Optimizing generalization on the train set: a novel gradient-based framework to train parameters and hyperparameters simultaneously

Abstract

Generalization is a central problem in Machine Learning. Most prediction methods require careful calibration of hyperparameters carried out on a hold-out validation dataset to achieve generalization. The main goal of this paper is to present a novel approach based on a new measure of risk that allows us to develop novel fully automatic procedures for generalization. We illustrate the pertinence of this new framework in the regression problem. The main advantages of this new approach are: (i) it can simultaneously train the model and perform regularization in a single run of a gradient-based optimizer on all available data without any previous hyperparameter tuning; (ii) this framework can tackle several additional objectives simultaneously (correlation, sparsity,...) via the introduction of regularization parameters. Noticeably, our approach transforms hyperparameter tuning as well as feature selection (a combinatorial discrete optimization problem) into a continuous optimization problem that is solvable via classical gradient-based methods; (iii) the computational complexity of our methods is \( O(npK) \) where \( n, p, K \) denote respectively the number of observations, features and iterations of the gradient descent algorithm. We observe in our experiments a significantly smaller runtime for our methods as compared to benchmark methods for equivalent prediction score. Our procedures are implemented in PyTorch (code is available for replication).

Introduction and Related works

Generalization is a central problem in machine learning. Regularized or constrained Empirical Risk Minimization (ERM) is a popular approach to achieve generalization \([31]\). Ridge \([26]\), Lasso \([55]\) and Elastic-net \([58]\) 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 positiveness,...). This usually involves introducing hyperparameters that need to be properly calibrated, which requires a good estimate of the generalization risk. The most common approach is data-splitting that partitions the available data into a training/validation-set. The validation-set is used to evaluate the generalization error of a model built using only the training-set. Another approach is based on unbiased estimation of the generalization error of a model (SURE \([52]\), AIC \([2]\), \( C_p \)-Mallows \([37]\)) on the training-set. Several hyperparameter tuning strategies are designed to achieve generalization: Grid-search, Random search \([5]\) or more advanced hyperparameter optimization techniques \([6, 4, 45]\). For instance, BlackBox optimization \([10]\) is used when the evaluation function is not available \([32]\). It includes in particular Bayesian...
hyperparametric optimization such as Thompson sampling [38, 51, 54]. Note that this technique either scales exponentially with the number of hyperparameters, or requires a smooth convex optimization space [46]. Highly non-convex optimization problems can be tackled by Population based methods (Genetic Algorithms [13, 44, 39], Particle Swarm [35, 34]) for a high computational cost. Another family of advanced methods, called gradient-based techniques, take advantage of gradient optimization techniques [16] 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/evaluating graph. It requires differentiating a potentially lengthy optimization process which is known to be a major bottleneck [42]. Gradient approximation is used to circumvent this difficulty, through implicit differentiation [33, 7]. All these advanced methods require data-splitting and the evaluation of the trained model on a hold-out validation-set unlike our approach.

We can cite other methods that improve generalization during the training phase without using a hold-out validation-set. For instance, Stochastic Gradient Descent and the related batch learning techniques [3] 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. Note that this method and the availability of massive datasets played a crucial role in the success of Deep neural networks. Although it has been shown that batch size has a positive impact on generalization [22], it cannot maximize generalization on its own. Model aggregation is another popular approach to achieve generalization. It concerns for instance Random Forest [24, 9], MARS [20] and Boosting [19]. 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. Note that XGBOOST [14] 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 [18, 17]. However these methods still require optimization and/or constraints in order to generalize. It implies the introduction of numerous hyperparameters that need to be calibrated on an hold-out validation-set for instance via Grid-search. Tuning these hyperparameters requires expensive human expertise and/or computational resources. We present a novel approach based on a different understanding of the generalization notion. This allows us to derive several training procedures that are fully automatic and do not require data splitting to achieve generalization. The underlying intuition is that 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 patterns when none exist, we will refer to this situation as the non-informative case. The rest of the paper is organized as follows. In Section 1, we present our novel approach in the regression setting. Based on this approach, we develop in Section 2 a framework for the linear regression setting and build procedures able to capture specific structures. In Section 3, we carry out an extensive numerical study that highlights several interesting points about this new framework. Finally we discuss possible directions for future work in Section 4.

1 A novel approach for generalization

We place ourselves in the regression setting where our goal is to recover \( \mathbb{E}[Y|x] \) from a sample of observations of \( (x, Y) \). Let consider a train-sample \( D = \{(x_1, Y_1), \cdots, (x_n, Y_n)\} \) of size \( n \), where the pairs \( (x_i, Y_i) \) are independent and take values in \( X \times Y \). Let denote by \( Y \) the \( n \times p \) design matrix such that \( X^\top = (x_1, \cdots, x_n) \). In the regression setting, we often want to recover \( \mathbb{E}[Y|x] = f_\beta(X) \) from \( D = (X, Y) \), where \( f_\beta : X \to \mathbb{R}^+ \) is a function which belongs to a considered class of models \( F \). This is usually done by minimizing the following empirical risk (ER) w.r.t. the parameter \( \beta \): \( \text{ER}(X, Y, \beta) = \frac{1}{n} \sum_{i=1}^n L(Y_i, f_\beta(x_i)) \), where \( L: Y \times \mathbb{R}^+ \to \mathbb{R}^+ \) is a loss function. In practice, the correlation between \( x \) and \( Y \) is unknown and may actually be very weak. In that case, \( x \) provides very little information about \( Y \) and we expect from a good procedure to avoid building a spurious connection between \( x \) and \( Y \). Therefore, by understanding generalization as “do not fit the data in non-informative cases”, we suggest creating a artificial dataset that preserves the marginal distributions, but such that the link between \( x \) and \( Y \) has been completely removed. A simple way to do so is to construct an artificial one \( \tilde{D} = (\tilde{X}, \tilde{Y}) = (X, \pi(Y)) \) by applying a permutation \( \pi \in \mathfrak{S}_n \) (the set of permutations of \( n \) points) on the components of \( Y \) of the initial dataset \( D \) where for any \( y \in \mathbb{R}^n \), we set \( \pi(y) = \)
Formally, it will result in the addition of a term to ER. As the new dataset $\tilde{D}$ is built directly on the train-set, generalization can be achieved without any data splitting. Formally, this amounts to adding to ER a term that achieves generalization. We called this new risk measure the ER-$G$. With this approach, novel criteria that need no hold-out validation-set can be developed and used in the same way as SURE, AIC, $C_p$-mallows to perform various tasks (enforce generalization, model selection, feature engineering). The ER-$G$ approach can also be used to derive novel procedures if we have access to a family of closed-form estimators $\{\beta_0\}_\theta$ depending on a regularization parameter $\theta$. From now on and for the sake of notation simplicity, we will write $ER(X, Y, \theta)$ for $ER(X, Y, \hat{\beta}_\theta)$.

**ER-$G$-Approach**

Fix $T \in \mathbb{N}^*$. Let $\{\pi_t\}_{t=1}^T$ be $T$ permutations in $\mathcal{G}_n$. (i) The ER-$G$ criterion is defined as

$$ER-G(X, Y, \theta) = ER(X, Y, \theta) + \frac{1}{T} \sum_{t=1}^T \left| ER(X_0, Y, \theta) - ER(X, \pi_t(Y), \theta) \right|,$$

where $X_0 = (1_n | 0_{n \times (p-1)})$ and $1_n$ is the one $n$-dimensional vector.

(ii) The ER-$G$ procedure is given for a family of closed-form solution $\{\beta(\theta)\}_\theta$ by

$$\hat{\beta}_{ER-G} = \beta(\hat{\theta}) \quad \text{with} \quad \hat{\theta} = \arg \min_\theta ER-G(X, Y, \theta).$$

**Discussion.** The ER-$G$ criterion (1) performs a trade-off between the first term which fits the data while the second term prevents overfitting. The quantity $ER(X_0, Y, \theta)$ corresponds to the risk of the best estimator when no features $x$ is included in the model. For instance, for the regression linear model with the quadratic loss, this term is simply the standard deviation of $Y$. Thus, the second term in (1) states that a model should not perform better than the intercept model in non-informative cases.

An empirical study (See Figure 3) about the impact on the generalization performances of the value of $T$ was carried out in the linear regression model considered in Section 2. It revealed that this parameter has virtually no impact. Therefore, $T$ is not an hyperparameter that requires tuning. We set $T = 30$ in our experiments which is largely sufficient to achieve generalization. In addition, this approach allows us to enforce several additional structures simultaneously (sparsity, correlation, group sparsity, low-rank,...) just by considering an appropriate family of models encoded into $\theta$. We call $\theta$ the regularization parameter as we do not calibrate it on a hold-out validation-set which is a requirement for hyperparameters. Indeed, in our approach, we can tune $\theta$ directly on the train set. Feature selection is by essence a discrete optimization problem whereas the ER-$G$ criterion transforms this task into a continuous optimization problem (see Section 2) that is solvable via an unique classical gradient-based methods.

A joint effort by the communities of electronic engineering, computer science and numerical optimization has resulted into the combined optimization of the software (graph-based computation, automatic differentiation) and hardware architecture (GPU’s, TPU’s) in order to compute gradients efficiently. Since our method is purely gradient based on a specifically designed derivation graph, it can immediately benefits from this optimized tensorized computation environment. The message that we want to convey in this paper is the following. It is possible to achieve generalization on the train-set via the ER-$G$ criterion. Although we illustrate the potential of the ER-$G$ approach only in the linear regression setting in Section 2, we believe it was interesting to provide here a general approach to investigate other Machine Learning settings. Of course, we are aware that adapting this approach to include other models will require significant work. Indeed, the ER-$G$ procedures currently depends on a closed-form family of models. We are currently developing an approach to remove this restriction and extend it to more general families of models and other settings such as the classification problem. The ER-$G$ criterion (1) contains two antagonistic terms which result into large oscillations on the loss landscape (w.r.t. $\theta$) in our experiments. This was due to an inappropriate choice of $L$ (e.g. quadratic loss) that resulted in instability in the generalization performance. To remediate this issue, it is important to choose a uniformly continuous loss function so that the criterion does not oscillate too abruptly w.r.t. $\theta$. In that regard, the quadratic loss (not uniformly continuous) was not a good candidate and we used instead the square root of the quadratic loss in

$$(y_{\pi(1)}, \ldots, y_{\pi(n)})^T.$$
Note that this loss is differentiable w.r.t. \( \theta \) as long as \( Y \neq X\hat{\beta}_0 \). See the Appendix for other possible choices of loss functions. Moreover, we observed in our experiments that the loss function \( L \) does not need to be convex to return interesting results (See Section 2).

## 2 Linear regression setting

From now, we place ourselves in the linear regression setting where \( \mathcal{X} = \mathbb{R}^p \), \( Y = \mathbb{R} \) and \( \mathcal{F} = \{ f_\beta(x) = \langle x, \beta \rangle, \beta \in \mathbb{R}^p \} \) is the class of linear functions. We consider the linear regression model:

\[
Y = X\beta^* + \xi, \tag{3}
\]

where \( X^T = (x_1, \cdots, x_n) \) is the \( n \times p \) design matrix and the \( n \)-dimensional vectors \( Y = (Y_1, \cdots, Y_n)^T \) and \( \xi = (\xi_1, \cdots, \xi_n)^T \) are respectively the response and the noise variables. Throughout this paper, the noise level \( \sigma > 0 \) is unknown. We specify the \( ER\sim G \) approach in the linear model setting with the square root quadratic loss with \( ||v||_2 = (\frac{1}{n} \sum_{i=1}^{n} v_i^2)^{1/2} \) for any \( v = (v_1, \ldots, v_n)^T \in \mathbb{R}^n \). Since our framework is defined for centered and rescaled response \( Y \), the standard deviation term \( ER(X_0, Y, \theta) = 1 \).

**BKKs’ FRAMEWORK**

Fix \( T \in \mathbb{N}^* \). Let \( \{\pi^t\}_{t=1}^T \) be \( T \) permutations in \( \mathcal{S}_n \). (i) **BKKs criterion** is defined as

\[
BKKs_\beta(\theta) = ||Y - X\beta(\theta, X, Y)||_2 + \frac{1}{T} \sum_{t=1}^{T} \left[ 1 - ||\pi^t(Y) - X\beta(\theta, X, \pi^t(Y))||_2 \right]. \tag{4}
\]

(ii) **BKKs procedure** is given for a closed-form family of estimators \( \{\beta(\theta)\}_\theta \) by

\[
\hat{\beta} = \beta(\hat{\theta}, X, Y) \quad \text{with} \quad \hat{\theta} = \arg \min_\theta BKKs_\beta(\theta). \tag{5}
\]

There is no particular meaning behind the name BKK as it was the result of a private joke.

Minimizing the first term w.r.t. \( \theta \) corresponds to the objective “Fit the data as well as possible”. Minimizing the second term achieves the following: “Avoid overfitting by selecting only the intercept in non-informative cases”. Optimizing these two terms simultaneously on the training set \( D \) yields the generalization property of the BKKs procedure.

From the adaptation of the \( ER\sim G \) approach to the linear setting, we can derive several criteria to take into account different underlying structures. Ridge is one of the most popular closed-form family of estimators \( \{\beta^R(\lambda, X, Y)\}_{\lambda>0} \):

\[
\beta^R(\lambda, X, Y) = (X^T X + \lambda I_p)^{-1} X^T Y, \quad \lambda > 0. \tag{6}
\]

From a computational point of view, the matrix inversion is not expensive in our setting as long as the covariance matrix can fully fit on the GPU. Then, the extreme level of parallelization removes the dependency between computational time and the number of features as seen in our experimental results in the Appendix. Otherwise, additional learning schemes (e.g. feature bagging [25], block batch learning [57], Least Mean Squares Solvers [36]) should be implemented.

From [1], we can derive our first criterion by taking \( BKK(\lambda) := BKKs_{\beta^R}(\lambda) \). The BKK procedure is designed to tackle strongly correlated features. The BKKs criterion may be seen as a novel hyperparameter tuning criterion without hold-out validation-set. Experiments for the Ridge family [6] reveal that our approach achieved significantly faster running times over cross-validation for equivalent generalization performances.

A novel family of closed-form estimators is designed to enforce sparsity in the trained model. To this end, we introduce a quasi-sparsifying operator in Definition 1.

**Definition 1.** Let \( \{\beta^S(\lambda, \kappa, \gamma, X, Y)\}_{(\lambda, \kappa, \gamma) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \times \mathbb{R}^p} \) be a family closed-form of estimators defined as follows:

\[
\beta^S(\lambda, \kappa, \gamma, X, Y) = S(\kappa, \gamma)\beta^R(\lambda, XS(\kappa, \gamma), Y), \tag{7}
\]
Parameter initialization

0

10

0

10

0

10

30

0

0

performances. This is not usually the case with other approaches. BKKs procedures remain the same for all the datasets we considered for consistently good prediction even more striking fact is that the initial values (see Table 1 for the main ones) to implement our iterations to achieve convergence [27]. We observed in our experiments that at most a few dozen are highly non-convex, we can still use ADAM without any significant increase in the number of algorithm without a hold-out validationization parameters while simultaneously training the model in a single run of the gradient descent

In this paper, we choose to compute the O

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Definition 2. Let \( \{ \beta^A(\lambda, \kappa, \gamma, \mu, \mathbf{X}, \mathbf{Y}) \}_{(\lambda, \kappa, \gamma, \mu) \in \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R}_+ \times \mathbb{R}} \) be a closed-form family of estimators defined as follows:

\[
\beta^A(\theta, \mathbf{X}, \mathbf{Y}) = S(\mu) \times \beta^R(\lambda, \mathbf{X}, \mathbf{Y}) + (1 - S(\mu)) \times \beta^S(\lambda, \kappa, \gamma, \mathbf{X}, \mathbf{Y}),
\]

where \( \beta^R(\lambda, \mathbf{Y}) \) and \( \beta^S(\lambda, \kappa, \gamma, \mathbf{X}, \mathbf{Y}) \) are defined in [6] and [7] respectively and \( S \) is the sigmoid family (7). By aggregating the families (6) and (7), we can build another closed-form family of estimators (Definition 2). It essentially consists in an interpolation between \( \beta^R \) and \( \beta^S \) estimators, where the level of interpolation is quantified via the introduction of a new regularization parameter \( \mu \in \mathbb{R} \).

Definition 2. Let \( \{ \beta^A(\lambda, \kappa, \gamma, \mu, \mathbf{X}, \mathbf{Y}) \}_{(\lambda, \kappa, \gamma, \mu) \in \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R}_+ \times \mathbb{R}} \) be a closed-form family of estimators defined as follows:

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\]

where \( \beta^R(\lambda, \mathbf{Y}) \) and \( \beta^S(\lambda, \kappa, \gamma, \mathbf{X}, \mathbf{Y}) \) are defined in [6] and [7] respectively and \( S \) is the sigmoid family (7).

From (8), we can derive our last criterion by taking \( \text{ABKK}(\lambda, \kappa, \gamma, \mu) := \text{BKK}_{\beta^A}(\lambda, \kappa, \gamma, \mu) \) which can handle both correlation and sparsity.

Discussion. The BKKs criteria enable us to develop fully automatic procedures to tune regularization parameters while simultaneously training the model in a single run of the gradient descent algorithm without a hold-out 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. Note that the computational complexity of our method grows only arithmetically w.r.t. the number of regularization parameters. In this paper, we choose to compute the BKKs procedures with ADAM. Although \( S\text{BKK} \) and \( \text{ABKK} \) are highly non-convex, we can still use ADAM without any significant increase in the number of iterations to achieve convergence [27]. We observed in our experiments that at most a few dozen iterations are required to compute our procedures resulting in a significantly faster running time. An even more striking fact is that the initial values (see Table 1 for the main ones) to implement our BKKs procedures remain the same for all the datasets we considered for consistently good prediction performances. This is not usually the case with other approaches.

| Optimization parameters | Parameter initialization |
|-------------------------|-------------------------|
| Tolerance               | 10^{-4}                 |
| Max. iter.              | 10^3                    |
| Learning rate           | 0.5                     |
| Adam \( \beta_1 \)      | 0.5                     |
| Adam \( \beta_2 \)      | 0.9                     |

Table 1: Parameters for the BKKs procedures.

\[\text{For } \mu \in \mathbb{R}, S(\mu) \text{ takes values in } (0, 1) \text{ and is actually observed in practice to be close to 0 or 1.}\]
3 Numerical experiments

In this section, we compare our $BKKs$ procedures against cross-validation on Ridge, Lasso and Elastic-net (implemented as RidgeCV, LassoCV and ElasticnetCV in Scikit-learn [43]) on simulated and real datasets. Our procedures are implemented in PyTorch ([41]) on the centered and rescaled response $Y$. Complete details and results can be found in the Appendix. Our Python code is released as an open source package for replication on github/AnonymousSubmissionNeurips2020/.

**Synthetic data.** We generate observations $(x, Y) \in \mathbb{R}^p \times \mathbb{R}$, $p = 80$ s.t. $Y = x^\top \beta^* + \epsilon$, with $\epsilon \sim \mathcal{N}(0, \sigma)$, $\sigma = 10$ 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 $n_{\text{train}} = 100$ and a test-dataset of size $n_{\text{test}} = 1000$. 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.

**Real data.** We test our methods on several commonly used real datasets (UCI [3] and Svmlib [12] repositories). See Appendix for more details. Each selected UCI dataset is splitted randomly into a 80% train-dataset and a 20% test-dataset. We repeat this operation $M = 100$ times to produce $M$ pairs of train/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.

**Performances evaluation criteria.** For each procedure and each train dataset, we construct the corresponding model $\hat{\beta}_{\text{train}}$ based on $D_{\text{train}} = (X_{\text{train}}, Y_{\text{train}})$. The generalization performances of all the considered procedures are evaluated using the hold-out test-sets $D_{\text{test}} = (X_{\text{test}}, Y_{\text{test}})$ by computing their $R^2$-scores as follows

$$R^2(\hat{\beta}_{\text{train}}) = 1 - \frac{\|Y_{\text{test}} - X_{\text{test}} \hat{\beta}_{\text{train}}\|_2}{\|Y_{\text{test}} - \hat{Y}_{\text{test}}\|_2} \leq 1, \quad (9)$$

where $\hat{Y}_{\text{test}}$ is the empirical mean of $Y_{\text{test}}$.

The higher the value of the $R^2$-score, the better the generalization performance of a procedure.

For the $M = 100$ repetitions of each synthetic scenario and each real dataset, we implement all the procedures and record their $R^2$-scores and running times. Boxplots summarize our findings. The empirical mean is represented with a green triangle. To check for statistically significant margin in $R^2$-scores and running times between different procedures, we use the Mann-Whitney test (as detailed in [30] and implemented in scipy [56]). The boxplots highlighted in yellow correspond to the best procedures according to the Mann-Whitney (MW) test.

**Comparison of the different procedures.** Figure[1] and[2] concerns the running times of each procedure respectively on the synthetic datasets and on the real datasets. For the synthetic data, the running times of the $BKKs$ procedures are always significantly smaller than those of the cross-validated benchmark procedures for equivalent to better $R^2$-scores (see Appendix for $R^2$-scores results). For the UCI datasets, the $BKKs$ always obtain the highest $R^2$-scores according to the MW test. For the 20news datasets, the $BKKs$ are always within 0.05 of the best. Figure[2] reveals that the $BKKs$ are always significantly faster to compute for all real datasets according to the MW test. The $BKK$ procedures achieved an average speed-up up to 20 times over the benchmark procedures for the 20news datasets and up to 123 times for the UCI datasets.

**Impact of parameter $T$ and number of iterations.** Figure[3] plots the impact of parameter $T$ on the performances of all the $BKKs$ procedures on the synthetic data.
We observe that the generalization performance ($R^2$-score) increases significantly as soon as $T = 1$. Starting from $T \approx 10$, the $R^2$-score has converged to 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) as compared to the usual risk $ER (T = 0)$. Note that larger values of $T$ are neither judicious nor needed in this approach. It is also a pleasant surprise that the needed number of iterations for ADAM to converge is divided by 3 starting from the first added permutation ($T = 1$). Furthermore, the number of iterations remained stable (below 20) starting from $T = 1$.

We fixed $T = 30$ in our experiments even though $T = 10$ may have been sufficient. Figure 4 contains the boxplots of the number of ADAM iterations for the BKKs procedures on the real datasets. The number of iterations required for convergence is always about a few dozen in our experiments even for $SBKK$ and $ABKK$ which are highly non-convex. This was already observed in other non-convex settings [27].
4 Conclusion and future work

In this paper, we introduce in the regression setting the new ER-G approach based on a different understanding of generalization. Exploiting this idea, criteria and procedures can be derived and implemented with a low computational complexity, via gradient descent applied only once on the train-set without any hold-out validation-set. Within ER-G, additional structures can taken into account without any significant increase in the computational complexity.

By applying ER-G in the specific linear model setting, we developed a new framework in which several new criteria and procedures were derived. The resulting BKKs are compatible with gradient-based optimization methods which fully exploit automatic graph-differentiation libraries (such as pytorch [40] and tensorflow [1]). Noticeably, we ran these experiments using ADAM with a set parameters and stopping criterion that are outside of the range of values commonly found in the literature (far from PyTorch default parameters). Training new models in the BKKs framework requires no tedious initialization. Indeed, we used the same fixed hyperparameters for ADAM and initialization values of the regularization parameters (see Table 1) for all the datasets we considered. Empirical investigations on the BKKs procedures revealed substantial gains in running time while matching the generalization performances of cross-validated benchmark procedures. Moreover, ADAM converges after a very small number of iterations even for non-convex criteria (SBKK and ABKK).

The values of Adam parameters and the striking gain in running time due to the introduction of permutations, especially their impact on the behavior of the gradient descent methods, may deserve further investigation. Other common optimizers (ADAdelta[15], ADAboost [19], RMSProp introduced in [21]) will also be considered as well as techniques commonly used in deep learning (Stochastic Gradient Descent [8], batch learning [22], cycling learning rates [49]). Preliminary results suggest that significant gains in generalization performances should be added to the advantages already highlighted in this paper. In ongoing work, we also adapt the ER-G approach to models with no closed-form estimators and classification tasks. In future work, we will investigate extensions of this method to non-linear models and times series. We believe our approach can also be extended to other types of data (image, text, graphs). Note that our procedures give a promising direction to design fast differentiable optimization methods for the regularization of neural networks as our computational complexity is arithmetic w.r.t. the number of hyperparameters. Deep neural networks produce state-of-the-art results on most machine learning benchmarks [17, 23, 28, 29, 47, 48, 53], but it is not yet the case on the U.C.I benchmark (as described in [18]) for small datasets (less than 1000 observations as shown in [28]). Moreover, training Deep neural networks requires heavy computational resources and manual supervision by experts given the huge number of hyperparameters to tune when working on new problems (see [50]). Our ER-G approach may potentially lead to significant improvements in generalization performance of Deep neural networks and help accelerate their democratization beyond circles of experts.
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