J(\beta^*) \cap \hat{J}(\hat{\beta})) + \# (J^c(\beta^*) \cap \hat{J}(\hat{\beta}))}{p}$$

Our simulations confirm $\hat{\beta}^S$ is a quasi-sparse vector. Indeed we observe in Figure 14 a sharp decline of the coefficients $|\hat{\beta}^S_j|$. Thus we set the threshold $\hat{\tau}$ at $10^{-3}$.

Overall, $\hat{\beta}^S$ and $\hat{\beta}^A$ perform better for support recovery than the benchmark procedures. Moreover in Scenario
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Figure 14. Coefficients values (blue) and threshold (red) with \( p = 80 \).

**B** favorable to LASSO, our procedures perform far better (Figure 15).

Figure 15. Support recovery performance analysis in **Scenario B** (best in yellow according to MW).

Figure 16. Support recovery performance analysis in **Scenario C** (best in yellow according to MW).

3. Conclusion and future work

In this paper, we introduced in the linear regression setting the new **MLR** approach based on a different understanding of generalization. Exploiting this idea, we derived a novel criterion and new procedures which can be implemented directly on the **train**-set without any hold-out **validation**-set. Within **MLR**, additional structures can be taken into account without any significant increase in the computational complexity.

We highlighted several additional advantageous properties of the **MLR** approach in our numerical experiments. The **MLR** approach is computationally feasible while yielding statistical performances equivalent or better than the cross-validated benchmarks. We provided numerical evidence of **MLR** criterion’s ability to generalize from the first added permutation. Besides, the strength of our **MLR** procedures stems from their compatibility with gradient-based optimization methods. As such, these procedures can fully benefit from automatic graph-differentiation libraries (such as pytorch [Paszke et al., 2017] and tensorflow [Abadi et al., 2015]).

In our numerical experiments, adding more permutations improves the convergence of the ADAM optimizer while preserving generalisation. As a matter of fact, \( T \) does not require any fine-tuning. In that regard, \( T \) is not a hyper-parameter. Likewise, the other hyperparameters require no tedious initialization in this framework. The same fixed hyperparameters for ADAM and initialization values of the regularization parameters (see Table 1) were used for all the considered datasets. Noticeably, these experiments were run using high values for learning rate and convergence threshold. Consequently, only a very small number of iterations were needed, even for non-convex criteria (**MLR_{\beta s}** and **MLR_{\beta A}**).

The **MLR** approach offers promising perspectives to address an impediment to the broader use of deep learning. Currently, fine-tuning DNN numerous hyper-parameters often involves heavy computational resources and manual supervision from field experts [Smith, 2018]. Nonetheless, it is widely accepted that deep neural networks produce state-of-the-art results on most machine learning benchmarks based on large and structured datasets [Escalera and Herbrich, 2018, He et al., 2016, Klambauer et al., 2017, Krizhevsky et al., 2012, Silver et al., 2016, Simonyan and Zisserman, 2014, Szegedy et al., 2015]. By contrast, it is not yet the case for small unstructured datasets, (eg. tabular datasets with less than 1000 observations ) where Random Forest, XGBOOST, MARS, etc are usually acknowledged as the state of the art [Shavitt and Segal, 2018].

These concerns are all the more relevant during the ongoing global health crisis. Reacting early and appropriately to new streams of information became a daily challenge. Specifically, relying on the minimum amount of data to produce informed decisions on a massive scale has become the crux of the matter. In this unprecedented situation, transfer learning and domain knowledge might not be relied on to address these concerns. In that regard, the minimal need for calibration and the reliable convergence behavior of the **MLR** approach are a key milestone in the search for fast reliable regularization methods of deep neural networks, especially in the small sample regime.

Beyond the results provided in this paper, we successfully extended the **MLR** approach to deep neural networks. Neural networks trained with the **MLR** criterion can reach state of the art results on benchmarks usually dominated by Random Forest and Gradient Boosting techniques. Moreover, these results were obtained while preserving the fast, smooth and reliable convergence behavior displayed in this
paper. We also successfully extended our approach to classification on tabular data. All these results are the topics of a future paper which will be posted on Arxiv soon. In an ongoing project, we are also adapting our approach to tackle few-shots learning and adversarial resilience for structured data (images, texts, graphs). We believe we just touched upon the many potential applications of the MLR approach in the fields of Machine Learning, Statistics and Econometrics.

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