Sign-Constrained Regularized Loss Minimization

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Abstract

In practical analysis, domain knowledge about analysis target has often been accumulated, although, typically, such knowledge has been discarded in the statistical analysis stage, and the statistical tool has been applied as a black box. In this paper, we introduce sign constraints that are a handy and simple representation for non-experts in generic learning problems. We have developed two new optimization algorithms for the sign-constrained regularized loss minimization, called the sign-constrained Pegasos (SC-Pega) and the sign-constrained SDCA (SC-SDCA), by simply inserting the sign correction step into the original Pegasos and SDCA, respectively. We present theoretical analyses that guarantee that insertion of the sign correction step does not degrade the convergence rate for both algorithms. Two applications, where the sign-constrained learning is effective, are presented. The one is exploitation of prior information about correlation between explanatory variables and a target variable. The other is introduction of the sign-constrained to SVM-Pairwise method. Experimental results demonstrate significant improvement of generalization performance by introducing sign constraints in both applications.

Introduction

The problem of regularized loss minimization (e.g. Hastie et al. (2009)) is often described as

$$
\min \ P(w) \ \text{wrt} \ w \in \mathbb{R}^d,
$$

where

$$
P(w) := \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \Phi(X^T w),
$$

$$
X := [x_1, \ldots, x_n] \in \mathbb{R}^{d \times n},
$$

aiming to obtain a linear predictor $\langle w, x \rangle$ for an unknown input $x \in \mathbb{R}^d$. Therein, $\Phi: \mathbb{R}^n \rightarrow \mathbb{R}$ is a loss function which is the sum of convex losses for $n$ examples: $\Phi(z) := \sum_{i=1}^n \phi_i(z_i)$ for $z := [z_1, \ldots, z_n]^T \in \mathbb{R}^n$. This problem covers a large class of machine learning algorithms including support vector machine, logistic regression, support vector regression, and ridge regression.

In this study, we pose sign constraints (Lawson and Hanson, 1995) to the entries in the model parameter $w \in \mathbb{R}^d$ in the unconstrained minimization problem (1). We divide the index set of $d$ entries into three exclusive subsets, $\mathcal{I}_+$, $\mathcal{I}_0$, and $\mathcal{I}_-$, as $\{1, \ldots, d\} = \mathcal{I}_+ \cup \mathcal{I}_0 \cup \mathcal{I}_-$ and impose on the entries in $\mathcal{I}_+$ and $\mathcal{I}_-$,

$$
\text{for } h \in \mathcal{I}_+, \quad w_h \geq 0, \quad \text{for } h' \in \mathcal{I}_-, \quad w_{h'} \leq 0.
$$

Sign constraints can introduce prior knowledge directly to learning machines. For example, let us consider a binary classification task. In case that $h$-th explanatory variable $x_h$ is positively correlated to a binary class label $y \in \{\pm 1\}$, then a positive weight coefficient $w_h$ is expected to achieve a better generalization performance than a negative coefficient, because without sign constraints, the entry $w_h$ in the optimal solution might be negative due to small sample problem. On the other hand, in case that $x_h$ is negatively correlated to the class label, a negative weight coefficient $w_h$ would yield better prediction. If sign constraints were explicitly imposed, then inadequate signs of coefficients could be avoided.

The strategy of sign constraints for generic learning problems has rarely been discussed so far, although there are extensive reports for non-negative least square regression supported by many successful applications including sound source localization (Lin et al., 2004), tomographic imaging (Ma, 2013), spectral analysis (Zhang et al., 2007), hyperspectral image super-resolution (Dong et al., 2016), microbial community pattern detection (Cai et al., 2017), face recognition (Ji et al., 2009; He et al., 2013), and non-negative image restoration (Henrot et al., 2013; Landi and Piccolomini, 2012; Wang and Ma, 2007; Shashua and Hazan, 2005). In most of them, non-negative least square regression is used as an important ingredient of bigger methods such as non-negative matrix factorization (Lee and Seung, 2001; Wang et al., 2017; Kimura et al., 2016; Févotte and Idier, 2011; Ding et al., 2006).

Several efficient algorithms for the non-negative least square regression have been developed. The active set method by Lawson and Hanson (1995) has been widely used in many years, and several work (Kim et al., 2010, 2007; Bierlaire et al., 1991; Portugal et al., 1994; Moré and Toraldo, 1991; Lin and Moré, 1999; Morigi et al., 2007) have accelerated optimization by combining the active set method with the projected gradient approach. Interior point methods (Bellavia et al., 2006; Hönkenschloss et al., 1999; Kanzow and Klug, 2006) have been proposed as an alternative algorithm for non-negative least square regression. However, all of them cannot be applied to generic regularized loss minimization problems.

In this paper, we present two algorithms for the sign-constrained regularized loss minimization problem with
generic loss functions. A surge of algorithms for unconstrained regularized empirical loss minimization have been developed such as SAG (Roux et al., 2012; Schmidt et al., 2016), SVRG (Johnson and Zhang, 2013), Prox-SVRG (Xiao and Zhang, 2014), SAGA (Defazio et al., 2014a), Kaczmarz (Needell et al., 2015), EMGD (Zhang et al., 2013), and Finito (Defazio et al., 2014b). This study focuses on two popular algorithms, Pegasos (Shalev-Shwartz et al., 2011) and SDCA (Shalev-Shwartz and Zhang, 2013). A prominent characteristic of the two algorithms is the fact that they can be expressed as 

$$w_{t+1} := \frac{1}{t}w_t - \frac{1}{t\lambda}X_{A_t}\nabla \Phi(X_{A_t}^\top w_t; A_t).$$

which approximates the objective function $P(w)$. The current solution $w_t$ is moved toward the opposite gradient direction as

$$w_{t+1/2} := w_t - \frac{1}{\lambda t'}\nabla P_t(w_t) = \frac{t - 1}{t}w_t - \frac{1}{k\lambda}X_{A_t}\nabla \Phi(X_{A_t}^\top w_t; A_t).$$

At the projection-onto-ball step, the norm of the solution is shortened to be $\frac{1}{\sqrt{k\lambda\|w_{t+1/2}\|}}$ if the norm is over $\frac{1}{\sqrt{k\lambda\|w_{t+1/2}\|}}$:

$$w_{t+1} := \min \left(1, \frac{\|w_t\|}{\sqrt{k\lambda\|w_{t+1/2}\|}}\right)w_{t+1/2}.$$

### Assumption 2.1

Throughout this paper, the following assumptions are used:

(a) $\Phi(\cdot)$ is a convex function.  
(b) $\frac{1}{n}\Phi(0) \leq r_{\text{loss}}$.  
(c) $\forall s \in \mathbb{R}^n$, $\Phi(s) \geq 0$.  
(d) $\forall i, \|x_i\| \leq R$.

Most of widely used loss functions satisfy the above assumptions. Several examples of such loss functions are described in Table 1. If the hinge loss is chosen, the learning machine is a well-known instance called the support vector machine. If the square error loss is chosen, the learning machine is called the ridge regression. We denote the optimal solution to the constraint problem by $w_* := \arg\min P(w)$. We assume two types of loss functions: $L$-Lipschitz continuous function and $(1/\gamma)$-smooth function. Function $\phi_i : \mathbb{R} \to \mathbb{R}$ is said to be an $L$-Lipschitz continuous function if

$$\forall s, \forall \delta \in \mathbb{R}, \quad |\phi_i(s + \delta) - \phi_i(s)| \leq L|\delta|.$$  

Such functions are often said shortly to be $L$-Lipschitz in this paper. Function $\phi_i : \mathbb{R} \to \mathbb{R}$ is a $(1/\gamma)$-smooth function if its derivative function is $L$-Lipschitz. For an index subset $A \subseteq \{1, \ldots, n\}$ and a vector $v \in \mathbb{R}^n$, let $v_A$ be the subvector of $v$ containing entries corresponding to $A$. Let $X_A$ be a sub-matrix in $X$ containing columns corresponding to $A$. Let $\Phi(\cdot; A) : \mathbb{R}^{|A|} \to \mathbb{R}$ be defined as

$$\Phi(s_A; A) := \sum_{i \in A} \phi_i(s_i).$$

### 3 Sign-Constrained Pegasos

In the original Pegasos algorithm (Shalev-Shwartz et al., 2011), $\phi_i$ is assumed to be the classical hinge loss function (See Table 1 for the definition). Each iterate consists of three steps: the mini-batch selection step, the gradient step, and the projection-onto-ball step. Mini-batch selection step chooses a subset $A_t \subseteq \{1, \ldots, n\}$ from $n$ examples at random. The cardinality of the subset is predefined as $|A_t| = k$. Gradient step computes the gradient of

$$P_t(w) := \frac{1}{2}\|w\|^2 + \frac{1}{k}\Phi(X_{A_t}^\top w; A_t).$$
### Table 1: Loss functions and their properties. Suppose $0 \leq \gamma \leq 1$. Let $y := [y_1, \ldots, y_n]^\top$.

| Name                  | Definition                                                                 | Label    | Type               | $r_{\text{loss}}$ |
|-----------------------|---------------------------------------------------------------------------|----------|--------------------|--------------------|
| Classical hinge loss  | $\phi_i(s) := \max(0, 1 - y_i s)$                                        | $y_i \in \{\pm 1\}$ | 1-Lipschitz        | 1                  |
| Smoothed hinge loss   | $\phi_i(s) := \begin{cases} 1 - y_i s - 0.5 \gamma & \text{if } y_i s \in (-\infty, 1 - \gamma], \\ (1 - y_i s)^2/(2\gamma) & \text{if } y_i s \in (1 - \gamma, 1), \\ 0 & \text{if } y_i s \in [1, +\infty). \end{cases}$ | $y_i \in \{\pm 1\}$ | $(1/\gamma)$-smooth | $1 - \frac{\gamma}{2}$ |
| Logistic loss         | $\phi_i(s) := \log(1 + \exp(-y_i s))$                                    | $y_i \in \{\pm 1\}$ | 0.25-smooth        | $\log(2)$          |
| Square error loss     | $\phi_i(s) := 0.5(s - y_i)^2$                                            | $y_i \in \mathbb{R}$ | 1-smooth           | $\|y\|^2/(2n)$     |
| Absolute error loss   | $\phi_i(s) := |s - y_i|$                                                | $y_i \in \mathbb{R}$ | 1-Lipschitz        | $\|y\|_1/n$        |

### Algorithm 1: Generic Sign-Constrained Pegasos

**Require:** Data matrix $X \in \mathbb{R}^{d \times n}$, loss function $\Phi : \mathbb{R} \to \mathbb{R}$, regularization parameter $\lambda \in \mathbb{R}$, sign constraint parameter $c \in \{\pm 1\}^d$, and mini-batch size $k$.

1: begin 
2: $w_1 := 0_d$: \{Initialization\} 
3: for $t := 1, \ldots, T$ do 
   4: Choose $A_t \subseteq \{1, \ldots, n\}$ uniformly at random such that $|A_t| = k$.
   5: $w_{t+1/3} := \frac{1}{n} X A_t \nabla \Phi(X_{A_t} w_{t-1}; A_t)$;
   6: $w_{t+2/3} := w_{t+1/3} + c \odot (-c \odot w_{t+1/3})$;
   7: $w_{t+1} := \min \left(1, \sqrt{\frac{\lambda}{r_{\text{loss}}}} \|w_{t+2/3}\|^{-1}\right) w_{t+2/3}$;
8: end for 
9: return $\bar{w} := \sum_{t=1}^{T} w_t / T$;
10: end.

The projection-onto-ball step plays an important role in getting a smaller upper-bound of the norm of the gradient of the regularization term in the objective, which eventually reduces the number of iterates to attain an $\epsilon$-approximate solution (i.e., $P(\bar{w}) - P(w_*) \leq \epsilon$).

In the algorithm developed in this study, we simply insert between those two steps, a new step that corrects the sign of each entry in the current solution $w$ as

$$
\begin{align*}
w_h &\leftarrow \begin{cases}
\max(0, w_h) & \text{for } h \in \mathcal{I}_+,
\min(0, w_h) & \text{for } h \in \mathcal{I}_-,
\end{cases} \\
w_h &\quad \text{for } h \in \mathcal{I}_0,
\end{align*}
$$

which can be rewritten equivalently as $w \leftarrow w + c \odot (-c \odot w)_+$ where the operator $(-)_{+}$ is defined as $\forall x \in \mathbb{R}^d$, $(x)_+ := \max(0, x)$.

The algorithm can be summarized as Algorithm 1. Here, the loss function is not limited to the classical hinge loss. In the projection-onto-ball step, the solution is projected onto $\sqrt{\frac{\lambda}{r_{\text{loss}}}}$-ball instead of $(1/\sqrt{\lambda})$-ball to handle more general settings. Recall that $r_{\text{loss}} = 1$ if $\phi_i$ is the hinge loss employed in the original Pegasos. It can be shown that the objective gap is bounded as follows.

### Theorem 1

Consider Algorithm 1. If $\phi_i$ are $L$-Lipschitz continuous, it holds that

$$
\mathbb{E}[P(\bar{w})] - P(w_*) \leq \left(\sqrt{r_{\text{loss}} \lambda} + LR\right)^2 \frac{1 + \log(T)}{\lambda T},
$$

See Subsection A.1 for proof of Theorem 1. This bound is exactly same as the original Pegasos, yet Algorithm 1 contains the sign correction step.

### 4 Sign-Constrained SDCA

The original SDCA is a framework for the unconstrained problems (1). In SDCA, a dual problem is solved instead of the primal problem. Namely, the dual objective is maximized in an iterative fashion with respect to the dual variables $\alpha := [\alpha_1, \ldots, \alpha_n]^\top \in \mathbb{R}^n$. The problem dual to the unconstrained problem (1) is given by

$$
\min_{\alpha \in \mathbb{R}^n} D(\alpha) \text{ wrt } \alpha \in \mathbb{R}^n,
$$

where

$$
D(\alpha) := -\frac{\lambda}{2} \left\| \frac{1}{\lambda n} X \alpha \right\|^2 - \frac{1}{n} \Phi^*(-\alpha).
$$

To find the maximizer of $D(\alpha)$, a single example $i$ is chosen randomly at each iterate $t$, and a single dual variable $\alpha_i$ is optimized with the other $(n - 1)$ variables $\alpha_1, \ldots, \alpha_{i-1}, \alpha_{i+1}, \ldots, \alpha_n$ frozen. If we denote by $\alpha^{(t-1)} \in \mathbb{R}^n$ the value of the dual vector at the dual iterate (t - 1), the dual vector is updated as $\alpha^{(t)} := \alpha^{(t-1)} + \Delta \alpha e_i$ where $\Delta \alpha \in \mathbb{R}$ is determined so that $\Delta \alpha \in \argmax_{\Delta \alpha \in \mathbb{R}} D_t(\Delta \alpha; \omega^{(t-1)})$ where

$$
\omega^{(t-1)} = \frac{1}{n} X \alpha^{(t-1)}
$$

and

$$
D_t(\Delta \alpha; \omega) := -\frac{\lambda}{2} \left\| \omega + \frac{\Delta \alpha}{\lambda n} x_i \right\|^2 - \frac{1}{n} \phi_i^*(-\alpha_i^{(t-1)} - \Delta \alpha).
$$

In case of the hinge loss, the maximizer of $D_t(\cdot; \omega^{(t-1)})$ can be found within $O(d)$ computation. The primal variable $\omega^{(t)}$ can also be maintained within $O(d)$ computation by $\omega^{(t)} := \omega^{(t-1)} + \frac{\Delta \alpha}{\lambda n} x_i$. 

3
Now let us move on the sign-constrained problem. In addition to Algorithm 1 that is derived from Pegasos, we present another algorithm based on SDCA for solving the minimizer of $P(w)$ subject to the sign constraint $c \odot w \geq 0_d$. Like Algorithm 1 that has been designed by inserting the sign correction step into the original Pegasos iterate, the new algorithm has been developed by simply adding the sign correction step in each SDCA iterate. The resultant algorithm is described in Algorithm 2.

For some loss functions, maximization at step 5 in Algorithm 2 cannot be given in a closed form. Alternatively, step 4 can be replaced to

$$
4: \quad \Delta \alpha := s, \quad \text{where} \quad s := \text{Clip}_{[0, s_{\text{lb}}]}\left(\frac{1}{2} + \frac{z(t)\alpha_i + \phi_i^+(z(t)) - \phi_i^-(-\alpha_i) + \phi_i(z(t))}{\gamma q^2} \right) s_{\text{lb}}.
$$

Therein, we have defined $s_{\text{lb}} := \lambda n \gamma / (\lambda n \gamma + R^2)$, $z(t) := \langle w(t-1), x_i \rangle$, $q^2 := -\nabla \phi_i^+(z(t)) - \alpha_i(t-1)$, and $\text{Clip}_{[a, b]}(x) := \max(a, \min(b, x))$. See Subsection A.4 for derivation of (16).

We have found the following theorem that states the required number of iterates guaranteeing the expected primal objective gap below a threshold $\epsilon$ under the sign constraints.

**Theorem 2.** Consider Algorithm 2. In case that $\phi_i$ are $L$-Lipschitz continuous (i.e. (6)), it holds that $\text{E}[P(\tilde{w})] - P(w_*) \leq \epsilon$ if $T$ and $T_0$ are specified so that

$$
T_0 \geq \frac{4G}{\lambda \epsilon} \max \left\{ 0, \left( n \log \frac{2mn \log G}{\epsilon} \right) \right\}
$$

and

$$
T \geq T_0 + \max \left\{ n, \frac{G}{\lambda \epsilon} \right\}
$$

where $G := 4R^2L^2$. If $\phi_i$ are hinge loss functions, then $G := R^2L^2$. In case that $\phi_i$ are $(1/\gamma)$-smooth, $\text{E}[P(\tilde{w})] - P(w_*) \leq \epsilon$ is established if

$$
T > T_0 \geq \left( n + \frac{R^2}{\lambda \gamma} \right) \log \left( \left( n + \frac{R^2}{\lambda \gamma} \right) \frac{T_0}{T_0 \epsilon} \right).
$$

See Subsections A.6 for proof of Theorem 2. Theorem 2 suggests that the convergence rate of Algorithm 2 is not deteriorated compared to the original SDCA in both cases of $L$-Lipschitz and smooth losses, despite insertion of the sign correction step.

### 5 Multiclass Classification

In this section, we extend our algorithms to the multi-class classification setting of $m$ classes. Here, the model parameter is a $W \in \mathbb{R}^{d \times m}$ instead of a vector $w \in \mathbb{R}^d$. The loss function for each example $x_i \in \mathbb{R}^d$ is of an $m$-dimensional vector. Here, the prediction is supposed to be done by taking the class with the maximal score among $s_1 := \langle w_1, x \rangle, \ldots, s_m := \langle w_m, x \rangle$. Here, without loss of generality, the set of the class labels are given by $\mathcal{Y} := \{1, \ldots, m\}$. Several loss functions $\phi_i^m : \mathbb{R}^m \rightarrow \mathbb{R}$ are used for multiclass classification as follows.

- **Soft-max loss:**

  $$
  \phi_i^m(s) := \log \left( \sum_{y \in \mathcal{Y}} \exp(s_y - s_y) \right)
  $$

  Therein, $y_i$ is the true class label of $i$-th example.

- **Max-hinge loss:**

  $$
  \phi_i^m(s) := \max_{y \in \mathcal{Y}} (s_y - s_y + \delta_{y,y_i}).
  $$

- **Top-k hinge loss** (Lapin et al., 2015):

  $$
  \phi_i^m(s) := \frac{1}{k} \sum_{j=1}^k \left( \langle I - 1e_{y_i}, s + 1 - e_{y_j} \rangle \right).
  $$

  Therein, $x_{[j]}$ denotes the $j$-th largest value in a vector $x \in \mathbb{R}^m$.

The objective function for learning $W \in \mathbb{R}^{d \times m}$ is defined as

$$
P^m(W) := \frac{\lambda}{2} \lVert W \rVert_F^2 + \frac{1}{n} \sum_{i=1}^n \phi_i^m(W^\top x_i).
$$

The learning problem discussed is minimization of $P^m(W)$ with respect to $W$ subject to sign constraints

$$
\forall (h, j) \in \mathcal{E}_+, \quad W_{h,j} \geq 0,
$$

$$
\forall (h', j') \in \mathcal{E}_- \quad W_{h',j'} \leq 0,
$$

with two exclusive set $\mathcal{E}_+$ and $\mathcal{E}_-$ such that

$$
\mathcal{E}_+ \cup \mathcal{E}_- \subseteq \{(h, j) \in \mathbb{N}^2 | h \in [1,d], j \in [1,m]\}.
$$

Introducing $C \in \{0, \pm 1\}^{d \times m}$ as

$$
C_{h,j} := \begin{cases} +1 & \text{for } (h, j) \in \mathcal{E}_+, \\ -1 & \text{for } (h, j) \in \mathcal{E}_-, \\ 0 & \text{o.w.} \end{cases}
$$

the feasible region can be expressed as

$$
\mathcal{S}^m := \{ W \in \mathbb{R}^{d \times m} | C \odot W \geq O_{d \times m} \}.
$$
The goal is here to develop algorithms that find

$$W^*_t := \arg \min_{W \in S^n} P^m(W).$$

(28)

Define $$\Phi^m(\cdot; A) : \mathbb{R}^{m \times k} \to \mathbb{R}$$ as

$$\Phi^m(S_A; A) := \sum_{i \in A} \phi^m_i(s_i)$$

(29)

where $$S_A$$ is the horizontal concatenation of columns in $$S := [s_1, \ldots, s_n] \in \mathbb{R}^{m \times n}$$ selected by a minibatch $$A$$. We here use the following assumptions: $$\Phi^m(\cdot)$$ is a convex function; $$\Phi^m(O) \leq n_{\text{loss}}; \forall S \in \mathbb{R}^{m \times n}, \Phi^m(S) \geq 0; \forall i, \|s_i\| \leq R.$$

By extending Algorithm 1, an algorithm for minimization of $$P^m(W)$$ subject to the sign constraints can be developed as described in Algorithm 3.

The SDCA-based learning algorithm can also be developed for the multiclass classification task. In the algorithm, the dual variables are represented as a matrix $$A := [a_1, \ldots, a_n] \in \mathbb{R}^{m \times n}$$. At each iterate $$t$$, one of $$n$$ columns, $$a_i$$, is chosen at random instead of choosing one of a dual variable to update the matrix as $$A^{(t)} := A^{(t-1)} + \Delta a e_i^T$$ where we have used the iterate number ($$t$$) as the superscript of $$A$$. To determine the value of $$\Delta a$$, the following auxiliary function is introduced:

$$D_t(\Delta a; W) := -\frac{\|x_i\|^2}{2\lambda^2 n} \|\Delta a\|^2 - \langle W^r x_i, \Delta a \rangle - \phi_i^*(r - \phi_i^{(t-1)} - \Delta a).$$

(30)

For both algorithms (Algorithms 3 and 4), we can bound the required number of iterations similar to those presented in Theorems 1 and 2.

6 Experiments

In this section, experimental results are reported in order to illustrate the effects of the sign constraints on classification and to demonstrate the convergence behavior.

6.1 Prediction Performance

The pattern recognition performance of the sign-constrained learning was examined on two tasks: Escherichia coli (E. coli) prediction and protein function prediction.

E. coli Prediction The first task is to predict E. coli counts in river water. The E. coli count has been used as an indicator for fecal contamination in water environment in many parts of the world (Scott et al., 2002). In this experiment, the data points with E. coli counts over 500 most probable number (MPN)/100 mL are assigned to positive class, and the others are negative. The hydrological and water quality monitoring data are used for predicting E. coli counts to be positive or negative.

For ensuring the microbial safety in water usage, it is meaningful to predict E. coli counts on a real-time basis. The concentration of E. coli in water, which is measured by culture-dependent methods (Kobayashi et al., 2013), has been used to monitor the fecal contamination in water environment, and has been proved to be effective to prevent waterborne infectious diseases in varied water usage styles. On the other hand, the real-time monitoring of E. coli has not yet been achieved. It takes at least ten hours to obtain E. coli counts by culture-dependent methods, and also at least several hours are needed to measure the concentration of E. coli by culture-independent methods (Ishii et al., 2014b,a), such as polymerase chain reaction. Since it is possible to measure the some of the hydrological and water quality data with real-time sensors, the real-time prediction of E. coli counts will be realized if the hydrological and water quality data are available for the E. coli count prediction.

Many training examples are required to obtain a better generalization performance. A serious issue, however, is that measuring the concentration of E. coli is time-consuming and the cost of reagents is expensive. We here demonstrate that this issue can be relaxed by exploiting the domain knowledge hoarded in the field of water engineering.

The hydrological and water quality data contain nine explanatory variables, WT, pH, EC, SS, DO, BOD, TN, TP, and flow rate. The explanatory variable pH is divided into two variables, pH$^+$, $\leq \text{max}(0, \text{pH} - 7)$ and pH$^-$, $\leq \text{max}(0, 7 - \text{pH})$. It is well-known, in the field of water engineering, that E. coli...
is increased, as WT, EC, SS, BOD, TN, and TP are larger, and as pH\textsuperscript{+}, pH\textsubscript{-}, DO, and the flow rate are smaller. From this fact, we restrict the sign of entries in the predictor parameter \( w \) as follows.

- Coefficients \( w_h \) of six explanatory variables, WT, EC, SS, BOD, TN, and TP must be non-negative.
- Coefficients \( w_h \) of four explanatory variables, pH\textsuperscript{+}, pH\textsubscript{-}, DO, flow rate must be non-positive.

We actually measured the concentrations of \textit{E. coli} 177 times from December 5th, 2011 to April 17th, 2013. We obtained 177 data points including 88 positives and 89 negatives. We chose ten examples out of 177 data points at random to use them for training, and the other 167 examples were used for testing. The prediction performance is evaluated by the precision recall break-even point (PRBEP) (Joachims, 2005) and the ROC score. We compared the classical SVM with the sign-constrained SVM (SC-SVM) to examine the effects of sign constraints. We repeated this procedure 10,000 times and obtained 10,000 PRBEP and 10,000 ROC scores.

SC-SVM achieved significant improvement compared to the classical SVM. SC-SVM achieved PRBEP and ROC score of 0.808 and 0.863 on average over 10,000 trials, whereas those of the classical SVM were 0.757 and 0.810, respectively. The difference from the classical SVM on each trial is plotted in the histograms of Figure 1. Positive improvements of ROC scores were obtained in 8,932 trials out of 10,000 trials, whereas ROC scores were decreased only for 796 trials. For PRBEP, positive improvements were obtained on 7,349 trials, whereas deteriorations were observed only on 1,069 trials.

### Protein Function Prediction

In the field of molecular biology, understanding the functions of proteins is positioned as a key step for elucidation of cellular mechanisms. Sequence similarities have been a major mean to predict the function of an unannotated protein. At the beginning of this century, the prediction accuracy has been improved by combining sequence similarities with discriminative learning. The method, named SVM-Pairwise (Liao and Noble, 2003), uses a feature vector that contains pairwise similarities to annotated protein sequences. Several other literature (Liu et al., 2014; Ogul and Mumcuoglu, 2006; Lanckriet et al., 2004b,a) have also provided empirical evidences for the fact that the SVM-Pairwise approach is a powerful framework. Basically, if \( n \) proteins are in a training dataset, the feature vector has \( n \) entries, \( x_1, \ldots, x_n \). If we suppose that the first \( n_+ \) proteins in the training set are in positive class and the rest are negative, then the first \( n_+ \) similarities \( x_1, \ldots, x_{n_+} \) are sequence similarities to positive examples, and \( x_{n_++1}, \ldots, x_n \) are similarities to negative examples. The \( n \)-dimensional vectors are fed to SVM and get the weight coefficients \( w := [w_1, \ldots, w_n]^T \).

Then, the prediction score of the target protein is expressed as

\[
\sum_{i=1}^{n_+} w_i x_i + \sum_{i'=n_++1}^{n} w_i x_i. \tag{31}
\]

The input protein sequence is predicted to have some particular cellular function if the score is over a threshold. It should be preferable that the first \( n_+ \) weight coefficients \( w_1, \ldots, w_{n_+} \) are non-negative and that the rest of \( (n-n_+) \) weight coefficients \( w_{n_++1}, \ldots, w_n \) are non-positive. The SVM-Pairwise approach does not ensure those requirements. Meanwhile, our approach is capable to explicitly impose the constraints of

\[
w_1 \geq 0, \ldots, w_{n_+} \geq 0, \quad \text{and} \quad w_{n_++1} \leq 0, \ldots, w_n \leq 0. \tag{32}
\]

This approach was applied to predict protein functions in \textit{Saccharomyces cerevisiae} (\textit{S. cerevisiae}). The annotations of the protein functions are provided in MIPS Comprehensive Yeast Genome Database (CYGD). The dataset contains 3,583 proteins. The Smith-Waterman similarities available from \url{https://noble.gs.washington.edu/proj/sdp-svm/} were used as sequence similarities among the proteins. The number of categories was 12. Some proteins have multiple cellular functions. Indeed, 1,343 proteins in the dataset have more than one function. From this reason, we pose 12 independent binary classification tasks instead of a single multi-class classification task. 3,583 proteins were randomly split into half to get two datasets. The one was used for training, and the other was for testing. For 12 classification tasks, we repeated this procedure 100 times, and we obtained 100 ROC scores.

Table 2 reports the ROC scores averaged over 100 trials and the standard deviations for 12 binary classification tasks. The sign constraints significantly surpassed the classical training for all 12 tasks. Surprisingly, we observed that the ROC score.
of SC-SVM is larger than that of the classical SVM in every trial.

6.2 Convergence

We carried out empirical evaluation of the proposed optimization methods, the sign-constrained Pegasos (SC-Pega) and the sign-constrained SDCA (SC-SDCA), in order to illustrate the convergence of our algorithms to the optimum. For SC-Pega, we set the mini-batch size to $k = 10$ and $k = 100$. In this experiments, we used the smoothed hinge loss with $\gamma = 0.01$ and $\lambda = 1/n$. We used three datasets; Covtype ($n = 581,012$ and $d = 54$), W8a ($n = 49,749$ and $d = 300$), and Phishing ($n = 11,055$ and $d = 68$). The three datasets are for binary classification and available from LIBSVM web site (https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/).

Figure 2 depicts the primal objective gap against epochs, where the primal objective gap is defined as $P(w) - P(w_*)$. As expected in theoretical results, SC-SDCA converged to the optimum faster than SC-Pega except on the dataset Phishing. No significant difference between different mini-batch sizes is observed.

7 Conclusions

In this paper, we presented two new algorithms for minimizing regularized empirical loss subject to sign constraints. The two algorithms are based on Pegasos and SDCA, both of which have a solid theoretical support for convergence. The sign-constrained versions, named SC-Pega and SC-SDCA, respectively, enjoy the same convergence rate as the corresponding original algorithms. The algorithms were demonstrated in two applications. The one is posing sign constraints according to domain knowledge, and the other is improving the SVM-Pairwise method by sign constraints.

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A Proofs and Derivations

A.1 Proof of Theorem 1

Shalev-Shwartz et al. (2011) have used the following lemma, given below, to obtain the bound.

**Lemma A.1** (Hazan et al. (2007)). Let \( f_1, \ldots, f_T \) be a sequence of \( \lambda \)-strongly convex functions. Let \( \mathcal{C} \) be a closed convex set and define \( \Pi_{\mathcal{C}}(w) := \text{argmin} \| w' - w \| \). Let \( w_1, \ldots, w_{t+1} \) be a sequence of vectors such that \( w_1 \in \mathcal{C} \) and for \( t \geq 1 \), \( w_{t+1} := \Pi_{\mathcal{C}}(w_t - \nabla f_t(\lambda t)) \). Assume that \( \forall t \in \mathbb{N}, \| \nabla f_t \| \leq G \). Then, for \( \forall u \in \mathcal{C} \), it holds that

\[
\frac{1}{T} \sum_{t=1}^{T} f_t(w_t) \leq \frac{1}{T} \sum_{t=1}^{T} f_t(u) + \frac{(1 + \log(T))G^2}{2\lambda T}. \tag{33}
\]

We, too, have used Lemma A.1 to obtain Theorem 1 for our sign-constrained learning problem (5). To this end, we find the following lemma.

**Lemma A.2.** Let \( \mathcal{B} \) be \( \frac{r_{\text{loss}}}{\sqrt{\lambda}} \)-ball defined as

\[
\mathcal{B} := \left\{ w \in \mathbb{R}^d \mid \| w \| \leq \sqrt{\frac{r_{\text{loss}}}{\lambda}} \right\}. \tag{34}
\]

and \( \mathcal{S} \) be the set defined in (3). Then, the intersection of the two sets are closed and convex. It holds that

\[
w_{t+1} = \Pi_{\mathcal{B} \cap \mathcal{S}} \left( w_t - \frac{1}{\lambda t} \nabla P_t(w_t) \right) \tag{35}
\]

for \( \forall t \in \mathbb{N} \). Furthermore, the optimal solution \( w_* := \text{argmin}_{w \in \mathcal{S}} P(w) \) is in the intersection of the two sets. Namely,

\[
w_* \in \mathcal{B} \cap \mathcal{S}. \tag{36}
\]

See Subsection A.2 for proof of Lemma A.2. The above lemma suggests that the setting of \( f_t := P_t \), \( \mathcal{C} := \mathcal{B} \cap \mathcal{S} \) and \( u := w_* \) fulfills the assumptions of Lemma A.1. An upper bound of the norm of the gradient of \( f_t \) is given by

\[
\| \nabla f_t(w_t) \| = \| \nabla P_t(w_t) \| \leq \sqrt{r_{\text{loss}} \lambda + LR}. \tag{37}
\]

See Subsection A.3 for derivation of (37). By setting \( G = \sqrt{r_{\text{loss}} \lambda + LR} \), Theorem 1 is established.

A.2 Proof of Lemma A.2

**Lemma A.2** states the following three claims.

- \( \mathcal{B} \cap \mathcal{S} \) is a closed and convex set.
- (35) is hold.
- (36) is hold.

Apparently, \( \mathcal{B} \cap \mathcal{S} \) is a closed and convex set because the both sets are closed and convex. We shall show (35) and then (36).

**Proof of (35)** To prove (35), it suffices to show the projection from a point \( z \in \mathbb{R}^d \) onto the set \( \mathcal{B} \cap \mathcal{S} \) is given by

\[
\Pi_{\mathcal{B} \cap \mathcal{S}}(z) = \min \left\{ 1, \sqrt{\frac{r_{\text{loss}}}{\lambda \| \Pi_{\mathcal{S}}(z) \|} } \right\} \Pi_{\mathcal{S}}(z). \tag{38}
\]

The projection problem can be expressed as

\[
\min \frac{1}{2} \| x - z \|^2 \quad \text{wrt} \quad x \in \mathbb{R}^d \tag{39}
\]

subject to \( \| x \| \leq r_{\text{loss}} / \lambda, ~ c \odot x \geq 0_d \).

With non-negative dual variables \( \beta \in \mathbb{R}^d \) and \( \eta \in \mathbb{R}_+ \), the Lagrangian function is given by

\[
\mathcal{L}_{\mathcal{B} \cap \mathcal{S}}(x, \beta, \eta) := \frac{1}{2} \| x - z \|^2 - \langle \beta, c \odot x \rangle + \frac{\eta}{2} (\| x \|^2 - \frac{r_{\text{loss}}}{\lambda}). \tag{40}
\]

Let \( (x_*, \beta_*, \eta_*) \) be the saddle point of \( \min_{x} \max_{\beta, \eta} \mathcal{L}_{\mathcal{B} \cap \mathcal{S}}(x, \beta, \eta) \). Then, \( x_* = \Pi_{\mathcal{B} \cap \mathcal{S}}(z) \). At the saddle point, it holds that \( \nabla_x \mathcal{L}_{\mathcal{B} \cap \mathcal{S}} = 0 \), yielding

\[
x = \frac{1}{\eta + 1} (z + c \odot \beta). \tag{41}
\]

The dual objective is written as

\[
\mathcal{D}_{\mathcal{B} \cap \mathcal{S}}(\beta, \eta) = \min_{x} \mathcal{L}_{\mathcal{B} \cap \mathcal{S}}(x, \beta, \eta)
\]

\[
= \mathcal{L}_{\mathcal{B} \cap \mathcal{S}} \left( \frac{1}{\eta + 1} (z + c \odot \beta), \beta, \eta \right) \tag{42}
\]

\[
= -\frac{1}{2(\eta + 1)} \| z + c \odot \beta \|^2 + \frac{\eta}{2\lambda} + \frac{1}{2} \| z \|^2.
\]

This implies that \( \mathcal{D}_{\mathcal{B} \cap \mathcal{S}}(\cdot, \cdot) \) is maximized when \( \beta = (\neg c \odot z)_+ \). Note that this does not depend on the value of \( \eta \). Substituting this into (41), we have

\[
x = \frac{1}{\eta + 1} (z + c \odot (\neg c \odot z)_+) = \frac{1}{\eta + 1} \Pi_{\mathcal{S}}(z), \tag{43}
\]

where the last equality follows from the fast that \( \Pi_{\mathcal{S}}(z) = z + c \odot (\neg c \odot z)_+ \) which can be shown as follows. The Lagrangian function for the problem of projection of \( z \) onto \( \mathcal{S} \) is given by \( \mathcal{L}_{\mathcal{S}}(x, \beta) = \mathcal{L}_{\mathcal{B} \cap \mathcal{S}}(x, \beta, 0) \), and, with a similar derivation, the dual objective is \( \mathcal{D}_{\mathcal{S}}(\beta) = \mathcal{D}_{\mathcal{B} \cap \mathcal{S}}(\beta, 0) \) which is maximized at \( \beta = (\neg c \odot z)_+ \) yielding \( \Pi_{\mathcal{S}}(z) = z + (\neg c \odot z)_+ \).
Next, we find the optimal $\eta$. The dual objective is
\[
D_{B \cap S}((-c \odot z) +, \eta) = -\frac{1}{2} \|\Pi_S(z)\|^2(\eta + 1)^{-1} - \frac{r_{\text{loss}}}{2\lambda} \eta + \frac{1}{2} \|z\|_2^2 \tag{44}
\]
with the derivative
\[
\nabla_\eta D_{B \cap S}((-c \odot z) +, \eta) = \frac{1}{2} \|\Pi_S(z)\|^2(\eta + 1)^{-2} - \frac{r_{\text{loss}}}{2\lambda}. \tag{45}
\]

Setting the derivative to zero and noting that $\eta$ is a non-negative variable, we get
\[
\eta_* = \max \left(0, \sqrt{\frac{\lambda}{r_{\text{loss}}}} \|\Pi_S(z)\| - 1\right). \tag{46}
\]

Substituting this into (43), we obtain
\[
\Pi_{B \cap S}(z) = x_* = \frac{1}{1 + \max(0, \sqrt{\lambda/r_{\text{loss}} \|\Pi_S(z)\|} - 1)} \Pi_S(z) = \min \left\{1, \sqrt{\frac{\sqrt{\lambda} \|\Pi_S(z)\|}{r_{\text{loss}}}} \right\} \Pi_S(z). \tag{47}
\]
Thus, (38) is established.

**Proof of (36)** We use the following problem dual to (5):
\[
\max \quad -\frac{\lambda}{2} \left\| \Pi_S \left( \frac{X \alpha}{\lambda n} \right) \right\|^2 - \frac{1}{n} \Phi^*(-\alpha) \quad \text{wrt} \quad \alpha \in \mathbb{R}^n. \tag{48}
\]
Let $\alpha_*$ be the solution optimal to the dual problem (48).

The primal optimal solution can be recovered by
\[
w_* = \Pi_S \left( \frac{1}{\lambda n} X \alpha_* \right) \tag{49}
\]
with no duality gap. The loss term in the objective of the dual problem is bounded from above as
\[
-\frac{1}{n} \Phi^*(-\alpha) = -\frac{1}{n} \max_{s \in \mathbb{R}^n} \langle s, -\alpha \rangle - \Phi(s)
= -\frac{1}{n} \min_{s \in \mathbb{R}^n} \langle s, \alpha \rangle + \Phi(s)
= -\frac{1}{n} (\langle 0, \alpha \rangle + \Phi(0)) = -\frac{1}{n} \Phi(0) \leq r_{\text{loss}}. \tag{50}
\]

The square norm of the primal optimal solution is bounded as
\[
\|w_*\|^2 = \frac{1}{2} \|w_*\|^2 + \frac{1}{2} \|w_*\|^2
\leq \frac{1}{2} \|w_*\|^2 + \frac{1}{\lambda} \left( \Phi^*(-\alpha_*) \right)
= \frac{1}{2} \|w_*\|^2 + \frac{1}{\lambda} \Pi_S \left( \frac{X \alpha_*}{\lambda n} \right) \tag{51}
\]
where the first inequality follows from the third and fourth equalities, and the last inequality follow from Assumption 2.1(c), no duality gap, (49), and (50), respectively. Therefore, $w_* \in S$. Furthermore, $w_*$ is feasible so $w_* \in S$. Hence, (36) is established.

### A.3 Derivation of (37)

This inequality leads to a bound of the norm of the gradient of the loss term in $P_{1}(\cdot)$ can be bounded as
\[
\left\| \frac{\partial}{\partial \mathbf{w}} \Phi(\mathbf{X}_i^\top \mathbf{w} ; \mathbf{A}_i) \right\| = \left\| \sum_{i \in \mathcal{A}_t} \mathbf{x}_i \nabla \psi_i((\mathbf{x}_i, \mathbf{w})) \right\|
\leq \sum_{i \in \mathcal{A}_t} \| \mathbf{x}_i \| \| \nabla \psi_i((\mathbf{x}_i, \mathbf{w})) \| \leq kLR. \tag{52}
\]

Using this, (37) is derived as
\[
\| \nabla f_i(w_i) \| = \| \nabla P_{1}(w_i) \|
\leq \lambda \| w_i \| + \frac{1}{k} \left\| \frac{\partial}{\partial \mathbf{w}} \Phi(\mathbf{X}_i^\top \mathbf{w} ; \mathbf{A}_i) \right\|
\leq \lambda \sqrt{\frac{r_{\text{loss}}}{\lambda}} + \frac{kLR}{k} \leq \sqrt{r_{\text{loss}} \lambda} + LR. \tag{53}
\]

### A.4 Derivation of (16)

Exploiting proof techniques used in ProxSDCA (Shalev-Shwartz and Zhang, 2016), we here limit the form of $\Delta \alpha$ to $s q$ where $q := u_i - \alpha_i^{(t-1)}$ and $u_i \in -\partial \psi_i(z_i)$.

Denote by $\mathcal{D}_0(\alpha)$ the objective function of the dual problem (48). Suppose that $i$-th example is chosen at $t$-th iterate. The new value of the regularization term in $\mathcal{D}_0(\alpha)$ is given by
\[
\frac{\lambda}{2} \left\| \Pi_S \left( \frac{X (\alpha + sq \mathbf{e}_i)}{\lambda n} \right) \right\|^2 \geq -\frac{\lambda}{2} \left\| \Pi_S \left( \mathbf{w}^{(t-1)} \right) + \frac{sq}{\lambda n} \mathbf{x}_i \right\|^2
\geq -\frac{\lambda}{2} \left\| \mathbf{w}^{(t-1)} \right\|^2 - \frac{s}{n} q - \frac{1}{2\lambda} \left( \frac{s}{n} \right)^2 R^2 q^2. \tag{54}
\]
where the first inequality follows from the following inequality
\[
\forall \mathbf{v}, \forall \Delta \in \mathbb{R}^d, \quad \|\Pi_S(\mathbf{v}) + \Delta\| \geq \|\Pi_S(\mathbf{v})\|, \tag{55}
\]
and the second inequality is derived from the fact of $\mathbf{w}^{(t-1)} = \Pi_S \left( \mathbf{w}^{(t-1)} \right)$ and the assumption of $\| \mathbf{x}_i \| \leq R$. We shall prove (55) in Subsection A.5.
The improvement of the dual objective is expressed as
\[ D^0(\alpha^{(t-1)}) + sqe_i - D^0(\alpha^{(t-1)}) \]
\[ = -\frac{\lambda}{2} \| \Pi_S X(\alpha + sqe_i) \|_2^2 + \frac{\lambda}{2} \| w^{(t-1)} \|_2^2 \]
\[ - \frac{1}{n} \phi_i(-\alpha_i - sq) + \frac{1}{n} \phi_i(-\alpha_i) \]
\[ \geq -\frac{1}{2\lambda} (\frac{s}{n})^2 R^2 q^2 + \frac{(1 - s)s\gamma^2}{2n} \]
\[ + \frac{s}{n} (z^{(t)} \alpha_i + \phi_i^*(-\alpha_i) - \phi_i^*(u_i) - z^{(t)} u) \]
\[ = \frac{s^2}{2n} \gamma^2 s_{\text{h}}^{-1} + \frac{s}{n} \left( z^{(t)} \alpha_i + \phi_i^*(-\alpha_i) + \phi_i(z^{(t)}) + \frac{\gamma q^2}{2} \right) \]
\[ \text{Thus, the value of } s \text{ maximizing the lower-bound can be given by} \]
\[ s = \text{Clip}_{[0,s_{\text{h}}^{-1}]} \left( \frac{1}{2} + \frac{z^{(t)} \alpha_i + \phi_i^*(-\alpha_i) + \phi_i(z^{(t)})}{\gamma q^2} \right) s_{\text{h}}. \]
\[ \text{Thus, } (16) \text{ is derived.} \]

### A.5 Derivation of (55)

For \( h = 1, \ldots, d \), letting
\[ b_h(\Delta; v) := \begin{cases} 0.5(\Delta + (v)_+)^2 & \text{for } h \in I_+, \\ 0.5(\Delta + v)^2 & \text{for } h \in I_0, \\ 0.5(\Delta + (-v)_+)^2 & \text{for } h \in I_-, \end{cases} \]
\[ a_h(v) := \begin{cases} 0.5(v)_+^2 & \text{for } h \in I_+, \\ 0.5(v)_0^2 & \text{for } h \in I_0, \\ 0.5(-v)_+^2 & \text{for } h \in I_-, \end{cases} \]
both the sides in (55) can be rewritten as
\[ \text{LHS of (55)} = \sum_{h=1}^{d} b_h(\Delta_h; v_h), \]
\[ \text{RHS of (55)} = \sum_{h=1}^{d} a_h(v_h + \Delta_h) \]
To show the inequality (55), it suffices to show that
\[ \forall h = 1, \ldots, d, \forall v, \forall \Delta \in \mathbb{R}, \ b_h(\Delta; v) \geq a_h(v + \Delta). \]

### A.6 Proof of Theorem 2

A key observation that leads to the discovery of Theorem 2 is the following lemma:

**Lemma A.3.** Let \( g : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\} \) be defined as
\[ g(w) := \frac{1}{2} \| w \|_2^2 + \delta_S(w) \]
where \( \delta_S(\cdot) \) is the indicator function of the feasible region \( S \) given in (3). Namely, \( \delta_S(w) = \infty \) if \( w \notin S \); otherwise \( \delta_S(w) = 0 \). Then, with \( d \)-dimensional vector \( c \) defined in (4), the gradient of its convex conjugate (Rockafellar, 1970) is expressed as
\[ \nabla g^*(\bar{w}) = \bar{w} + c \odot (-c \odot \bar{w})_+. \]

See Subsections A.7 for proof of Lemma A.3.

The function \( g \) defined in Lemma A.3 is 1-strongly convex. Then, if we view \( g \) as a regularization function in replacement of the square L2-norm regularizer, the sign-constrained optimization problem (5) can be rewritten as
\[ \min \ \lambda g(w) + \frac{1}{n} \Phi(X^T w) \quad \text{wrt } \ w \in \mathbb{R}^d. \]

This is a class of optimization problems targeted by a variant of SDCA named Prox-SDCA (Shalev-Shwartz and Zhang,
2016) which maintains the convergence rate of the vanilla SDCA yet the regularization function can be extended to be a 1-strongly convex function. The difference from the vanilla SDCA is that the primal variable is recovered from the gradient of the convex conjugate of \( g(\cdot) \) at the end of each iterate. It can be seen that Algorithm 2 is generated by applying Prox-SDCA to our problem setting with \( g \) defined in Lemma A.3. From this observation, Theorem 2 is established.

\[ \Box \]

A.7 Proof of Lemma A.3

The convex conjugate of \( g \) is

\[
g^*(\bar{w}) = \max_{w \in \mathbb{R}^d} (\langle \bar{w}, w \rangle - g(w))
\]

\[
= \max_{w \in \mathbb{R}^d} \left( \langle \bar{w}, w \rangle - \frac{1}{2} \|w\|^2 - \delta_S(w) \right)
\]

\[
= \max_{w \in S} \left( \langle \bar{w}, w \rangle - \frac{1}{2} \|w\|^2 \right) \quad (72)
\]

\[
= \frac{1}{2} \|\bar{w}\|^2 - \frac{1}{2} \min_{w \in S} \|w - \bar{w}\|^2.
\]

We use Danskin’s theorem to get the derivative as:

\[ \nabla g^*(\bar{w}) = \Pi_S(\bar{w}). \quad (73) \]