On gradient descent training under data augmentation with on-line noisy copies

Katsuyuki Hagiwara
Faculty of Education, Mie University
1577 Kurima-Machiya-cho, Tsu, 514-8507, Japan
hagi@edu.mie-u.ac.jp

Abstract. In machine learning, data augmentation (DA) is a technique for improving the generalization performance. In this paper, we mainly considered gradient descent of linear regression under DA using noisy copies of datasets, in which noise is injected into inputs. We analyzed the situation where random noisy copies are newly generated and used at each epoch; i.e., the case of using on-line noisy copies. Therefore, it is viewed as an analysis on a method using noise injection into training process by DA manner; i.e., on-line version of DA. We considered the training process under three training situation which are the full-batch training under the sum of squared errors, the full-batch and mini-batch training under the mean squared error. We showed that, in all cases, training for DA with on-line copies is approximately equivalent to the $\ell_2$ regularization training whose regularization parameter corresponds to the variance of injected noise. On the other hand, we showed that DA with on-line copies yields apparent acceleration of training in full-batch under the sum of squared errors and the mini-batch under the mean squared error; i.e., the learning rate is multiplied by the number of noisy copies plus one. The apparent acceleration and regularization effect come from the original part and noise in a copy data respectively. These results are confirmed in a numerical experiment. In the numerical experiment, we found that our result can be applied to usual off-line DA in under-parameterization scenario and can not in over-parametrization scenario. Moreover, we experimentally investigated the training process of neural networks under DA with off-line noisy copies and found that our analysis on linear regression is possible to be applied to neural networks.

Keywords: gradient decent, data augmentation, input noise injection, linear regression, neural networks

1 Introduction

1.1 Background

Data augmentation (DA) is a technique for increasing the number of data and applied in many deep learning applications; e.g., image [18] including major convolutional neural network architectures such as [11] and successors, speech[17]
and natural language processing[12] and so on. Despite of many reports showing the effectiveness of DA, it is not so clear how and why it works.

Generally, DA is known as a strategy for avoiding over-fitting and improving robustness. It is brought about by increasing the number of data which is meaningful in some sense. In image tasks, augmented data are often made by geometric transformation of the original data such as rotation, scale and position changes and so on. DA by these processings may append the new data sets which are possible to appear in prediction phase. In an another viewpoint, we may be able to say that this provides a robustness in terms of change of view of objects. This effect seems to be bias reduction in the generalization error. On the other hand, there is a DA technique that appends new data sets whose inputs are disturbed by noise. This is possible to keep robustness in terms of input changes in some sense; e.g., injection of noise into training inputs to overcome adversarial examples [16]. In addition to the robustness, it is often pointed out that this type of DA provides a regularization effect by referring [1]. Therefore, it may reduce variance in the generalization error. Note that it is not clear the distinction of effect of popular DA techniques using interpolation of data such as [13]. This paper concerns with the DA technique using noise injection into inputs.

1.2 Contribution

In this paper, we study a naive DA technique using noise injection into input data. More precisely, a set of pairs of input disturbed by noise and output for the original input are appended to the original data set. We call this augmented data set a noisy copy of the original data set; i.e., if the number of data is $n$ and the number of copy sets is $K$, the number of whole data under augmentation is $(K + 1)n$, where 1 for the original data. Obviously, this increases the number of data as desired. Note that noise is injected only input data here while there is a method for disturbing also labels[14]. We focus on a training process under DA using a noisy copies. We consider gradient descent (GD) of linear regression. Although this is a quite simple setting, it is often assumed in the analysis related to neural networks and learning, especially in over-parametrization scenario; e.g., [8, 10]. It is also related to the analysis of randomized neural network; e.g. [7]. Unfortunately, it is not straightforward to analyze the GD training process under the above setting of DA even when assuming linear regression. As argued later precisely, this is because weight update at any epoch is correlated to injected noise since noise is injected before training and fixed in training. We refer to this type of noisy copy as off-line noisy copy. Note that this is a natural setting in the context of DA. In this paper, we consider the DA with on-line noisy copy which is randomly drawn and injected at each epoch in training. Indeed, this can be viewed as a kind of noise injection in training process as argued later. Therefore, from another point of view, we analyze a method using noise injection into training process by DA manner; i.e., on-line version of DA.

In this paper, we analyzed the GD update of linear regression under DA with random on-line noisy copies. The main contribution of this paper is as follows.
For the full-batch training under the sum of squared errors, we showed that the GD update at an epoch is approximately equivalent to that of the $\ell_2$ regularization (ridge regression) with $K + 1$ times learning rate, where $K$ is the number of copies.

For the full-batch training under the mean squared error, we showed that the GD update at an epoch is approximately equivalent to that of the $\ell_2$ regularization.

For the mini-batch training under the mean squared error, by ignoring the update term including the square of the learning rate, we showed that the GD update at an epoch is approximately equivalent to that of the $\ell_2$ regularization with $K + 1$ times learning rate.

These results rely on the evaluation based on the expected value in three cases and, additionally, almost surely convergence for the second case. Note that the results here do not depend on whether the scenario is under-parametrization or over-parametrization. In this paper, these results were confirmed in a simple numerical experiment.

In all results, the regularization parameter is proportional to the variance of noise; i.e., the smoothing effect is high when the noise variance is large. This result is intuitively natural while it is explicitly formulated here due to the analysis of a simple linear regression.

On the other hand, apparent acceleration is found in the full-batch training under the sum of squared errors and the mini-batch training. This seems to be natural because, in DA, similar data sets are presented several times in one epoch. However, this is not straightforward since it can not be observed in the full-batch under the mean squared error. Especially, a simple and interpretable result in the mini-batch training is approximately obtained and may not be trivial, in which approximation is valid when the learning rate is small or the update term is small.

In our result, apparent acceleration applies also to DA with off-line noisy copies, which is natural situation of DA. On the one hand, the regularization effect of off-line case can not be specified while it exists as shown in our numerical experiment. It is stochastically determined by noise injected before training. However, the numerical experiment revealed that the regularization effects for both type of DA are very similar in under-parametrization scenario while they are not in over-parametrization scenario. This is because, in the over-parameterization scenario, over-fitting to noise injected before training is serious; i.e., the training process depends largely on the injected noise.

The important point in our result for linear regression is that there is nothing but apparent acceleration and regularization in the effect of DA. And, the regularization effect by DA is important for generalization while the increase in the total number of data by DA may not so important other than apparent acceleration of training. It is worthwhile to note that the original input data and noise in copy contribute to apparent acceleration and effect of regularization respectively.
Furthermore, for layered neural networks, we execute a simple numerical experiment of the full-batch and mini-batch GD training under the mean squared error criterion. We compared the training curves with off-line DA and without DA for each training condition. The results are summarized below.

- In the full-batch training, apparent acceleration is not observed when introducing DA while the effect of regularization is observed.
- In the mini-batch training, both of apparent acceleration and effect of regularization are observed.

The training process of neural networks was very similar to that of linear regression. This may imply that our findings for linear regression are possible to apply to neural networks. Therefore, we need to take this into account in applying DA with off-line noisy copies in the deep learning software such as Keras[3]. On the other hand, it is worthwhile to note that a mixture of apparent acceleration and regularization effect by DA may has a different effect on training process of neural networks. This is because there are bottlenecks in training of neural networks; e.g. [5]. Unlike linear regression, the error surface of neural networks is complex. Because of this, there may exist the effects that are not appeared in the analysis of linear regression; i.e., the other than a simple acceleration and regularization. The investigation of this is left as a future work.

2 Related works

As a work on DA with off-line noisy copies, noise injection into the input is shown to be equivalent to the training under a cost function with a regularization term[1]. It is not argued the introduction of noisy copies and the training process. [21] experimentally showed that, in classification tasks, input noise injection can reduce over-fitting compared to the early stopping and as weight decay. However, there is no analysis on the training process under DA with noisy copies. On the other hand, we considered DA with on-line noisy copies. Indeed, this can be viewed as a kind of noise injection in training process, in which noise is injected into inputs, weights and hidden output; e.g. [15, 9, 2, 4, 16]. In this direction, there are a lot of works to overcome adversarial examples especially in images; e.g., [16]. Among these, [4] is the most relevant work that provided an asymptotic characterization of the training and generalization errors of input noise injection under a random feature model. This is more general than our result since it considered a nonlinear model while it is not considered a difference in training criterion. Also, our result is more simple and interpretable due to the restriction to a linear regression problem. Nevertheless, it may be meaningful for understanding the training process of neural networks since it includes an over-parameterized case; e.g., [10]. Actually, our experimental result showed that the analysis on linear regression seems to be applicable to the training of neural networks. Despite of our simple setting of linear regression, we can not find similar works to ours. This is because the DA based on-line input noise injection may be minor in practices.
3 Gradient descent of linear regression

We consider a linear regression problem. Let $y$ and $X$ be an $n$-dimensional response (output) vector and an $n \times m$ matrix of predictors (inputs). $n$ is the number of data and $m$ is the number of input variables (input dimension). The $i$th element of $y$ is denoted by $y_i$ and the $(i,j)$ element of $X$ is denoted by $x_{i,j}$; i.e. the $i$th data of the $j$th variable. In the context of DA below, $(X, y)$ is referred to as the original data. Let $w$ is an $m$-dimensional weight (coefficient) vector, whose $j$th element is denoted by $w_j$.

We consider gradient descent (GD) under an error function (criterion) on $w$, in which we assume that the loss function is squared error. We define

$$S(w) := \| y - Xw \|^2, \quad (1)$$

which is the sum of squared errors (SSE). For example, GD according to the SSE is an algorithm, in which, by starting from an initial vector $w(0)$, the $t$th step (epoch) of the update is given by

$$w(t) = w(t-1) - \eta \Delta_S(t-1) \quad (2)$$

$$\Delta_S(t-1) := \frac{\partial S(w)}{\partial w} \bigg|_{w=w(t-1)} = -2X^\top (y - Xw(t-1)), \quad (3)$$

where $\eta > 0$ is a constant step size or learning rate. Note that training according to $S(w)$ is the full-batch (FB) training on data $(X, y)$. If the error function is the $\ell_2$ regularized cost function with SSE defined by

$$C(w) := S(w) + \lambda \|w\|^2, \quad (4)$$

the update term is given by

$$\Delta_C(t-1) := \Delta_S(t-1) + 2\lambda w(t-1). \quad (5)$$

4 Data augmentation with noisy copies

4.1 Data augmentation

We now consider a data augmentation (DA) by adding the $K$ pairs of noisy copies of input matrix $X$ and the corresponding output $y$.

Let $k$ and $t$ be indexes of noisy copy and epoch (step) in training, where $k \in \{1, \ldots, K\}$ and $t \in \{0, 1, \cdots \}$. Let $U_{t,k}$ be an $n \times m$ random matrix whose elements are samples from $N(0, \tau^2/n)$, where $\tau > 0$ and $K$ is the number of copies. We define $U_{t,0} = O_{n,m}$, where $O_{n,m}$ is an $n \times m$ zero matrix. We then define

$$X_{K,t} = \begin{bmatrix} X + U_{t,0} \\ X + U_{t,1} \\ \vdots \\ X + U_{t,K} \end{bmatrix}, \quad y_K = \begin{bmatrix} y \\ \vdots \\ y \end{bmatrix}, \quad (6)$$
where $y_K$ consists of a $K + 1$ times repetition of $y$. We also define $y_0 = y$ and $X_0 = X$. We refer to $(X_{0,t}, y_0) = (X, y)$ as the original data. We assume that samples in $\{U_{t,k} \mid 1 \leq k \leq K, 0 \leq t \}$ are mutually independent. For simplicity, we assume that $(X, y)$ and the initial value of the weight vector are non-stochastic. We focus on the stochastic behavior originated from $U_{t,k}$’s.

We explicitly refer to $U_{t,k}$ as on-line noise. On the other hand, we write $U_k = U_{t,k}$ if noisy copies are unchanged during training. This may be usual case of DA. In this case, we refer to $U_k$ as off-line noise.

### 4.2 FB training under SSE

For a weight vector $w$, we define SSE for augmented data by

$$ S_{\text{SSE},K,t}(w) := \|y_K - X_{K,t}w\|^2, \quad (7) $$

where we set $S_{\text{SSE},0,t}(w) := S(w)$; i.e., $S_{\text{SSE}}$ is the SSE for the original data, which is defined in (1). The GD training under $S_{\text{SSE},K,t}$ is a FB training and the GD step is given by

$$ w(t) = w(t - 1) - \eta \Delta_{\text{SSE}}(t - 1) \quad (8) $$

$$ \Delta_{\text{SSE}}(t - 1) := \frac{\partial S_{\text{SSE},K,t}(w)}{\partial w} \bigg|_{w = w(t - 1)}. \quad (9) $$

Since

$$ S_{\text{SSE},K,t}(w) = \|y - Xw\|^2 + \sum_{k=1}^{K} \|y - (X + U_{t,k})w\|^2 $$

$$ = S(w) + \sum_{k=1}^{K} \{\|y - Xw\|^2 + \|U_{t,k}w\|^2 + 2(y - Xw)^\top U_{t,k}w\} $$

$$ = (K + 1)S(w) + \sum_{k=1}^{K} \{\|U_{t,k}w\|^2 + 2y^\top U_{t,k}w - 2w^\top X^\top U_{t,k}w\} $$

holds, by the definition of $S$, we obtain

$$ \Delta_{\text{SSE}}(t - 1) = (K + 1) \left[ \Delta_S(t - 1) + \frac{2}{K + 1} r_{\text{SSE}}(t - 1) \right] \quad (11) $$

$$ r_{\text{SSE}}(t - 1) := \sum_{k=1}^{K} \{U_{t,k}^\top y - (X^\top U_{t,k} + U_{t,k}^\top X - U_{t,k}^\top U_{t,k})w(t - 1)\}, \quad (12) $$

where $\Delta_S$ is defined in (3).
Regardless of on-line or off-line noise, as found in (11), the update term under $S_{K,t}^{\text{SSE}}$ is $K + 1$ times larger than that under $S$ which is SSE for the original data. Since $\Delta_S^{\text{SSE}}$ is multiplied by the learning rate, the effect of adding noisy copies to the training data can be viewed as the use of $(K + 1)\eta$; i.e., the role of increasing the learning rate. Obviously, this can be avoided by normalizing $U_{t,k}$. We discuss this later.

On the other hand, the behavior of $r_S^{\text{SSE}}(t - 1)$ may not so clear. We consider the case of $m \leq n$. Let $\hat{w}$ and $L(X)$ be the least squares estimator under the original data and the linear subspace spanned by the column vector of $X$. $X\hat{w}$ is given by the orthogonal projection of $y$ onto $L(X)$. Then, in the GD training under $S$, $w(t)$ is updated so that $Xw(t)$ moves toward the $X\hat{w}$ on $L(X)$. In case of injecting noise, this happens on $L(X + U_{t,k})$. In other words, injection of $U_{t,k}$ disturbs the convergence to the least squares estimate on $L(X)$. However, generally, we cannot specify whether it improves the generalization performance or not; i.e., it depends on the linear subspace generated by $X + U_{t,k}$.

We consider the influence of $r_S^{\text{SSE}}(t - 1)$. If $U_{t,k} = U_k$ then $r_S^{\text{SSE}}(t - 1)$ is deterministic during the training; i.e., in case of off-line noise. In this case, it is difficult to analyze the probabilistic behavior of this term since $U_k$ is correlated with $w(t - 1)$. However, if $U_{t,k}$ is randomly drawn at each step, $U_{t,k}$ is independent of $w(t - 1)$. This is because $w(t - 1)$ is a function of $\{U_{k,s} | 1 \leq k \leq K, 0 \leq s < t\}$ which is independent of $U_{t,k}, k = 1, \ldots, K$. In this case, by (12), we obtain

$$E_U[t_k, (r_S^{\text{SSE}}(t - 1))] = K\tau^2 w(t - 1)$$

since the elements of $U_{t,k}$ are i.i.d. according to $N(0, \tau^2/n)$, where $E_U[t_k]$ is the expectation with respect to the joint probability distribution of the elements of $U_{t,k}$. Therefore, we obtain

$$E_U[t_k, (r_S^{\text{SSE}}(t - 1))] = (K + 1) \left[ \Delta_S(t - 1) + 2\frac{K\tau^2}{K + 1} w(t - 1) \right].$$

The update rule according to $S_{t,k}^{\text{SSE}}$ is essentially equivalent to the rule under the $\ell_2$ regularized cost which is given by (4), in which the regularization parameter is $\lambda = K\tau^2/(K + 1)$. However, there is a difference in learning rate. In the update under $S_{t,k}^{\text{SSE}}$, it is automatically multiplied by $(K + 1)$; i.e., the learning rate depends on the number of copies. It implies that apparent acceleration occurs and the effect is notable when the number of copies is large.

Since we present a similar data several times at one epoch in the DA setting, apparent acceleration is intuitively understood. However, it is not straightforward as found in the next analysis.

### 4.3 FB training under mean squared errors

We next consider to employ the mean squared error (MSE) instead of the SSE above. It is defined by

$$S_{t,k}^{\text{MSE}}(w) := \frac{1}{(K + 1)n} S_{t,k}^{\text{SSE}}(w),$$

(15)
since the number of data is $(K + 1)n$ in this case. We define $S_{0,t}(w) = \frac{1}{n} S(w)$ that is the MSE for the original data. Note that this is FB training. The GD step for $S_{K,t}^{\text{MSE}}$ is given by

$$w(t) = w(t - 1) - \eta \Delta_{K,t}^{\text{MSE}}(t - 1)$$

(16)

$$\Delta_{K,t}^{\text{MSE}}(t - 1) := \left. \frac{\partial S_{t,k}^{\text{MSE}}(w)}{\partial w} \right|_{w = w(t - 1)}.$$ 

(17)

By (10), we obtain

$$S_{t,k}^{\text{MSE}}(w) = \frac{1}{n} S(w) + \frac{1}{n} \frac{1}{K + 1} \sum_{k=1}^{K} \{ \| U_{t,k} w \|^2 + 2 y^\top U_{t,k} w - 2 w^\top X^\top U_{t,k} w \}.$$ 

(18)

and

$$\Delta_{K,t}^{\text{MSE}}(t - 1) = \frac{1}{n} \Delta_{t} S(t - 1) + \frac{2}{n} \frac{K}{K + 1} r_{K,t}^{\text{MSE}}(t - 1)$$

(19)

$$r_{K,t}^{\text{MSE}}(t - 1) := \frac{1}{K} \sum_{k=1}^{K} \{ U_{t,k}^\top y - (X^\top U_{t,k} + U_{t,k}^\top X - U_{t,k}^\top U_{t,k}) w(t - 1) \}.$$ 

(20)

By the same story as in case of the SSE, we obtain

$$E_{U_{t,k}}[r_{K,t}^{\text{MSE}}(t - 1)] = \tau^2 w(t - 1)$$

(21)

and, therefore,

$$E_{U_{t,k}}[\Delta_{K,t}^{\text{MSE}}(t - 1)] = \frac{1}{n} \Delta_{t} S(t - 1) + 2 \frac{\tau^2}{n} \frac{K}{K + 1} w(t - 1).$$

(22)

The update under $S_{K,t}^{\text{MSE}}$ is essentially equivalent to the update under the $\ell_2$ regularized cost which is given by $S(w)/n + \lambda \| w \|^2$, in which the regularization parameter is $\lambda = \tau^2 K/(K + 1)n$. In this case, the learning rate is not affected by $K$. This is because of the normalization by $K + 1$ in $S_{K,t}^{\text{MSE}}$.

In this case, the other type of the probabilistic behavior makes sense as shown in [4]. We fix $n$ and $m$. Note that all elements of the matrix in $\{ U_{t,k} \mid k = 1, \ldots, K \}$ are mutually independent and those are also mutually independent of the elements of $y$, $X$ and $w(0)$. Let $u_{t,k}^{i,j}$ be the $(i,j)$ element of $U_{t,k}$. Since $u_{t,k}^{i,j}$, $k = 1, \ldots, K$ are i.i.d. according to $N(0, \tau^2/n)$, we obtain

$$\lim_{K \to \infty} \frac{1}{K} \sum_{k=1}^{K} u_{t,k}^{i,j} = 0 \text{ almost surely.}$$

Therefore, $\lim_{K \to \infty} \sum_{k=1}^{K} U_{t,k} = O_{n,m}$ almost surely. On the other hand, we define $Z_{t,k,j_1,j_2} = \sum_{i=1}^{n} u_{t,k}^{i,j_1} u_{t,k}^{i,j_2}$. Note that the elements in $U_{t,k}$ are i.i.d according to $N(0, \tau^2)$ for any $k$ and $t$. Therefore, for any $j_1$ and $j_2$, $Z_{t,k,j_1,j_2}$, $k = 1, \ldots, K$ are i.i.d with $E[Z_{t,k,j_1,j_2}] = 0$ if $j_1 \neq j_2$ and
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with $\mathbb{E}[Z_{t,k,j_1,j_2}] = \tau^2$ if $j_1 = j_2$. Therefore, $\lim_{K \to \infty} \sum_{k=1}^{K} U_{t,k}^\top U_{t,k} = \tau^2 I_m$ almost surely, where $I_m$ is the $m \times m$ identity matrix. As a result, we obtain

$$\lim_{K \to \infty} r_K(t-1) = \tau^2 w(t-1)$$  \hfill (23)

almost surely and, therefore,

$$\lim_{K \to \infty} \Delta_{K}^\text{MSE}(t-1) = \frac{1}{n} \Delta_{\tau}(t-1) + 2 \frac{\tau^2}{n} w(t-1)$$  \hfill (24)

almost surely. By (22), this is consistent with $\mathbb{E}_{U_{t,k}} \left[ \Delta_{K}^\text{MSE}(t-1) \right]$ for a large $K$.

In [4], it appears a different regularization term that comes from a nonlinearity of random feature model.

This result on MSE is important. Since we present a similar data several times at one epoch in the DA setting, the training speed under DA seems to be high compared to presenting only the original data. However, the above result implies that there is no apparent acceleration effect under the MSE setting. This result, together with the result for the previous SSE setting, it may depends on the training criterion. The next question is what happens in the mini-batch (MB) setting which is a standard setting in deep learning.

### 4.4 MB training under MSE

We first consider the mini-batch (MB) training for the original data.

Let $\rho$ be the MB size and $Q$ be the number of MB, where $0 < \rho < n$. We assume that the number of the original data is divisible by $\rho$; i.e., $\rho = n/Q$. We then set $B_q = \{(q-1)\rho + 1, \ldots, q\rho\}$ for $q = 1, \ldots, Q$. $\{B_1, \ldots, B_Q\}$ be a partition of $\{1, \ldots, n\}$; i.e., $\{1, \ldots, n\} = \bigcup_{q=1}^{Q} B_q$ and $B_q \cap B_{q'} = \emptyset$ for $q \neq q'$. $B_q$ is the set of indexes of the $q$th MB of the original data.

Let $x_i$ be the $i$th row vector of $X$. Let $X[B_q]$ be a $\rho \times m$ input sub matrix whose row vectors are $\{x_i \mid i \in B_q\}$ with keeping the order. Let $y[B_q]$ be an output vector whose elements are $\{y_i \mid i \in B_q\}$ with keeping the order. We define

$$S_q^\text{MB}(w) := \frac{1}{\rho} \|y[B_q] - X[B_q]w\|^2$$  \hfill (25)

which is the MSE for the $q$th MB. By setting $w(t,0) = w(t-1)$, the update in the MB training at $t$th epoch is that we repeat

$$w(t,q) = w(t,q-1) - \eta \Delta_q^\text{MB}(t)$$  \hfill (26)

$$\Delta_q^\text{MB}(t) := \left. \frac{\partial S_q^\text{MB}(w)}{\partial w} \right|_{w=w(t,q-1)}$$  \hfill (27)

$$= -2X[B_q]^\top (y[B_q] - X[B_q]w(t,q-1))$$  \hfill (28)
for \( q = 1, \ldots, Q \) and we obtain \( \mathbf{w}(t) = \mathbf{w}(t, Q) \). We define

\[
\Delta_{a, b}^{\text{MB}}(t) := \sum_{j=a}^{b} \Delta_{j}^{\text{MB}}(t). \tag{29}
\]

Then, this process can also be written as

\[
\mathbf{w}(t) = \mathbf{w}(t - 1) - \eta \Delta_{1:Q}^{\text{MB}}(t). \tag{30}
\]

We next consider to apply the MB training for the whole data including noisy copies. To achieve this, we may set \( A_p = \{ (p - 1)\rho, \ldots, p\rho \} \) for \( p = 1, \ldots, P_K \), where \( P_K = Q(K + 1) \). Roughly speaking, at the \( t \)th epoch, we repeat the update by starting from \( \mathbf{w}(t - 1) \) and choosing \( (\mathbf{X}_{t, k}[A_p], \mathbf{y}_{K}[A_p]) \) as the MB. This sequential construction of the MB can also be written by the double-loop in which the outer loop is for \( k \) and inner loop is for the MB. We describe this procedure below.

For a weight vector \( \mathbf{w} \), we define the error function in the MB training by

\[
S_{k, q}^{\text{MB}}(\mathbf{w}) := \frac{1}{\rho} \| \mathbf{y}[B_q] - (\mathbf{X}[B_q] + \mathbf{U}_{t, k}[B_q])\mathbf{w} \|^2, \tag{31}
\]

where \( S_{0, q}^{\text{MB}}(\mathbf{w}) = S_{q}^{\text{MB}}(\mathbf{w}) \). We define the update rule of the MB training under DA as follows. For a fixed \( k \), we define

\[
\mathbf{w}(t, k, q) = \mathbf{w}(t, k, q - 1) - \eta \Delta_{k, q}^{\text{MB}}(t) \tag{32}
\]

\[
\Delta_{k, q}^{\text{MB}}(t) := \left. \frac{\partial S_{k, q}^{\text{MB}}(\mathbf{w})}{\partial \mathbf{w}} \right|_{\mathbf{w}(t, k, q - 1)} \tag{33}
\]

for \( q = 1, \ldots, Q \), where \( \mathbf{w}(t, k, 0) = \mathbf{w}(t, k - 1, Q) \). We define \( \mathbf{w}(t, k) := \mathbf{w}(t, k, Q) \). Now, in this algorithm, by setting \( \mathbf{w}(t, 0, 0) = \mathbf{w}(t - 1) \) and repeating (32) with (33) at each \( k \), we obtain \( \mathbf{w}(t, k) \) for \( k = 0, 1, \ldots, K \) successively. After all, we set \( \mathbf{w}(t) = \mathbf{w}(t, K) \) which is a resulting weight vector at epoch \( t \). To clarify this algorithm, the pseudo code is given in Fig.1.

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**Fig. 1.** Code for the MB training

| Line | Description                                      |
|------|--------------------------------------------------|
| 1.   | \( \mathbf{w}(t, 0, 0) = \mathbf{w}(t - 1) \)  |
| 2.   | for \( (k \in \{0, 1, \ldots, K\}) \) {         |
| 3.   | for \( (q \in \{1, \ldots, Q\}) \) {           |
| 4.   | Obtain \( \mathbf{w}(t, k, q) \) by (32) with (33) |
| 5.   | }                                                |
| 6.   | \( \mathbf{w}(t, k) = \mathbf{w}(t, k, Q) \)    |
| 7.   | }                                                |
| 8.   | \( \mathbf{w}(t) = \mathbf{w}(t, K) \)          |
For simplicity, we write $X[B_q] = X_q$, $U_{t,k}[B_q] = U_{t,k,q}$ and $y[B_q] = y_q$ below. Since

$$\frac{\partial S_{k,q}^{MB}(w)}{\partial w} = - \frac{2}{\rho} (X_q + U_{t,k,q})^\top (y_q - (X_q + U_{t,k,q})w)$$

$$= - \frac{2}{\rho} X_q^\top (y_q - X_qw) - \frac{2}{\rho} U_{t,k,q}^\top (y_q - X_qw)$$

$$+ \frac{2}{\rho} X_q^\top U_{t,k,q}w + \frac{2}{\rho} U_{t,k,q}^\top U_{t,k,q}w$$

holds, we obtain

$$\Delta_{0,q}^{MB}(t) = - \frac{2}{\rho} X_q^\top (y_q - X_qw(t,0,q-1))$$

(35)

for $k = 0$ and

$$\mathbb{E}_{U_{t,k,q}} \left[ \Delta_{k,q}^{MB}(t) \right] = - \frac{2}{\rho} X_q^\top (y_q - X_qw(t,k,q-1)) + \frac{2\tau^2}{n} w(t,k,q-1).$$

(36)

for $k \geq 1$ since $U_{t,k,q}$ and $w(t,k,q-1)$ are mutually independent. We use this fact for simplifying the description below.

We define

$$\Delta_{k,a,b}^{MB}(t) := \sum_{j=a}^{b} \Delta_{k,j}^{MB}(t).$$

(37)

When $k = 0$, by the definition of DA here, the update under the augmented data is the same as that under the original (noiseless) data. We then have

$$w(t,0,q) = w(t,0,q-1) - \eta \Delta_{0,q}^{MB}(t)$$

(38)

by (32), where $w(t,0,0) = w(t-1)$. By this relationship, we obtain

$$w(t,0,Q) = w(t,0,q) - \eta \Delta_{0,q+1:Q}^{MB}$$

(39)

and we then set $w(t,1,0) = w(t,0,Q)$.

For $k \geq 1$, by setting $w(t,k,0) = w(t,k-1,Q)$, we obtain

$$w(t,k,q) = w(t,k-1,Q) - \eta \Delta_{k,1,q}^{MB}(t)$$

(40)

by (32) again. We also obtain

$$w(t,k-1,Q) = w(t,k-1,0) - \eta \Delta_{k-1,1,Q}^{MB}(t),$$

(41)
where \( w(t, k - 1, 0) = w(t, k - 2, Q) \) for \( k \geq 2 \) and \( w(k, 0, 0) = w(t - 1) \) for \( k = 1 \). As a result, we obtain

\[
\begin{align*}
\text{(40)}: & \quad w(t, k, q) = w(t, k - 1, Q) - \eta \Delta_{k,q}^\text{MB}(t) \\
\text{(41)}: & \quad w(t, k, q) = w(t, k - 2, Q) - \eta \Delta_{k-1,q}^\text{MB}(t) - \eta \Delta_{k,q}^\text{MB}(t) \\
\text{(42)}: & \quad \ldots \\
\text{(43)}: & \quad w(t, 1, 0) = w(t, 0, 0) - \eta \sum_{j=1}^{k-1} \Delta_{j+1,q}^\text{MB} - \eta \Delta_{k-1,q}^\text{MB}(t) \\
\text{(44)}: & \quad w(t, k, q) = w(t, k, q - 1) - \eta \Delta_{k,q}^\text{MB}(t) + C \eta
\end{align*}
\]

where the last line comes from (39). This equation links the \( q \)th update of the \( k \)th copy to the \( q \)th update of the original data at epoch \( t \). Therefore, we obtain

\[
\begin{align*}
\text{(45)}: & \quad w(t, k, q) = w(t, 0, q) - C \eta \quad (43)
\end{align*}
\]

by focusing on \( \eta \), where \( C \) is a constant that does not include \( \eta \) but, of course, is related to the other factors. On the other hand, the update equation at \((t, k, q)\) is given by

\[
\begin{align*}
\text{(46)}: & \quad w(t, k, q) = w(t, k, q - 1) - \eta \Delta_{k,q}^\text{MB}(t) + C' \eta
\end{align*}
\]

where \( w(t, k, 0) = w(t, k - 1, Q) \). By (36) and (43), we obtain

\[
\begin{align*}
\mathbb{E}_{U_{t,k q}} \left[ \Delta_{k,q}^\text{MB}(t) \right] = & \frac{1}{\rho} \left\{ -2X_q^\top (y_q - X_y w(t, k, q - 1)) \right\} + \frac{2\tau^2}{n} w(t, k, q - 1) \\
= & \frac{1}{\rho} \left\{ -2X_q^\top (y_q - X_y w(t, 0, q - 1)) \right\} + \frac{2\tau^2}{n} w(t, 0, q - 1) + C' \eta \\
= & \Delta_{0,q}^\text{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) + C' \eta
\end{align*}
\]

for a constant \( C' \). Therefore, by (44), we obtain

\[
\begin{align*}
\mathbb{E}_{U_{t,k q}} [w(t, k, q)] = & \ w(t, k, q - 1) - \eta \left[ \Delta_{0,q}^\text{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right] + C'' \eta^2
\end{align*}
\]
By ignoring the term including $\eta^2$, we obtain

$$E_{U_{t,k,q}}[w(t, k, q)] \simeq w(t, k, q - 1) - \eta \left[ \Delta_{0,q}^{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right]$$

(47)

for $k \geq 1$. The important point of this equation is that the update term is not related to $k$ and it is calculated for the original data that is the case of $k = 0$ in DA. Note that we have

$$w(t, 0, Q) = w(t, 0, 0) - \eta \Delta_{0,1:Q}^{MB}(t) = w(t - 1) - \eta \Delta_{0,1:Q}^{MB}(t)$$

(48)

for $k = 0$. Therefore, by setting $(k, q) = (K, Q)$ and removing the symbol of the expectation, we approximately obtain

$$w(t) = w(t, K, Q)$$

$$\simeq w(t, K, 0) - \eta \sum_{q=1}^{Q} \left[ \Delta_{0,q}^{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right]$$

$$= w(t, K - 1, Q) - \eta \left[ \Delta_{0,1:Q}^{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right]$$

$$\simeq w(t, K - 1, 0) - 2\eta \left[ \Delta_{0,1:Q}^{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right]$$

$$\cdots$$

$$= w(t, 1, 0) - K\eta \left[ \Delta_{0,1:Q}^{MB}(t) + \frac{2\tau^2}{n} w(t, 0, q - 1) \right]$$

$$\simeq w(t, 0, 0) - \eta (K + 1) \Delta_{0,1:Q}^{MB}(t) + K \sum_{q=1}^{Q} \frac{2\tau^2}{n} w(t, 0, q - 1)$$

$$= w(t - 1) - (K + 1)\eta \left[ \Delta_{0,1:Q}^{MB}(t) + \frac{K}{K + 1} \sum_{q=1}^{Q} \frac{2\tau^2}{n} w(t, 0, q - 1) \right],$$

(49)

where the 6th line comes from $U_{t,0} = O_{n,m}$. This implies that the update in the MB training under DA is equivalent to obtaining $w(t) = w(t, Q)$ by

$$w(t, q) = w(t, q - 1) - \eta (K + 1) \left[ \Delta_{0,q}^{MB}(t) + \frac{K}{K + 1} \frac{2\tau^2}{n} w(t, q - 1) \right],$$

(50)

where we set $w(t, 0) = w(t - 1)$. Actually, it is easy to see that this leads to (49). This is the $\ell_2$ regularization training under $S_{MB}^Q(w) + \lambda \|w\|^2$ for the original data, in which the regularization parameter is $\lambda = K\tau^2/(K + 1)n$. However, the learning rate is $(K + 1)\eta$ which is larger than that in the naive training and increases as $K$ increases. Hence, apparent acceleration can be found also in the MB training.
We should mention the fact that this simple result is obtained by ignoring the term including $\eta^2$. This is true if $\eta$ is very small. Additionally, since the term including $\eta^2$ is a function of the update terms, this approximation can be precise when the amount of the update is small. Obviously, such a situation occurs in the later stage of training if the weight vector normally converges. Note that if we turn our attention to neural networks, small amount of update of weights are suggested; e.g., [10].

On the other hand, the MB training updates the weight vector several times at each epoch. Therefore, it seems to be capable of accelerating the training. However, it is not straightforward since the update is made for a part of data, by which it includes a kind of stochastic fluctuation. Nevertheless, our result supports this intuition with a simple and explicit form that is approximately derived under a stochastic evaluation.

5 Numerical experiments

5.1 Example of linear regression

We consider a multiple regression. $x_{i,j}$, $i = 1, \ldots, n$, $j = 1, \ldots, m$ are sampled from $N(0, \sigma_x^2)$ and $y_i = x_{i,1} - x_{i,2} + \varepsilon_i$, where $\varepsilon_i \sim N(0, \sigma^2)$. The number of original data and input variables are set to $n = 20$ and $m = 15$ respectively. This is an under-parametrization scenario while $n$ is relatively small. For DA, we set $Q = 4$, thus $\rho = 5$. In DA, $u_{t,k}^{i,j}$ is sampled from $N(0, \tau^2)$. Note that any sampling here is at random. We set $\sigma_x = 0.5$, $\sigma = 0.2$ and $\tau = 1.0$. The training curves on the original training data under the SSE, MSE and MB based training are shown in Fig. 2. The number of epochs is 1000. The number of noisy copies is $K = 4$ for (a), (b) and (c). For the MB training, we show the result of $K = 1$ in (d). If the two weight updates are the same then their training errors on original data are the same. Therefore, in Fig. 2, we show the transition of the MSE on the original data. In each figure, we show the training curves of the naive GD (GD in the figure), GD with the $\ell_2$ regularization (GD-REG), GD under DA with off-line noisy copies (GD-DA (off-line)) and GD under DA with on-line noisy copies (GD-DA (on-line)). For normalization, we set the learning rate $\eta = 0.001$ in the SSE training, $\eta = 0.001n$ in the MSE training and $\eta = 0.001Q$ the MB training, where $Q$ is the number of mini-batches. By this normalization, for example, the training curves are consistent in (a) and (b) for naive GD. In the regularization method, the values of the learning rate and regularization parameter are set to the values derived in this paper. For example, in the MB training, the learning rate is $(K + 1)\eta$ and $\lambda = K\tau^2/(K + 1)n$.

In Fig. 2, we can observe the following facts.

- In all cases, the training curve under DA with on-line noisy copies is well consistent with that under the $\ell_2$ regularization training except a small fluctuation. This result supports our probabilistic analysis.
- In all cases, the training curve of GD under DA with off-line noisy copies is different from that under the $\ell_2$ regularization training. This is because the
noise and updated weight vector are correlated as explained in the previous section. The difference is notable at the later stage of training while it is not observed in the early steps of training. This is because the correlation is small in this portion; i.e., in an extreme case, at the initial state, they are uncorrelated. And, it becomes larger as epoch increases. Therefore, the degree of the regularization is different for on-line and off-line noise. This determines the error in the later stage of training.

- In (a), (c) and (d), the training curves of GD under DA (both of on-line and off-line) show the steep reduction in the early steps of training. This is caused by a large learning rates that is brought about by the number of copies in DA. It is not observed in (b); i.e., under MSE. Of course, for GD under DA, the error reduction is small at the later stage in training. This is caused by the regularization which avoids the over-training. The degree of over-fitting is controlled by the variance of noise in DA since it exactly corresponds to the regularization parameter.

- By comparing (c) and (d), we can verify that the increase of the number of copies brings us apparent acceleration which is caused by the increase of the learning rate and contributes the early stage of training. On the other hand, in this example, $K/(K+1)$ is 0.8 for $K = 4$ and 0.5 for $K = 1$. Therefore, the corresponding regularization parameter is relatively different and this causes a difference in the training errors at the later stage. This is negligible when $K$ is large.

Our calculation can be applied regardless of the under-parametrized or over-parametrized cases for original data; i.e., $n > m$ or $n < m$. We show the result of the MB training in the over-parametrized case. The setting of the numerical experiment is the same as above except that the learning rate is 0.0001Q (it is smaller), the number of epochs is 3000, $\tau = 2$ and $m = 100$, in which we append 85 irrelevant input variables to the previous input. Since $n = 20 < m$, this is an over-parametrized case. Note that a true relation is included in assumed models here. We show the training curves for the cases of $K = 2$ and $K = 5$ in (a) and (b) of Figure. 3 respectively. The number of whole data (data including noisy copies) is $3n = 60$ for the former and $6n = 120$ for the latter. Therefore, under the DA, the former is the over-parametrized case and the latter is the under-parametrized case. As seen in the figure, the training curves of GD-DA (on-line) for both cases are almost consistent. Since adding on-line noisy copies is equivalent to the $\ell_2$ regularization, DA with noisy copies may be effective for avoiding over-training regardless of the under-parametrization or over-parameterization scenarios. However, the increase in the total number of data by DA may not so important other than the apparent acceleration of training. On the other hand, the regularization effects for both type of DA are very similar in under-parametrization scenario. However, they are not in over-parametrization scenario. This is because, in the over-parameterization scenario, over-fitting to noise injected before training is serious; i.e., the training process depends largely on the injected noise.
Fig. 2. Training curves for naive GD (GD), GD under the $\ell_2$ regularization (GD-REG), GD under DA with off-line noise (GD-DA (off-line)) and GD under DA with on-line noise (GD-DA (on-line)). (a) SSE training, (b) MSE training, (c) MB training ($K = 4$), (d) MB training ($K = 1$).

5.2 Example of neural networks

As pointed out in recent works, wide neural networks can be linearized under the GD training. Therefore, our result on linear regression is possible to be applied to neural networks. We test this through simple numerical examples for real datasets.

We use the two benchmark datasets from UCI repository[6], which are the Auto-MPG (miles per gallon) and SIEC (steel industry energy consumption) datasets. The number of data is 78 for Auto-MPG and 1752 SIEC which are 20[%] and 5[%] of the available data respectively. The architecture of neural network is 4-layer for both datasets, in which the number of nodes at each layer is 8-32-32-1 for Auto-MPG and 6-64-64-1 for SIEC. For both datasets, the activation function is ReLU in the two hidden layers and linear in the output layer. We use a simple Stochastic GD (SGD) training which is implemented in Keras[3] since our purpose is to observe the property of the GD training. The
error function is the MSE with different batch size. The learning rates for both datasets are set to 0.00001 in the MB training and 0.0001 in the FB training. The number of epochs are set to 1000 for Auto-MPG and 500 for SIEC. In Fig. 4, we show the MSE based training curves for 5 runs of a naive SGD (referred to as SGD) and SGD under DA (referred to as SGD-DA) which is off-line DA with $K = 2$, $\tau$ is set to 0.2. Note that the training curves are the MSE errors for the training data; i.e., original data for SGD and augmented data for SGD-DA. We show the results of the MB and FB training. The batch size (BS) in the MB training are 20 for Auto-MPG and 100 for SIEC respectively. Therefore, the results in (a) and (c) correspond to the MB training and those in (b) and (d) correspond to the FB training under the MSE criterion in our analysis. We summarize the result below.

- As seen in (b) and (d) which are the FB settings, the rate of error reduction at the initial portion of training is the same for both cases; i.e., SGD and SGD-DA. On the other hand, the training is suppressed in SGD-DA. This is caused by the regularization effect by DA. Therefore, apparent acceleration of DA can not be observed under the setting of the FB training under the MSE criterion. This is consistent with our result on linear regression.
- As seen in (a) and (c) which are the MB settings, the regularization effect by DA can be observed. Additionally, the steep reduction of error at the initial portion of training is observed for SGD-DA. Thus, apparent acceleration caused by introducing DA is observed. This is also consistent with our result on linear regression.

In case of the MB training of linear regression, DA using noisy copies brings us the effects of regularization and apparent acceleration of training. The latter may not essential in linear regression problems since there is only one global minimum. However, in nonlinear regression problems including layered neural
networks, it affects the convergence property of training since the error surface of neural networks is complex.

6 Conclusions and future works

We analyzed the training process of the GD update for linear regression under DA with on-line noisy copies, in which noise of copy is injected into input. We especially evaluated the average behavior of the training process of the FB training under SSE, MSE and the MB training under MSE. This result was verified in a simple numerical experiment. We also experimentally investigated the effect of DA on neural networks. This numerical experiment suggests that our analysis on linear regression is possible to apply to neural networks. As a future work, we need to analyze the effect of DA with noisy copies on the training process of neural networks. The analysis on the regularization effect
of layered and convolutional neural networks may be followed by [4]. On the other hand, it is worthwhile to note that a mixture of apparent acceleration and regularization effect obtained by DA has a possibility of different effect on training process of neural networks. This is because there are bottlenecks in training of neural networks; e.g., [5]. Because of the complex error surface in neural networks, there is a possibility of the existence of the effect that is not appeared in the analysis of linear regression; i.e., the other than a simple apparent acceleration and regularization. We need to clarify it in the future work.

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References

1. Bishop, C.M. : Training with noise is equivalent to Tikhonov regularization. Neural Computation, 7, 108-116 (1995)
2. Camuto, A., Willetts, M., Şimsékli, U., Roberts, S., Holmes, C. : Explicit Regularisation in Gaussian Noise Injections. NeurIPS2020 (2020)
3. Chollet, F. et al., https://github.com/fchollet/keras (2015)
4. Dhifallah, O., Lu, Y. M. : On the inherent regularization effects of noise injection during training. ICML2021 (2021)
5. Dinh, L., Pascanu, R., Bengio, S., Bengio, Y. : Sharp minima can generalize for deep nets. PMLR2017, 1019-1028 (2017)
6. Dua, D., Graff, C., http://archive.ics.uci.edu/ml (2019)
7. Gallicchio,C., Scardapane, S. : Deep randomized neural networks. arXiv:2002.12287 (2020)
8. Hastie, T., Montanari, A., Rosset, S., Tibshirani, R.J. : Surprises in high-dimensional ridgeless least squares interpolation. arXiv:1903.08560 (2020)
9. Ho, K., Leung, C., Sum, J. : On weight-noise-injection training. ICONIP2008, 919–926 (2008)
10. Jacot, A., Gabriel, F., Hongler, C. : Neural tangent kernel: convergence and generalization in neural networks. In Advances in Neural Information Processing Systems, 8571–8580 (2018)
11. Krizhevsky, A., Sutskever, I., Hinton, G. E. : Imagenet classification with deep convolutional neural networks. NeurIPS2012, 1097–1105 (2012)
12. Li, B., Hou, Y., Che., W. : Data augmentation approaches in natural language processing: A survey. AI Open (2022)
13. Lim, S.H., Erichson, N.B., Utrera, F., Xu, W., Mahoney, M.W. : Noisy Feature Mixup, ICLR2022, arXiv:2110.02180 (2021)
14. Nishi, K., Ding, Y., Rich, A., Höllerer, T. : Augmentation Strategies for Learning with Noisy Labels. CVPR2021, arXiv:2103.02130 (2021)
15. Nitish, S., Hinton, G. E., Alex, K., Ilya, S., Ruslan, S. : Dropout: a simple way to prevent neural networks from overfitting. J. Mach. Learn. Res., 15, 1929–58 (2014).
16. Panda, P., Roy, K. : Implicit adversarial data augmentation and robustness with noise-based learning. Neural Networks, 141, 120-132 (2021)
17. Ramirez, J.M., Montalvo, A., Calvo, J.R. : A survey of the effects of data augmentation for automatic speech recognition systems. CIARP 2019, Lect. Notes Comput. Sci., 11896, 669-678 (2019)
18. Shorten, C., Khoshgoftaar, T.M. : A survey on image data augmentation for deep learning. Journal of Big Data, 6, 1-48 (2019)
19. Smith, S.L., Dherin, B., Barrett, D., De, S. : On the origin of implicit regularization in stochastic gradient descent. ICLR2021 (2021)
20. Zhang, C., Bengio, S., Hardt, M., Recht, B., Vinyals, O. : Understanding deep learning requires rethinking generalization. ICLR2017, arXiv:1611.03530 (2017)
21. Zur, R.M., Jiang, Y., Pesce, L.L., Drukker, K. : Noise injection for training artificial neural networks: A comparison with weight decay and early stopping. Med. Phys., 36, 4810-4818 (2009)