Fast SVM-based Feature Elimination Utilizing Data Radius, Hard-Margin, Soft-Margin

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Abstract

Margin maximization in the hard-margin sense, proposed as feature elimination criterion by the MFE-LO method, is combined here with data radius utilization to further aim to lower generalization error, as several published bounds and bound-related formulations pertaining to lowering misclassification risk (or error) pertain to radius e.g. product of squared radius and weight vector squared norm. Additionally, we propose additional novel feature elimination criteria that, while instead being in the soft-margin sense, too can utilize data radius, utilizing previously published bound-related formulations for approaching radius for the soft-margin sense, whereby e.g. a focus was on the principle stated therein as “finding a bound whose minima are in a region with small leave-one-out values may be more important than its tightness”. These additional criteria we propose combine radius utilization with a novel and computationally low-cost soft-margin light classifier retraining approach we devise named QP1; QP1 is the soft-margin alternative to the hard-margin LO. We correct an error in the MFE-LO description, find MFE-LO achieves the highest generalization accuracy among the previously published margin-based feature elimination (MFE) methods, discuss some limitations of MFE-LO, and find our novel methods herein outperform MFE-LO, attain lower test set classification error rate. On several datasets that each both have a large number of features and fall into the ‘large features few samples’ dataset category, and on datasets with lower (low-to-intermediate) number of features, our novel methods give promising results. Especially, among our methods the tunable ones, that do not employ (the non-tunable) LO approach, can be tuned more aggressively in the future than herein, to aim to demonstrate for them even higher performance than herein.

1 Introduction

For information on support vector machines (SVMs), interested readers can be referred to e.g. [3], [9], [1]. Our brief summary of SVMs below gives notation for our manuscript, which is similar to the notation in [1].

The labeled training data is \( \{(\mathbf{x}_n, y_n), n \in \mathcal{N}\} \) where \( \mathcal{N} \equiv \{1, \ldots, N\} \); sample \( \mathbf{x}_n \in \mathbb{R}^M \) has class label \( y_n \in \{\pm 1\} \). \( f(\mathbf{x}) \equiv \mathbf{w}^T \mathbf{x} + w_0, \mathbf{w} \in \mathbb{R}^M, w_0 \in \mathbb{R} \), is a hyperplane acting as a two-class decision function. With \( g_n \equiv g(\mathbf{x}_n) \equiv y_n f(\mathbf{x}_n), \frac{g_n}{||\mathbf{w}||} \) is the signed distance from \( \mathbf{x}_n \) to the decision boundary which is a separating one if \( g_n > 0 \forall n \) with margin defined as \( \gamma \equiv \frac{\min_n g_n}{||\mathbf{w}||} \). Hard-margin SVM is a linear or generalized linear two-class classifier defined via the optimization problem

\[
\min_{\mathbf{w}, w_0} \frac{1}{2} ||\mathbf{w}||^2 \quad \text{s.t.} \quad y_n f(\mathbf{x}_n) \geq 1, \forall n
\]

and soft-margin SVM is a linear or generalized linear two-class classifier defined via the optimization problem

\[
\min_{\mathbf{w}, w_0, \xi} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n \quad \text{s.t.} \quad \xi_n \geq 0; \quad y_n f(\mathbf{x}_n) \geq 1 - \xi_n; \forall n
\]
In the linear case, the SVM weight vector is given by
\[ \mathbf{w} \equiv \sum_{k \in \mathcal{S}} \lambda_k y_k \mathbf{s}_k, \]
where \( \mathcal{S} = \{ \mathbf{s}_k : k \in \mathcal{S} \equiv \{1, \ldots, T\} \} \), used to specify the SVM solution, is the set of support vectors which is a subset of the training points, and \( \lambda_k \) are the associated Lagrange multipliers.

The generalized linear (nonlinear) case involves nonlinear functions \( \phi_i(\cdot) \) and \( \phi_i(\mathbf{x}) \equiv [\phi_1(\mathbf{x}), \ldots, \phi_L(\mathbf{x})]^T \). Inner products between \( \phi_i(\mathbf{x}) \) and \( \phi_j(\mathbf{u}) \) that can be efficiently computed via a positive definite kernel function \( \mathbf{K}(\mathbf{x}, \mathbf{u}) \equiv \phi_i(\mathbf{x}) \phi_j(\mathbf{u}) \) are of particular interest; in this case, \( \phi_i(\cdot) \) and \( \mathbf{w} \) need not be explicitly defined since both the SVM discriminant function \( f \) and the weight vector squared 2-norm can be expressed solely in terms of the kernel:

\[ f(\mathbf{x}) = \sum_{k \in \mathcal{S}} \lambda_k y_k \mathbf{s}_k \mathbf{K}(\mathbf{s}_k, \mathbf{x}) + w_0 \quad (3) \]

\[ ||\mathbf{w}||^2 = \sum_{k \in \mathcal{S}} \sum_{l \in \mathcal{S}} \lambda_k y_k \lambda_l y_l \mathbf{s}_k \mathbf{K}(\mathbf{s}_k, \mathbf{s}_l). \quad (4) \]

This “kernel trick”, where a specified \( K \) is provided to SVM training, is the nonlinear kernel case.

Relating these SVM concepts to feature elimination algorithms, [1] proposed a so-called “strict margin maximization” (or, margin maximization in the hard-margin sense) method called ‘basic MFE’ that picks the feature elimination that preserves maximum (positive) margin in the reduced space as follows:

\[ m^* = \arg \max_{m \in \{n \in \mathcal{R} | \|\mathbf{s}_m\| > \|\mathbf{s}_n\| \}} \min_n g^n_m / ||\mathbf{w}^{-m}||; \]

and a second, counterpart method (MFE-Slack) based on generalization of strict margin maximization that picks the feature elimination with the smallest SVM objective function [2] in the reduced space via the discrete optimization problem

\[ (m^*, n^*) = \arg \min_{m \in \mathcal{R}} \min_{n \in \{l | l_{-m} > 0\}} \frac{1}{2} (||\mathbf{w}||^2)^{-m} (\rho^{-m,n_a})^2 + C \sum_{n=1}^N \xi^{-m,n_a}; \]

for each candidate \( m \) for elimination, every (correctly classified) sample is evaluated as the potential margin-setter \( n_a \), with both the weight vector squared norm (WVSN) and slacknesses evaluated post-feature-elimination, to pick the optimal \( (m^*, n^*) \) that, post-elimination, minimizes [2] over all discrete choices \( \{m, n_a\} \). A hybrid [1] (here MFEh) used ‘basic MFE’ when applicable (at steps data is separable) and MFE-Slack at other steps.

## 2 Related work: Little Optimization (LO)

To increase with little computation the margin maximization in the hard-margin sense that ‘basic MFE’ can obtain alone (in reduced space, under weights \((\mathbf{w}, w_0)\)), the LO approach [1] considered the parameterization \((a \mathbf{w}, b)\) where \( a \) and \( b \) are scalars to be optimized, with \( \mathbf{w} \) held fixed; i.e. posed the standard hard-margin SVM training problem but optimizing in this two-d \((a, b)\) space:

\[ \min_{a,b} a^2 s.t. \ y_n (a (\mathbf{w}^T \mathbf{x}_n) + b) \geq 1, \forall n; \quad (5) \]

Embedding LO into the elimination decision (to eliminate by largest post-LO margin in reduced space) [1] is herein referred to as MFE-LOe (or MFE-LO in some graphs).

**Correction to LO:** Before continuing, we now point out an error in how [1] solves (5) and correct the error. To give an intuitive graphical description, we now refer to Fig. 4 in [1]. In the illustrated halfspace \( a > 0 \), the entirety of the illustrated shaded region (defined by (i.e. lying to

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1Notation: During feature elimination, one or more features can be eliminated in one ‘step’; i.e. the elimination is ‘stepwise’. \( \mathcal{R} \) denotes the retained feature set at the start of a step. We denote a quantity (or variable) \( q \) under the step’s (candidate or actual) elimination of a set \( \mathcal{M} \) of features in multiple equivalent ways: \( q^{-\mathcal{M}} \) (i.e. \( q^{\mathcal{R}\setminus \mathcal{M}} \)) to simply only convey \( \mathcal{M} \); \( q^{-\mathcal{M},n_a} \) to convey the step index \( i \), at the left of \( \mathcal{M} \); \( q^{-\mathcal{M},n_a} \) to convey that the sample with the sample index \( n_a \) is being considered a ‘margin-setter’ (aka ‘anchor’) sample (discussed below), at the right of \( \mathcal{M} \). Use of superscript \(-m\) as an alternative to \(-\mathcal{M}\), where \( m \) is feature index (for a single feature), refers to 1-by-1 elimination of features.
the right of the intersection point of) the two thick lines) is not the correct feasible region of the problem; the correct feasible region is the smaller (shaded) cone defined by \( l_2 \) (going through \( w_0 = -1 \)). Notice that accordingly the statement in [1] that the feasible region is defined by the cone “bounded by the line \( l_2 \) with maximum slope in \( L_2 \) and the line \( l_1 \) with minimum slope in \( L_1 \)” is incorrect. The (correct) feasible region is defined by the cone bounded by the line with minimum slope in \( L_2 \) and the line with maximum slope in \( L_1 \). The LO solution, i.e. the (feasible) minimum \( a^2 \), lies at that cone’s tip; this tip is shown in the Figure as the intersection point of two lines immediately above the “\( C^+ \)” label shown in the Figure.

LO serves to perform light classifier retraining which has several generalization accuracy advantages compared to full (SVM) retraining (FSR aka FR). First, stepwise FSR (to stepwise attain the most optimal values for SVM margin or objective function) may cause the subset selection process to overfit; a limitation, especially for a dataset whose number of features is large since overfitting, a cumulative effect, is expected when a large number of elimination steps accumulate. In Fig. 3 across-trial average test set classification error rate (see: Sec. 5 which gives our experiment procedure) is plotted, as a function of the number of retained features (reduced going from right to left).\(^2\) In conjunction with Fig. 1, these results for MFEh-FRs (stepwise FSR subsequent to elimination decision by MFEh) and MFE-LO illustrate that although stepwise FSR can improve generalization, utilizing FSR throughout a large number of elimination steps is attaining less generalization accuracy than light classifier retraining; this result can perhaps be understood as a type of overfitting.

Fig. 2 redraws Fig. 1(a) to supplement each method’s across-trial average curve (\( \mu \)) with the \( \mu + \sigma \) curve (seen above the average curve) and the \( \mu - \sigma \) curve (seen below the average curve), where \( \sigma \) is the across-trial standard deviation; in this manuscript, to demonstrate results more precisely, we demonstrate standard deviation in this fashion. To illustrate there may not be much overfitting for a dataset with hugely fewer features (and hugely lower features-to-samples ratio), Fig. 4 demonstrates FR-based elimination outperforming elimination based on light classifier retraining (LO\(^3\)). LO is in both Fig. 3 (for large number of features) and Fig. 4 (for much smaller number of features), playing a reference role. Second, FSR can have more computational cost than light classifier retraining. For initial dimensionality \( M \) (e.g. 7000+ for gene data), at the \( i \)-th elimination step FSR trains an SVM for the very large feature dimensionality \( M - i \) (6999, 6998, \ldots); lower computational cost can be attained by light classifier retraining that is carried out by LO as well as carried out by our novel QP1 approach discussed shortly.

We propose and assess several novel feature elimination methods, including assessing them in comparison with these previously published MFE methods in [1] (MFE-LO, MFEh, MFE-Slack), and discuss the limitations of these previous three methods in doing so. Since MFE-LO is not usable at any feature elimination step at which the data is not separable (i.e. a step at which a (pre-LO) separating classifier is not possible or available), datasets that remain separable for most (ideally, vast majority) of the steps are the most suitable datasets for comparing the generalization performance of MFE-LO to other methods, irrespective of whether or not these other methods too require separability; especially these datasets include ‘small \( N \), large \( M \)’ datasets (discussed in previous work such as [1], [2], [7]). Accordingly, almost all results given herein, whenever comparing MFE-LO to our novel methods and to the methods in [1], are for such datasets. In fact, we give results for each of the three ‘small \( N \), large \( M \)’ gene datasets seen in [1] and other works. In Fig. 1 across-trial average test set classification error rate is plotted, as a function of the number of retained features (reduced going from right to left), illustrating MFE-LOe outperformed MFEh (and MFE-Slack, whose curve overlaps curve of MFEh).\(^4\) Extensive results for several datasets and extensive discussion are given in Sec. 5.

\(^2\)When in a graph we show two methods paired with a slash ‘/’, such as MFE-LO and MFE-Slack paired here, the first and second indicate, respectively, the method used when data is separable and nonseparable; in this particular Figure, the second method plays little role within the pairing, since this dataset was separable until only very few features remained as illustrated by Fig. 1(b).

\(^3\)QP1 shown is light classifier retraining that will shortly be discussed below.

\(^4\)The third method in this Figure will be discussed in Sec. 4.
Figure 1: (a) MFE-LOe achieved much lower across-trial average test set classification error rate i.e. better generalization than MFEh. (b) The (across-trial average) training set classification error rate curves illustrate that initially separable data remained separable longer under MFE-LOe than MFEh. SVM linear kernel case; Colon Cancer gene dataset with 2000 features and much fewer samples. Here, for the particular case of 1-by-1 elimination of features.
Figure 2

Figure 3: Stepwise light classifier retraining (LOe (MFE-LO)) attaining lower test set classification error rate than stepwise full SVM retraining (FR (MFEh-FRs)); here, for the particular case of 1-by-1 elimination of features. SVM linear kernel case; Colon Cancer gene dataset with 2000 features and much fewer samples. Zoomed to final 300 features retained.
3 QP1: slackness-incorporating light classifier retraining

We begin by making a central observation, not made in previously published related work (LO) \cite{1}: the moment one makes the modeling assumption that scalars $a$ and $b$ for the parameterization $(aw, b)$ is to be sought while holding $w$ fixed (such as made by LO in previous work), what is happening is that the data to work with is becoming 1d (scalar); notice in \cite{5} that the non-scalar (multi-dimensional) data variables $x_n$ (denoted $x_n^{-M}$ during the elimination process) from the original SVM optimization problem are transformed into scalar data variables $w^T_x n$ and can thus not only be explored via an optimization formulation that, unlike LO, is slackness-incorporating but also different ways to generate a solution for this slackness-incorporating formulation can be explored. Accordingly, in this Section, we discuss that what arises from incorporating slackness for such 1d data is a computationally exceptionally simple quadratic programming (QP) problem (relatively speaking, considering QP problems in general) for which a solution can be generated in one of multiple possible ways including our novel specialized computationally low-cost active-set method we present (but do not empirically utilize) herein\cite{5}, and we also show that additional ways to generate a solution conveniently arise from simply and conveniently employing distinct SVM solver approaches as we show shortly in this Section that the optimization formulation (the QP) is equivalent to the simple 1d soft-margin SVM (i.e. soft-margin SVM for scalar data). For example, when the abovementioned particular QP (i.e. the QP for scalar data) is handled as a 1d SVM, one way to generate a solution is to utilize an SVM solver such as LIBSVM \cite{4} and another way is \cite{11} which too solves the 1d soft-margin SVM problem. This second way, \cite{11}, has the built-in limitation that a support vector (a vector for which the discriminant function value $yf$ is 1, i.e. a vector “at the margin”\cite{11}) is assigned from within each of the two classes rather than from within solely one class; this is a limitation because it narrows the $(a, b, \xi)$ search

\footnote{For small- to medium-scale inequality constrained quadratic programming (ICQP) problems, it has been mentioned that active-set methods are the most effective \cite{10} generally; we took a specific active-set algorithm given in \cite{11} and specialized it for our particular novel ICQP problem \cite{11} which is discussed shortly, achieving much computational efficiency for the algorithm in doing so. Herein we present our active-set method work for mainly as a novel theoretical mathematical contribution (wherein our devised Lemmas and Theorems are presented) and do not actually utilize this algorithm in our current feature elimination experiments herein.}

\footnote{As \cite{11} stated (see: proof of Observation 4 in \cite{11}). “If $x_i$ is a support vector, then by definition $y_i(x_i \cdot w + b) = 1.$”}
space, when compared with SVM solvers such as LIBSVM and our abovementioned novel active-set method; in particular, candidate solutions encountered along the particular descent path that our method takes as a non-discrete optimization method include candidate solutions considered by the discrete optimization method [11], i.e. solutions at which \( y_i(\mathbf{x}_i \cdot w + b) = 1 \) is simultaneously fulfilled by two (training) samples (which, can be thought of as the “margin-setter” samples). To summarize, our mathematical analytical interest and contributions here are aligned more with the following three notions collectively than simply aligned with the more simplistic notion that it is possible to define (and then give some results for) a slackness version of LO (LO-Slack): 1) making the abovementioned central “data to optimize with is now 1d data” observation, not made by LO, 2) accordingly casting and treating the problem in a more general setting than LO did, as computationally low-cost quadratic programming for 1d data (QP1), and 3) accordingly providing an analysis of multiple approaches (each computationally low-cost) that can generate a solution for this particular setting. Our novel formulation, (6) (7) given below shortly, is thus quite suitably named QP1, not LO-Slack.\(^7\)

Given SVM linear weights \((w, w_0)\), we consider the parameterization \((aw, b, \xi)\), where \(a, b\), and \(N\) slacknesses are scalar parameters to be optimized, with \(w\) held fixed. We thus pose the soft-margin SVM problem (2) but only optimize in this \((a, b, \xi)\) parameter space:

\[
\min_{a, b, \xi} \frac{1}{2} a^2 ||w||^2 + C \sum_n \xi_n \text{s.t.} \xi_n \geq 0, \ y_n(aw^T \mathbf{x}_n + b) \geq 1 - \xi_n, \forall n;
\]

(6)

This formulation, QP1, is distinct from LO wherein, again, it was only in the hard-margin sense that margin maximization was posed, motivated, and discussed (focusing on [1], not the soft-margin sense [2]) i.e. for strictly satisfying the margin [1]; while [1] was careful to state, by contrast, that “strictly satisfying the margin could potentially lead to overfitting when training samples at the margin are outliers or even mislabeled samples. Optimizing the amount of slackness (by choosing the parameter \(C\)), e.g. via cross validation, may yield classifiers with better generalization than those based on strictly maximizing margin.” The fact that we formulated QP1 and are analytically discussing multiple computationally efficient solvers for QP1 herein are a contribution as it fills a substantial gap left by [1].

By contrast to LO, we focus on the soft-margin SVM (2); in our QP1 formulation, since \(w\) and thus also its norm \(||w||\) are held fixed, a change of variables \(w \equiv aw, \mathbf{z}_n \equiv \mathbf{x}_n/||w||\) shows the problem is equivalent to the simple 1d soft-margin SVM (i.e. soft-margin SVM for scalar data) which has little computational cost:

\[
\min_{w, b, \xi} \frac{1}{2} w^2 + C \sum_n \xi_n \text{s.t.} \xi_n \geq 0, \ y_n(wz_n + b) \geq 1 - \xi_n, \forall n
\]

(7)

Since QP1 (6) (7) requires little computation and contains hyperparameters e.g. \(C\) as part of its definition, QP1 can be performed in conjunction with each feature elimination step and hyper-parameter selection can be integrated into that step. Thus, across, as well as within, elimination steps, one can generate a set \(\{(a, b, \xi)\}\) of multiple (QP1 output) triplets i.e. a set \(\{(w, b)\}\) of classifiers (herein aka models; i.e. pairs of scalars \(w\) and \(b\)). However, for the task of picking among these a particular classifier (with its associated candidate feature elimination), picking the classifier with the smallest QP1 objective function may not be a great feature elimination criterion; that particular criterion is not our main focus herein and we overview it briefly and in an Appendix, so as to now move on to the notion that QP1 need not form a feature elimination criterion by itself and can instead, as a type of slackness-incorporating light classifier retraining (with little computational cost), be combined with other concepts to define a feature elimination criterion, such as we do in the upcoming Sec. 4.2 where we propose novel feature elimination criteria that combine QP1 with bounds that utilize data radius that aim to lower generalization error. A role of QP1 in such combinations is that QP1 serves to perform light classifier retraining which has several advantages

\(^7\)LO can be considered a specific type or instantiation of QP1; a special one that does not incorporate slackness i.e. QP1-NonSlack.
regarding generalization accuracy when compared to full SVM retraining (FSR) as well as when compared to the alternative LO method for light classifier retraining, as follows. First, stepwise FSR (to stepwise attain the most optimal values for SVM margin or objective function) may cause the subset selection process to overfit; a limitation, especially for a dataset whose number of features is large since overfitting, a cumulative effect, is expected when a large number of elimination steps accumulate. To illustrate there may not be much overfitting for a dataset with hugely fewer features (and hugely lower features-to-samples ratio), Fig. 4 demonstrates FSR-based methods outperforming light classifier retraining; see also our earlier above discussion of this Figure. Second, FSR has more computational complexity than QP1. For initial dimensionality \(M\) (e.g. 7000+ for gene data), at the \(i\)-th elimination step, FSR trains an SVM for the large feature dimensionality \(M - i\) (6999, 6998, \ldots), whereas our training essentially has the computational complexity of a 1d SVM (1, 1, \ldots). Moreover, by incorporating slackness, QP1 does not require margin maximization in the hard-margin sense whereas LO does require it; i.e. requiring margin maximization strictly in the hard-margin sense may lead to overfitting when training samples at the margin are outliers or even mislabeled samples, as mentioned above.

Like our QP1 approach, MFE-slack [1] also incorporates slackness into the feature elimination criterion. However, it can be easily noticed that in MFE-slack, unlike in QP1, originally designed relative magnitudes among SVM Lagrange multipliers and intercept \(u_0\) do not remain unchanged, since MFE-Slack scales a Lagrange multiplier and \(u_0\) by the same scalar (at each feature elimination step). This is a slight but significant limitation in MFE-slack, as our Figures demonstrated, which demonstrated that our QP1 approach, which does modify the abovementioned relative magnitudes (via jointly optimizing \(a\) and \(b\) (and the slacknesses \(\xi\))), is outperforming MFE-Slack.

As mentioned above, there are multiple approaches, such as LIBSVM, [11], and our active-set method in the Appendix, that can generate a solution for the 1d SVM problem (7); each is computationally low-cost, including being quite fast. However, each of these three has its own unique tradeoff between computational cost and how well the objective function is being optimized. In our experiments herein, we utilize the first (LIBSVM).

### 4 In feature elimination, utilizing bounds that utilize data radius

In earlier Sections, we discussed an approach that seeks scalars \(a\) and \(b\) for the parameterization \((a\mathbf{w}, b)\) while holding \(\mathbf{w}\) fixed (i.e. LO and QP1), whereby the data to work with within a feature elimination step becomes 1d (scalar). Next, aiming to further decrease generalization error, we define novel feature elimination methods by combining this approach with a utilization of data radius \(R\), essentially the radius of the smallest sphere containing all \(\phi(\mathbf{x})\), because, as we shortly discuss, \(R\) appeared as an integral part of several published bounds and bound-associated optimization formulations for characterizing generalization error that span the hard-margin and soft-margin settings. For information on bounds that utilize data radius, we refer interested readers first to e.g. [5] and [15]: [5] focuses on the ‘radius margin bound’ and ‘modified radius margin bound’ concepts (and associated optimization formulations) while making useful references to several other related work on bounds that utilize data radius (e.g. [13], [14], [17]), and [15] too discusses bounds that utilize data radius.

#### 4.1 Utilizing radius in the hard-margin classifier sense

For the hard-margin classifier case, several published bounds pertain to the product of squared radius and weight vector squared norm WVSN (\(R^2|\mathbf{w}|^2\)):

1) The first such bound we consider is an upper bound on the VC dimension \(h\). The bound \(h < R^2A^2 + 1\) for \(h\) (for the function family \(\{f_{w,b} : |w| \leq A\}\) for some scalar \(A\)) was discussed in e.g. [9, 10, 12]. Lowest upper bound on the VC dimension \(h\) is a known criterion for selecting among multiple functions (for machine learning) a particular one (so as to aim for lower generalization
error), such as during Structural Risk Minimization (SRM) e.g., when discussing how one can do SRM, [3] asked to find within a set of functions the particular one that, as [3] states, “gives maximum margin (and hence the lowest bound on the VC dimension.)” As seen in feature elimination that seeks to maximize margin in the hard-margin sense, such as LO, although a WVSN upper bound $A$ (i.e. $A^{-m}$) is not being computed explicitly, the WVSN itself is computed, and can be utilized as the available surrogate upper bound and define a new feature elimination method that picks the feature elimination for which the product of $R^2$ and WVSN$^9$ is smallest$^{10}$; further below, we revisit this method and elaborate.

2) A second bound, formed by the same product $R^2 ||w||^2$, is the leave-one-out (loo) radius margin bound $^5$

$$\text{loo} \leq 4R^2 ||w||^2$$

which, $^5$ stated holds for SVM without the bias term $b$ where $\text{loo}$ is the number of loo errors, $w$ is the solution of (11), and $R$ is the radius of the smallest sphere containing all $\phi(x)$. Thus, then stated that “extends the bound for the general case where $b$ is present” and also stated that “it has been shown (e.g. [13]) that $R^2$ is the objective value of the following optimization problem:"

$$\min_{\beta} 1 - \beta^T K \beta \text{ s.t. } 0 \leq \beta_n \forall n, e^T \beta = 1$$

An alternative to (11) to estimate data radius is to define $R^2$ as the maximum squared Euclidean distance between any two (training) points: e.g. during 1-by-1 elimination of features, $\max ||x_i^m - x_j^m||^2$. We elaborate on these two different data radius formulations further below.

3) Furthermore, another publication endorsing utilization of data radius for selecting among candidate functions was $^{15}$ which, giving a theorem on the expectation of error probability, wrote: “This theorem justifies the idea that the performance depends on the ratio $E\{R^2/M^2\}$ and not simply on the large margin $M$, where $R$ is controlled by the mapping function $\Phi(\cdot)$.” Since the maximization of margin $M$ (or, $1/||w||$, see e.g. (11)), central to SVM learning, is commonly formulated via the minimization of WVSN as seen in the hard-margin SVM formulation (11), we can thus see from $^{15}$ that performance can benefit from minimizing (the expectation of) the product of squared radius and WVSN. As discussed above in items 1 and 2, in the case of feature elimination the computation of the two items in this product is straightforward and computationally low-cost. Based on the importance of radius-based bounding discussed somewhat briefly above, given also that it was theoretically sound to propose for feature elimination the LO (or MFE-LO) method (that aims for, and formulates, margin maximization strictly in the hard-margin sense via minimizing the post-LO WVSN $(a^2)^{-M}(||w||^2)^{-M}$; see: equation (12) in (11)), it is also theoretically sound (once again strictly in the hard-margin sense) to propose minimizing the product of $R^2$ and the abovementioned WVSN quantity $a^2||w||^2$ i.e. “the product of squared radius and WVSN” that we have been discussing above:

$$m^* = \arg \min_{m \in \mathbb{R}[g^m > 0 \forall l]} \min_{a,b} (R^2)^{-m}(a^2)^{-m}(||w||^2)^{-m}$$

Here, by moving $(R^2)^{-m}$ and $(||w||^2)^{-m}$ to the left by considering their values need not depend on

$^8$For SRM, see e.g. [3].

$^9$The product $(R^2)^{-m}$WVSN$^{-m}$ in the particular case of 1-by-1 elimination of features; $(R^2)^{-M}$WVSN$^{-M}$ generally.

$^{10}$Of course, by contrast, when not doing feature elimination and no classifier to start from in order to guide the elimination is yet available (a scenario that requires all classifier weights to be simultaneously generated from scratch from training data), mathematically optimizing the product of squared radius and WVSN (i.e. the joint optimization of these two quantities) is not so straightforward (simultaneously with such generation); e.g. as the [3] full version provided for [3] writes “For our current implementation, solving each of $||w||^2$ ... $R^2$ ... is considered an independent problem. In the future $||w||^2$ and $R^2$ ... should be considered together. How to effectively pass information under one given parameter set to another is also worthy of investigation.”
the LO solver, (10) can be implemented as

\[ m^* = \arg \min_{m \in \{ \hat{m} \in \mathbb{R} | g - \hat{m} l > 0 \}} (R^2)^{-m} (\|w\|^2)^{-m} \min_{a,b} (a^2)^{-m} \]  

(11)

where the minimization on the right becomes easy to recognize as LO (5). Our novel method (10) (11) is named hBMFE-LO (“for hard-margin, Bound-Based MFE-LO”), where the “h” emphasizes that this method pertains to margin in the hard-margin sense; it is a method that combines MFE (Margin-maximizing (or Margin-based) Feature Elimination) [1] and upper bound on/for misclassification risk. Fig. 1, discussed earlier, illustrates hBMFE-LO outperformed MFE-LO which does not utilize radius. “ER” in the graph means the abovementioned Euclidean-based R calculation, which is an alternative to “tR” which means training-based (or, optimization-based) R calculation such as given by the optimization formulation (9). Extensive results for several datasets and extensive discussion are given in Sec. 5.

4.2 Utilizing radius in the soft-margin classifier sense

Practicality of the soft-margin SVM was discussed as being beneficial in past works and we cannot do justice to all of them here; see e.g. some useful references for SVM mentioned in our Introduction. [5] mentioned that the hard-margin SVM (1) is “not a form for practical use. It may not be feasible if \( \phi(x) \) are not linearly separable. In addition, a highly nonlinear \( \phi \) may lead to overfitting.” and mentioned next that thus practically they solve the soft-margin SVM formulation e.g. (2), which they refer to as “L1-SVM” (where “1” in “L1” states the exponent for the slackness variable in the objective function (2) [11]). These comments, in support of practically utilizing the soft-margin formulation (2) instead of the hard-margin formulation (1), are complemented by the following abovementioned comments [1]: “Optimizing the amount of slackness (by choosing the parameter \( C \), e.g. via cross validation, may yield classifiers with better generalization than those based on strictly maximizing margin.”

Before continuing, we note an additional important information in support of soft-margin SVM (i.e. in support of utilizing rather than not utilizing slackness variables), that is, additional to the above comments made in [5] and elsewhere for that support: slackness variables serve an important purpose even when data is separable because, e.g., 1) as noted in [11], strictly satisfying the margin may lead to overfitting when training samples at the margin are outliers or even mislabeled samples, 2) classifiers that separate the data (i.e. with zero classification error) and simultaneously allow some training samples to lie within (i.e. violate) the margin can be obtained and, due to reasons above, may generalize better than classifiers that do not allow slackness (i.e. margin violation) when separating the data with zero classification error. That is, in support of QP1, to contrast QP1 to LO, we note that incorporating slackness variables into the feature elimination model, as done by QP1, is important even when the data is expected to be separable, as this can alleviate overfitting, especially for data whose number of features is very large because overfitting can be a cumulative effect that stepwise accumulates over the course of elimination of a large number of features as during 1-by-1 elimination of features.

[5] stated that its goal is “to make radius margin bound, a theoretical bound of loo error, a practical tool”, and, based on its stated principle that “finding a bound whose minima are in a region with small loo values may be more important than its tightness” it proposed modified radius margin bounds for the soft-margin SVM (2) (aka L1-SVM as mentioned earlier) where, as [5] states, “the original bound is only applicable to the hard-margin case”. In particular, for the soft-margin SVM case, [5] considered, and discussed its generated results for, the following three heuristic bounds for L1-SVM (2):

\[ R^2 e^T \alpha + \sum_{n=1}^{N} \xi_n \]  

(12)

[5] also discusses and solves “L2-SVM” (for the case where the sum in the soft-margin SVM objective function is instead \( \sum_{n=1}^{N} \xi_n^2 \)) for which we do not perform experiments herein.
\begin{align*}
(R^2 + \frac{1}{C})(||w||^2 + C \sum_{n=1}^{N} \xi_n) \quad (13) \\
(R^2 + \frac{\Delta}{C})(||w||^2 + 2C \sum_{n=1}^{N} \xi_n) \quad (14)
\end{align*}

where \( \Delta \) was considered to be a positive constant close to one or one. For details in \([5]\), we refer interested readers to \([5]\). In this section, we focus on combining \((14)\) (using \( \Delta = 1 \)) with our tunable QP1 optimization approach to define an accordingly tunable novel feature elimination criterion that can potentially achieve better generalization than 1) MFE-LO (which is non-tunable), 2) radius-incorporating hBMFE-LO proposed above (which is non-tunable) and 3) eliminating using the QP1 criterion alone. That is, the classifier we are interested to plug into the formulation \((14)\) (i.e. values to plug in for the weight vector squared norm and slackness values in \((14)\)) is one that we shall obtain via our QP1 approach. Since QP1 would perform best when its tunability is utilized (by performing hyperparameter selection), at each feature elimination step our new novel feature elimination method, that combines QP1 with data radius utilization, performs hyperparameter selection (since QP1 only takes little computation) whereby many QP1 classifiers (i.e. \((a, b, \xi)\) triplets) are generated to select from, for that particular candidate feature elimination; e.g. in the case of 1-by-1 elimination of features (and when utilizing \((14)\) in particular), we thus propose the following novel feature elimination method:

\[
m^* = \arg \min_{m \in \mathbb{R}} \min_j ((R^2)^{-m} + \frac{1}{C_j})((w^2)^{-m} + 2C_j \sum_{n=1}^{N} \xi_n^{-m}) \quad (15)
\]

where \((w^2)^{-m}\) and \(\xi_n^{-m}\) are the “square of the scalar weight \(w\)” value and the scalar slackness \(\xi_n\) values generated by the QP1 training in the reduced space (i.e. when \(m\) is the candidate feature elimination being considered), and the set of indices \(j\) represents the set of hyperparameter value candidates. Since there are multiple ways to generate a solution for QP1 as well as generate the \(R^2\) value, there are multiple ways to implement the QP1-based feature elimination criterion given by \((15)\). The first way we discuss is named the QP1:lnm3-ER method, where “l” means LIBSVM is the means used by this particular way to generate a QP1 solution (i.e. we train a 1d SVM using LIBSVM; we can, in future work, alternatively train using our active-set method), “n” means we make no modifications to LIBSVM’s output for the 1d SVM (C-SVC) training (i.e. no modifications to the set of positive Lagrange multipliers assigned by LIBSVM and the samples they are assigned to\(^{12}\), “m” means model selection (here aka hyperparameter selection) is performed, “3” means we utilize the third of the above three L1-SVM heuristic bounds (i.e. bound \((14)\)), and “ER” was discussed above. In Fig. \([3]\) QP1:lnm3-ER is placed into the earlier Figure to compare generalization performance with those earlier methods. For a more potent illustration of the comparison of QP1:lnm3-ER to other methods, we also give Fig. \([4]\) wherein QP1:lnm3-ER essentially outperforms hBMFE-LO:ER even though these two curves are, once again, fluctuant; one would expect the QP1:lnm3-ER curve to become even lower by simply expanding the search used for the stepwise hyperparameter selection that QP1:lnm3-ER utilizes, by e.g. simply including additional candidate \(C\) values in the search set.

5 Results and Discussion

Note from author Yaman M. Aksu: Some shortcomings of this current particular version of this manuscript include the facts that I did not yet have time to: 1) provide discussion of the results that I am currently placing into this Results and Discussion section (though they are somewhat self-explanatory), 2) provide isolated (explicitly better organized) pseudocode for my novel specialized

\(^{12}\)Our experience with LIBSVM 1d SVM training is that sometimes the discriminant \(yf\) function value is not equal to 1 for any of the abovementioned vectors being assigned positive Lagrange multipliers.
Figure 5: QP1:lnm3-ER is placed into the earlier Figure for comparison.
Figure 6: Feature elimination starting with 7129 features. Duke Breast Cancer gene dataset. SVM linear kernel case.
active-set algorithm (in fact, algorithms, as there are variants) that are discussed in the Appendix, 3) provide more discussion on feature selection in especially the Introduction, 4) etc.

The common procedure used for training an initial SVM classifier, a first step for all feature elimination methods here, randomly split the dataset 50-50% into a non-heldout (training) set \( X \) and a heldout (test) set \( \bar{X} \) (with each split defining one ‘trial’), selected hyperparameters by 5-fold cross-validation \[8\] on \( X \), and used all of \( X \) to retrain the trial’s classifier for these selected values. In Figures we show across-trial averages. When features outnumber samples (e.g. 7129 \( \gg \) tens or hundreds), e.g. in gene, biomedical image, and other domains, it is highly probable that the training set will be separable while eliminating all the way down to relatively few features (e.g. hundreds, tens) \[6, 1\], and thus all methods herein may be able to eliminate all the way down to relatively few features without losing separability, whereas for intermediate dimensioned data separability may be lost sooner e.g. when half of the features is still left to eliminate.

For QP1, as mentioned above, at each feature elimination step we performed hyperparameter selection, to select from a set of candidate \( C_j \) values \[13\]: the set was \( \{C_{\text{init}}, C_{\text{init}}/2^1, \ldots, C_{\text{init}}/2^{30} \} \) where \( C_{\text{init}} \) denotes the \( C \) value that was used for training the initial SVM classifier (chosen in full feature space, by 5-fold cross-validation) prior to the feature elimination process\[13\]. Alternatively, in future work, training the initial classifier and performing feature elimination can be carried out jointly rather than separately, to jointly incorporate hyperparameter selection.

6 Appendix 1: QP1-specialized computationally low-cost active-set method

6.1 Introduction

Approaching QP1 as an inequality constrained quadratic programming (ICQP) problem in primal form, we specialized an active-set method whereby we make this method of obtaining a QP1 solution computationally low-cost as well. This method of obtaining a QP1 solution, which considers QP1 in primal form (i.e. takes descent steps to directly minimize (the primal form of) the QP1 objective function), is an alternative to considering QP1 a 1d SVM problem to be solved by an SVM solver in dual form.

In this introductory subsection, for the reader we provide an informative summary, based on \[10\], about how an ICQP problem

\[
q^* = \min_q \frac{1}{2}q^T G q + d^T q \quad s.t. \quad a_i^T q \geq t_i, \quad i \in I
\]  

(16)
can be solved via an active-set method; additional detail can be found in e.g. \[10\]. The notation in (16) is a standard one\[14\]. Then, after the Introduction, in Sec. 6.2, we focus on the forms, and properties, of these particular QP1-specific variables and matrices (e.g. \( q, G, d, a_i \)\[15\]), devise (given those particular matrices) our e.g. Lemmas and Theorem i.e. our mathematical contributions for finding a QP1 solution (especially, a computationally low-cost solution), and accordingly devise an active-set algorithm specialized for QP1 in particular that obtains a computationally low-cost solution for QP1.

For small- to medium-scale ICQP problems, it has been mentioned that active-set methods are the most effective \[10\] generally; we took a specific (and yet fairly general, as discussed below) active-set algorithm provided by \[10\] and specialized it in two central ways. The first specialization

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\[13\]Except the Leukemia dataset, for which a more balanced choice of \( C \) values was made wherein not only values smaller than \( C_{\text{init}} \) but also larger than \( C_{\text{init}} \) were included: \( \{C_{\text{init}} \cdot 2^5, \ldots, C_{\text{init}} / 2^{15} \} \).

\[14\]Shortly Sec. 6.2 will state these variables (e.g. \( q, G, d, a_i \)) for our particular QP problem QP1.

\[15\]Notice the matrices at hand here in QP1 exhibit much regularity i.e. contain numerous zeros and ones and we will make use of this in Sec. 6.2 e.g. \( G \) has a single nonzero element, and almost all of \( A \) and all of \( d \) are zeros and ones.
Figure 7: Average test set classification error rate for the Duke Breast Cancer gene dataset with 7129 features and much fewer samples. SVM linear kernel case.

(a) Zoomed to 300 features retained starting with 7129 features.

(b) Zoomed to 600 features retained starting with 7129 features.
Figure 8: This Figure redraws Fig. 7(a) (i.e. the across-trial average $\mu$) so as to also include, for each elimination method, the $\mu + \sigma$ curve (seen above the average curve $\mu$) and the $\mu - \sigma$ curve (seen below the average curve $\mu$), where $\sigma$ is the across-trial standard deviation of the elimination method.
Figure 9: Average test set classification error rate for the Leukemia gene dataset with 7129 features.

(a) Zoomed to 300 features retained starting with 7129 features.

(b) Zoomed to 600 features retained starting with 7129 features.
Figure 10: This Figure redraws Fig. 9(a) (i.e. the across-trial average $\mu$) so as to also include, for each elimination method, the $\mu + \sigma$ curve (seen above the average curve $\mu$) and the $\mu - \sigma$ curve (seen below the average curve $\mu$), where $\sigma$ is the across-trial standard deviation of the elimination method.
(a) Average test set classification error rate for the Colon Cancer gene dataset with 2000 features and much fewer samples. SVM linear kernel case.

(b) This Figure redraws Fig. 11(a) (i.e. the across-trial average $\mu$) so as to also include, for each elimination method, the $\mu + \sigma$ curve (seen above the average curve $\mu$) and the $\mu - \sigma$ curve (seen below the average curve $\mu$), where $\sigma$ is the
(a) Average test set classification error rate for the Splice Scale dataset with 60 features; a dataset for the low-to-intermediate number of features case. SVM linear kernel case.

(b) This Figure redraws Fig. 12(a) (i.e. the across-trial average $\mu$) so as to also include, for each elimination method, the $\mu + \sigma$ curve (seen above the average curve $\mu$) and the $\mu - \sigma$ curve (seen below the average curve $\mu$), where $\sigma$ is the across-trial standard deviation of the elimination method.
is that our work addresses an important matter about positive definiteness (pertaining to solving QP problems via an active-set approach\textsuperscript{16}) in two different ways\textsuperscript{17} even though it seems\textsuperscript{10} did not discuss the algorithm separately for these two separate ways in conjunction with presenting the algorithm.\textsuperscript{18} Our second specialization of the algorithm in\textsuperscript{10} is of course that we focus on our particular novel quadratic programming (QP) problem statement\textsuperscript{19} (i.e. our QP1 is a specific QP problem, defined by specific matrix forms) and create a computationally low-cost algorithm in doing so. Herein we present our active-set method work as a novel theoretical mathematical contribution (wherein our devised Lemmas and Theorems are presented) even though we do not actually utilize this algorithm in our current feature elimination experiments herein.

Usually a primal iterative active-set method starts with a feasible initial $q_0$ and ensures each $q_k$ (at iteration $k$) is feasible\textsuperscript{10}. An optimal active set (the active set for $q^*$\textsuperscript{19}) is sought, via such iterations, at each of which, one constraint is dropped or added to the current (iteration’s) estimate of this set, called the Working Set $W$ ($W^k$ at iteration $k$\textsuperscript{20}\textsuperscript{10}). Specifically, to ensure $q_{k+1}$ is feasible, the direction $p_k$ along which to move from $q_k$ to reach $q_{k+1}$ (i.e. $q_{k+1} = q_k + \delta_k p_k$ for some $\delta_k \in \mathbb{R}$) is computed such that constraints identified by a set $W^k$ are fulfilled as equalities i.e. $a_i^T p_k = 0 \forall i \in W^k$; this ensures feasibility of $q_{k+1}$ because these $W^k$ constraints are also fulfilled at $q_{k+1}$ due to $a_i^T q_{k+1} = a_i^T (q_k + \delta_k p_k) = a_i^T q_k + \delta_k a_i^T p_k = a_i^T q_k + t_i$, for any $\delta \in \mathbb{R}$. I.e., this is an equality-constrained QP (ECQP) subproblem (of the ICQP problem), with the above constraint set $W^k$:

$$p_k = \min_{p_k} \frac{1}{2} p_k^T G p_k + h_k^T p_k \quad s.t. \quad a_i^T p_k = 0 \forall i \in W^k \tag{17}$$

where $h_k \equiv Gq_k + d$ which can be evaluated prior to solving (17)\textsuperscript{10}. Let $A$ denote the matrix with $i$-th row $a_i^T$. Let $A^\Sigma$ denote the matrix whose only rows are a subset of $A$’s as specified by an index set $\mathcal{I}$; e.g. $A^{\Sigma^k}$ denotes the matrix whose only rows are $a_i^T$ for constraints $i \in W^k$ in (17).

Let $N(A^W)$ denote the null space of $A^W$; a complete set of basis vectors for $N(A^W)$ can be arranged as columns of a matrix, denoted $Z$ herein. By Lemma 16.1 in\textsuperscript{10}, the first-order necessary conditions for $p_k$ to be a solution of (17) can be fulfilled in conjunction with requiring the KKT matrix

$$
\begin{pmatrix}
G & -A^W^T \\
A^W & 0
\end{pmatrix}
$$

and assuming that $Z^TZGZ$ is positive definite; that is, by making the following two assumptions (requirements):

- $R1$: Require rows of $A^W$ to be linearly independent\textsuperscript{21}
- $R2$: Require $Z^TGZ$ to be positive definite.

\textsuperscript{10}\textsuperscript{10} gives an active-set algorithm, “Algorithm 16.1 (Active-Set Method for Convex QP)” (aka A16.1 herein). Since herein we utilize this algorithm, we now discuss it in the context of $R1$ and $R2$.

For $R2$: For solving the ECQP, the A16.1 algorithm only says “solve” and also a discussion of whether $R2$ shall be fulfilled does not seem to be provided in\textsuperscript{10} in conjunction with presenting the algorithm. Nevertheless, when applying A16.1 to our particular QP problem\textsuperscript{10} in Sec.\textsuperscript{20}\textsuperscript{20} we provide a way that focuses on the prospect of ensuring that $R2$ is fulfilled, due to the above Lemma 16.1 remark about the solution $p_k$ of the ECQP\textsuperscript{22}.

\textsuperscript{16}Specifically, the positive definiteness of $Z^TZGZ$, a matrix we discuss below.

\textsuperscript{17}The first way will require $Z^TZGZ$ to be positive definite; the second way will not.

\textsuperscript{18}Our work is, of course, helped by the fact that the QP problem has a more specific form than the general form\textsuperscript{10} used by\textsuperscript{10}, as in our case the matrices that appear in the problem definition have a specific, known form, as we shortly discuss.

\textsuperscript{19}The active set $\mathcal{A}(q)$, at some feasible $q$, identifies constraints $i$ fulfilled as equalities at $q$ i.e. $a_i^T q = 0$\textsuperscript{10}.

\textsuperscript{20}Notice that by definition of $W$ a constraint may be active without being in $W$.

\textsuperscript{21}That is, LICQ (Linear Independence Constraint Qualification) is fulfilled for active constraint gradients\textsuperscript{10}, whereby valid use of KKT conditions (to solve the constrained optimization problem at hand) is enabled.

\textsuperscript{22}Note that $R2$ is for the case $N(A^{W^k}) \neq \emptyset$ (i.e. the null space does not only contain the zero-vector, i.e.
For R1: (This paragraph too gives mathematical details that pertain to the perspective that the problem is an ICQP problem, rather than pertain to the perspective that the problem also happens to be an SVM problem; the reason we do not here yet intuitively associate these mathematical details with SVM is that such association is postponed to Sec. 6.2 as mentioned earlier.) The strategy of A16.1 for R1 to be fulfilled at every ICQP iteration k is to start (at k = 0) with an \( A^W \) that fulfills R1 and to shrink or grow \( A^W \) by at most a single row of \( A \) (i.e. a single constraint of the ICQP) at each iteration (if not keeping \( A^W \) the same) while ensuring the row chosen to grow \( A^W \) is linearly independent of the existing rows (of \( A^W \)). Specifically, in the event \( p_k^a \) is found to be nonzero, denoting \( B = \{ i \in W^k | a_i^T p_k^* < 0 \} \), in A16.1 \([10]\) the ratio \( R_i = (t_i - a_i^T q_k)/a_i^T p_k^* \) is computed for each \( i \in B \), so as to compute \( \delta_k \equiv \min_{i \in B} (1, R_i) \) and \( j \equiv \arg \min_{i \in B} (1, R_i) \), so that, accordingly, if \( \delta_k < 1 \), \( W^{k+1} \) is set to \( W^k \cup \{ j \} \), with \( j \) referred to as the “blocking constraint”.

It is a “blocking constraint” because, as can be easily seen from the definitions of \( B \) and \( R_i \) that pertain to the abovementioned movement along the direction \( p_k^a \), taking along that \( p_k^a \) direction a whole step \( 1p_k^a \) (i.e. \( \delta_k p_k^a \) for \( \delta_k = 1 \)) is being blocked by the fact that one of the constraints (i.e. a “blocking constraint”) is becoming active upon traveling merely a fraction \( \delta_k < 1 \) of that whole step; the directional distance traveled is thus \( \delta_k p_k^a \) where \( \delta_k < 1 \). Else if a whole step can be travelled (i.e. \( \delta_k = 1 \)), \( W^{k+1} \) is set to \( W^k \); i.e., without having to modify the Working Set, we have moved an amount \( \delta_k p_k^a \) from \( q_k \) and arrived the new location \( q_{k+1} \). Else in the event \( p_k^a \) is instead found to be zero, A16.1 states it has reached its terminating condition unless the Lagrange multiplier for a constraint \( i \in W^k \) was found to be negative in which case A16.1 sets \( W^{k+1} \) to \( W^k \setminus i \) \([10]\); i.e., A16.1 removes constraint \( i \) from the Working Set since by convention an initial global assumption requiring Lagrange multipliers to be nonnegative was made (as often is made when utilizing Lagrange multipliers).

### 6.2 Specializing Algorithm A16.1 \([10]\) to our particular QP problem QP1

By comparing (6) to (16), notice in our QP1 formulation \([6]\) that \( I = \{1, \ldots, 2N\} \), \( q \equiv [q_{\text{opt}}^T, \xi_1 \ldots \xi_N]^T \), where \( q_{\text{opt}} \equiv [a \ b]^T \), \( G \equiv \begin{pmatrix} (||w||^2)^{-M} & 0_{1 \times N+1} \\ 0_{N+1 \times 1} & 0_{N+1 \times N+1} \end{pmatrix} \), \( d \equiv [0 \ 0 \ C1_{1 \times N}]^T \), \( a_i^T \) is the \( i \)-th row of \( A \equiv \begin{pmatrix} V_{N \times 2} & I_{N \times N} \\ 0_{N \times 2} & I_{N \times N} \end{pmatrix} \), \( V_{N \times 2} \) consists of \( 1 \times 2 \) rows \( v_1, \ldots, v_N \) where \( v_n \equiv [y_n (w^{-M})^T x_n^{-M} \ y_n] \), \( y \equiv [y_1 \ldots y_N]^T \), \( t \equiv [t_1 \ldots t_{2N}]^T \equiv [1_{1 \times N} \ 0_{1 \times N}]^T \). As mentioned earlier, these matrices exhibit a specific, highly regular form defined by e.g. many zeros and ones in fixed spots.

In discussing the properties of ECQP (note: not ICQP), \([10]\) made the assumption (see: page 444) that in the ECQP the number of constraints is not greater than the number of unknowns (i.e. the number of optimization parameters). We shall refer to this restriction as Restriction 1. When the ECQP occurs within an active-set algorithm such as we discussed when giving (17), this means the assumption that the number of elements in the Working Set \( W \) is not greater than the number of optimization parameters. Accordingly, we now make the observation that the active-set algorithm A16.1 in \([10]\) would be suitable for QP1 if the number of elements in set \( W \) (or, equivalently, the number of rows in \( A^W \)) is ensured to not be greater than \( N + 2 \) which is the number of parameters in the parameter vector \((a,b,\xi_1,\ldots,\xi_N)\) of QP1. To mathematically appreciate the above assumption made by \([10]\), one can consider it from the LICQ perspective, in conjunction with R1 above, as follows. As mentioned above, to utilize LICQ when solving the optimization problem at hand, one can fulfill R1, but since R1 cannot be fulfilled in the event \( A^W \) has more rows than columns (i.e. a simple fact from linear algebra), \( A^W \) needs to be have fewer rows than columns to fulfill R1 and LICQ, and this leads us back to the abovementioned assumption in \([10]\).

Shortly we will return to discussing Restriction 1. Now, let us introduce a central point, a point that will be soon concluded by our Lemmas and Theorem; this introduction, before those \( Z^k \neq 0 \); below we will additionally address the possibility of \( N(A^{W_k}) = 0 \) (i.e. the null space contains only the zero-vector i.e. is “empty”, i.e. \( Z^k = 0 \)).
mathematical details enter the picture, is to highlight this central point with an intuitive and less mathematical description. The central point is that in our specialization of A16.1 currently our focus when calculating the step direction \( p_k^* \) and taking the step \( \delta_k p_k^* \) from \( q_k \) to \( q_{k+1} \) is \( i) \) to ensure a sample is a “doubly-active” sample at \( q_k \) i.e. a sample whose both constraints are active at \( q_k \) and \( ii) \) find the direction \( p_k^* \) that both decreases the objective function and keeps that sample doubly-active upon taking the step \( \delta_k p_k^* \), and thus we refer to \( p_k^* \) as the sample’s “direction of remaining doubly-active (DRD)”. While moving along that sample's DRD, a second sample can become doubly-active before a whole step \( 1p_k^* \) is completed, blocking further movement along that DRD (whereby, the computed \( \delta_k \) is less than 1 and reflects the amount of uninterrupted unblocked movement), in which case the next movement can take place along that second doubly-active sample’s DRD (which would likewise be found by transferring the “doubly-active sample” designation to solely this new sample, just like that designation was previously given to a single sample (the previous sample) in calculating the direction \( p_k^* \) along which was then moved). To summarize intuitively, given a sample designated to be the doubly-active sample, as much movement as possible is made (along a so-called “DRD” direction computed for that sample) while decreasing the objective function and keeping that sample doubly-active, and after that movement, if the movement was interrupted by the presence of a “blocking constraint”, at the point of interruption a switch in movement direction takes place to the DRD of the new sample; i.e. a switch from a single sample being margin-setter to a different single sample being margin-setter. Our Lemmas and Theorem below show that this approach is synonymous with fulfilling \( R1 \) and \( R2 \) that were discussed in Sec. 6.1.

The “doubly-active” property of a sample is represented and notated as follows. In our ICQP problem \((6)\), wherein each sample \( x_n \) is represented by a pair of companion constraints \( y_n (aw^Tx_n + b) \geq 1 - \xi_n \) and \( \xi_n \geq 0 \), each pair contributes two rows to \( A \) and there are \( N \) samples (or pairs), and thus \( A \) has a total of \( 2N \) rows. Notationwise, the row arrangement we consider for the \( 2N \)-row \( A \) is that the top \( N \)-row half and the bottom \( N \)-row half are respectively formed by the first constraint type \( (y(aw^Tx_n + b) \geq 1 - \xi) \) and the second constraint type \( (\xi \geq 0) \). As we elaborate shortly, similarly the row arrangement we consider for the \( A^W \) matrix is a block arrangement with three blocks (instead of two seen above for \( A \)) which, from top to bottom, correspond to the three categories that samples fall into according to whether \( W \) (at an iteration of the active-set algorithm) contains 1) only the first-type constraint for the sample 2) both constraint types for the sample 3) only the second-type constraint for the sample. The second category here is designating the doubly-active property of a sample. Shortly we elaborate on the notation.

Restriction 1 on the size of set \( W \) raises the nontrivial question about how the particular constraints (no greater than \( N + 2 \)) for the initial set \( W \) should be selected at algorithm initialization among all \( 2N \) constraints. During this initialization, recall that essentially a classifier, specified (defined) by the following two pieces of information, is input into the algorithm: \( i) \) the particular set \( P \) of training samples that were assigned positive Lagrange multipliers by some classifier generator and \( ii) \) the values of those multipliers. Consider, first, that this classifier generator may or may not explicitly provide identification information that identifies a particular sample \( x_n \) within that particular set \( P \) as being the “margin-setter” sample, that is, the sample that the initial iteration of the active-set algorithm would utilize as being the (initial) doubly-active sample. Here is one instance where this identification is not provided by the classifier generator; this generator, which may be a QP solver such as LIBSVM, may assign, as we have experienced when using LIBSVM (albeit with scalar training data), the value \( C \) to all multipliers within that set; the inconvenience that this scenario brings is that the generator, by assigning to every sample in \( P \) the same multiplier, is not indicating which samples in the set \( P \) are the margin violators, unlike the alternative scenario wherein margin violators become identified by the generator via the means of setting to \( C \) the multipliers for only some of the samples in \( P \) (with the multipliers of remaining \( P \) samples assigned a value less than \( C \), so as to identify those as “the sample(s) at the margin” as opposed to margin violators). Consider, second, that in some cases, when \( f(x_n) \) is computed under the

\[ \text{Before continuing, the reader could recall that this fact about all positive multipliers being upper-bounded by } C \text{ is a characteristic of the soft-margin SVM; see e.g. [3].} \]
provided information \(i\) and \(ii\) above, it may unfortunately be that the discriminant function value \(y_n f(x_n)\) does not compute precisely to 1 for any \(x_n\) within set \(P\), such as seen in our experience with LIBSVM, and thus trying to identify which samples in \(P\) have their \(y_n f(x_n)\) equal to 1 is not a reliable means, either (for determining which samples are at the margin (or are doubly-active) and which other samples aren’t). Thus, extra measures may need to be taken to make that determination. In particular, in the event that one finds out that \(i\) the generator that is generating and providing a classifier as input into our active-set algorithm has happened to set all positive multipliers to \(C\) and \(ii\) the discriminant \(y_n f(x_n)\) is not computing to 1 for any of those samples (with those positive multipliers), a normalization measure can be taken whereby one can utilize a scaling variable to scale to 1 the particular \(y_n f(x_n)\) that is both \(1\) the largest among the particular \(x_n\) that have the positive multipliers and \(2\) positive (to ensure that that particular \(x_n\) is a correctly classified sample.) To summarize this paragraph, it is possible, by taking measures, to provide to the active-set algorithm the designation of what the algorithm’s initial doubly-active sample is or could be, even in the event there may seem to be potential numerical obstacles; once this initial designation is made, the algorithm can proceed as described above i.e. by essentially largely mode-switching between \(i\) moving along the DRD of a current doubly-active sample and \(ii\) when becomes necessary (i.e. when a “blocking constraint” is encountered along the movement path), switching to a new doubly-active sample so as to then move along its DRD. We show below that this approach is computationally low-cost. Specifically, the computational complexity at an ICQP iteration is essentially the complexity of computing the single basis vector for the null space \(N(A^W)\) of a highly sparse \(N + 1 \times N + 2\) matrix \(A^W\).

Shortly, in Lemma 3 and Lemma 4, respectively, we show that 1) fulfilling \(R1\) requires that our \(W\) not contain both constraints of a sample for more than two samples and that 2) fulfilling \(R2\) requires every sample to be represented in \(W\) (i.e. \(W\) contains at least one of two constraints of every sample, whereas, by contrast, A16.1 modifies \(W\) freely without this requirement since it addresses a more general case). Regarding how \(R1\) and \(R2\) can be fulfilled, our theorem shows shortly that \(W\) would need to contain exactly either \(N + 1\) or \(N + 2\) constraints (from among the \(2N\) constraints of the ICQP) that are \(i\) linearly independent and \(ii\) include a constraint for each of the \(N\) samples. This points out that via specialization a more specific Working Set strategy has emerged for QP1 from A16.1’s; i.e. A16.1 allows, by contrast, \(A^W\) to have fewer than \(N + 1\) rows so long as they are linearly independent. To summarize, as part of specializing A16.1 to our particular QP problem QP1, our theorem is extending A16.1’s \(W\) strategy, making it become more specific.

In preparation for the lemmas, we now elaborate on the notation introduced above. We consider the index sets \(W_1\) and \(W_2\) that respectively specify which rows of \(A\)’s top \(N\)-row half (for the constraints of the form \(y(a w^T x + b) \geq 1 - \xi\)) and bottom \(N\)-row half (for the constraints of the form \(\xi \geq 0\)) form \(A^W\). Note that \(W_1\) and \(W_2\) contain relative (not absolute) row indexes for \(A\)

\(\begin{bmatrix}
A^{W_1}
B
A^{W_2} + N
\end{bmatrix}
\)

where \(A^{W_1} \equiv \left[ V^{W_1 m_1 x_2} I^{W_1 1 x_1 n}\right]\) (where \(m_{11} \equiv card(W_{11}), B \equiv \left(0_{m_{12} x_2}\right)\), \(A^{W_1} \equiv \left[ V^{W_1 m_1 x_2} I^{W_1 1 x_1 n}\right]\) (where \(m_{12} \equiv card(W_{12})\)), and \(A^{W_2 + N} \equiv \left[ V^{W_1 m_1 x_2} I^{W_1 1 x_1 n}\right]\)

\(\text{24}\) The reader can easily conclude, from linear algebra, that the null-space of an \(N + 1 \times N + 2\) full-row-rank matrix is one-dimensional and a subspace of \(\mathbb{R}^{N+2}\) and thus it has a single basis vector that has \(N + 2\) coordinates.

\(\text{25}\) The set of absolute indexes of the \(A\) rows that form \(A^W\) is given by \(W \equiv W_1 \cup (W_2 + N)\) where the plus sign denotes elementwise addition.

\(\text{26}\) This is because, by definition of the Working Set \(W\), a constraint may be active without being in \(W\).
\([0_{m2} \times 2 \, I_{W2}^{w2} \, m2 \times N]\) (where \(m2 \equiv \text{card}(W_{22})\)).

**Lemma 1:** Collectively, rows of (i) \(A_{W11}\), (ii) \(A_{W22+N}\), and (iii) the bottom half of \(B\) (i.e. \([0 \, I_{W12}\]) are linearly independent.

**Proof:** Among the final \(N\) columns of these rows, the column at which 1 appears (with the other \(N - 1\) columns being 0) differs from row to row. Q.E.D.

**Lemma 2:** If an \(m \times n\) matrix \(M\) is widened by placing into it \(k\) zero-columns (at column indexes \(i \in \{1, \ldots, n + k\}\) specified by a set \(I\)), a new complete set of null-space basis vectors can be constructed from the old without computation in two basic steps: 1) Grow each old \(n \times 1\) basis vector to \((n + k) \times 1\), with 0s placed at coordinates \(i \in I\). 2) Into the basis vector set, additionally put \(u_i\) for each \(i \in I\) (where \(u_i\) is the special unit vector with 0s except 1 at \(i\)-th coordinate). Consequently, in the new \(Z\), each row \(j \notin I\) is the corresponding row of the old \(Z\), augmented with only 0s.

**Proof:** Right-multiplying a matrix by a (column) vector produces the weighted sum of the matrix columns, with weights being the vector elements. Thus: 1) The fact that the outcome of \(V\) is a zero-column. Since such columns have column index \(\geq 2\) and \(V\) contains at least one 0. Thus, \(Z\) has two columns, \(z_{r1}^{T}\), which is real and symmetric and has 0 as an eigenvalue. Since \(Z^{T}GZ\) too is real and symmetric and has 0 as an eigenvalue. Q.E.D.

**Lemma 3:** Fulfilling R1 requires \(W_{12}\) to contain at most two samples (indexes).

**Proof:** \(A_{W12}\), which is \([V_{W12}^{w12} \times 2 \, I_{W12}^{w12} \, m2 \times N]\), is the top half of \(B\). Subtracting the bottom half of \(B\) from the top half of \(B\) reduces \(B\) to \(\begin{pmatrix} V_{W12} & 0 \\ 0 & I_{W12} \end{pmatrix}\) whose top half \([V_{W12} \, 0]\) can be row-rearranged as \(\begin{pmatrix} V_{W12}^{\text{dep}} & 0 \\ V_{W12}^{\text{ind}} & 0 \end{pmatrix}\) where \(V_{W12}^{\text{dep}}\) and \(V_{W12}^{\text{ind}}\) denote the two blocks composed of, respectively, linearly dependent and independent rows of \(V_{W12}\). Since \(V_{W12}\) has two columns, the number of rows of \(V_{W12}^{\text{ind}}\) is at most two. Because the last \(N\) columns of the above top half \([V_{W12}^{\text{dep}} \, 0]\) are zero, each row in this top half is linearly independent of the rows in set \(J\), where \(J\) denotes the set of rows in \(A_{W11}\) and \(A_{W22+N}\), due to Lemma 1. Collectively, again due to Lemma 1, the rows in set \(J\) and the rows of the bottom half \([0 \, I_{W12}^{w12}]\) of \(B\) are linearly independent because among the final \(N\) columns of all of these rows the column at which 1 appears, with the other \(N - 1\) columns being 0, differs from row to row. Thus, the linearly dependent rows of \(A_{W}\), if any, are the rows of the above bottom block \([V_{W12}^{\text{dep}} \, 0]\). Q.E.D.

**Lemma 4:** Fulfilling R2 requires every sample \(n\) to be represented in \(W\), i.e. \(n \in W_1 \cup W_2\) \(\forall n\).

**Proof:** By contradiction. Suppose \(n \notin W_1 \cup W_2\) for some sample \(n\). Then, column \(n + 2\) of \(A^W\) is a zero-column. Since such columns have column index \(\geq 2\), by Lemma 2 each of rows \(n \leq 2\) of \(Z\) is the corresponding row of \(\tilde{Z}\) augmented with only 0s (where \(\tilde{Z}\) is the null-space matrix that would result from first removing the zero-columns of \(A^W\)); i.e. \(z_{r1}\), the first row of \(Z\), contains at least one 0. Thus, \(z_{r1}^{T}z_{r1}\), which is real and symmetric, has 0 as an eigenvalue. Since \(Z^{T}GZ\) is ||\(w^{T-M}\)||\(z_{r1}^{T}z_{r1}\), \(Z^{T}GZ\) too is real and symmetric and has 0 as an eigenvalue. Q.E.D.

**Theorem 1:** At each ICQP iteration \(k\), fulfilling R1 and R2 would require \(W^k\) to contain exactly either \(N + 1\) or \(N + 2\) constraints (from among \(2N\) ICQP constraints) that i) are linearly independent and ii) include a constraint for each of the \(N\) samples.\(^{27}\) We refer to these conditions as \(C1\) and \(C2\).

**Proof:** By Lemma 3, fulfilling R1 requires \(W_{12}\) to be (a) empty or contain either (b) one or (c) two samples (sample indexes); i.e., \(A_{W12}\) is required to respectively be (a) empty or contain either (b) one or (c) two (linearly independent) rows. Under these three options wherein \(A^W\) is full-row-rank with at least \(N\) (linearly independent) rows due to collectively Lemmas 1, 3, 4, \(Z\) is,

\(^{27}\) Recall from above that A16.1\(^{[10]}\) allows, by contrast, \(A^W\) to have fewer than \(N + 1\) rows, so long as they are linearly independent; i.e. our Theorem has introduced a specialization of A16.1, extending its Working Set strategy.
respectively, two-column \( (A^W \text{ has } N \text{ rows}) \) or one-column \( (A^W \text{ has } N+1 \text{ rows}) \) or empty \( (A^W \text{ has } N+2 \text{ rows}) \). Option 1 does not fulfill \( R2 \) because, when the first row \( zr_1 \) of \( Z \) is two-column (i.e. \( zr_1 \equiv [z_1 z_2] \)), \( zr_1^T zr_1 \equiv \left( \begin{array}{c} z_1^2 \\ z_2^2 \end{array} \right) \) is not positive definite and thus neither is \( Z^T GZ \). This requires \( W_{12} \) (and thus both \( W_1 \) and \( W_2 \)) to be nonempty. Under option 2, \( zr_1 \) is a scalar \( z \) and \( R2 \) is fulfilled because \( Z^T GZ \), which is \( (|w|^2)^{-M} z^2 \), is a positive scalar (and thus positive definite). Under option 3, wherein \( R2 \) does not apply (since \( Z \) is empty), the KKT matrix is nonsingular because \( A^W \) is. Thus the option needs to be option 2 or 3; i.e. \( Z \) is one-column if not empty. Hence the two conditions stated in the Theorem. Q.E.D.

While the optimization parameter set is \( \{a, b, \xi_1, \ldots, \xi_N\} \) (i.e. includes slackness parameters \( \xi_n \) apart from the parameter pair \( (a,b) \)), at any iteration of the active-set algorithm the \( (a,b) \) part of the parameter set \( \{a, b, \xi_1, \ldots, \xi_N\} \) sufficiently specifies a found solution (where “found solution” means a feasible point that is either an interim iteration-specific solution or the found final solution for the algorithm), so long as it is ensured that the set \( W_{12} \) is not empty at that solution i.e. so long as there is a sample \( x_n \) ensured to be the single doubly-active sample discussed above. Utilizing Theorem 1, an active-set algorithm can ensure this. This may involve a (within-iteration) scaling of the \( (a,b) \) (i.e. \( q^{ot} \)) part of \( q \) so as to make equal to 1 the discriminant function value \( y_n f(x_n) \) for that sample \( x_n \) (since \( q^{ot} \) is the only part of \( q \) that determines that \( y_n f(x_n) \) value), since \( y_n f(x_n) \) being equal to 1 does ensure the sample is doubly-active. Upon such scaling via utilization of the \( q^{ot} \) part of \( q \), in order to accordingly adjust the remaining \( q \) coordinates the new slacknesses \( \xi_i = \max(0, 1 - g_i) \forall i \) can be calculated.

Now we discuss our specialization of A16.1 so as to fulfill \( C1 \) and \( C2 \), as well as show the constraint selection discussed in Theorem 1 is straightforward and computationally low-cost; in particular, we show we reduce the \( p_k^* \) computation to only \( N \) additions and 3 multiplications, given \( Z^k \). At initial iteration \( (k = 0) \), using the boundary (i.e. \( a = 1, b = 0 \)) information being input to the algorithm (aka, as we discussed earlier, the information identifying both a particular set \( P \) of samples as having positive Lagrange multipliers and the values of those multipliers), one of the correctly classified samples \( x_n \in P \) can be made and designated doubly-active (with scaling performed if necessary) and placed into \( W_{12} \); accordingly, the other \( N-1 \) samples, upon computing slackness for them, can be placed into either \( W_1 \) or \( W_2 \) based on individual slackness value. Such \( W^0 \) has \( N + 1 \) samples and fulfills \( C1 \) and \( C2 \). Subsequently, for \( k > 0 \), to fulfill \( C1 \) and \( C2 \), our specialization of \( W \) modifications is as follows. We only need to compute \( p_k^* \) when \( W \) contains \( N+1 \) constraint\(^ {28} \), in which case \( Z^k \) is one-column \( (Z^k \equiv [z_1 \ldots z_{N+2}]^T) \); i.e. the null space \( N(A^W) \) of \( A^W \) is a one-dimensional subspace of \( \mathbb{R}^{N+2} \). To compute \( p_k^* \), we employ the “null-space method” used for solving ECQP problems\(^ {10} \); the approach is based on taking an input \( p_k^{in} \in N(A^W) \) (that fulfills \( A^W p_k^{in} = 0 \) of \( 17 \)); e.g. due to \( Z^k \) being one-column, \( p_k^{in} \) can be set to a multiple of \( Z^k \), e.g. \( Z^k \) itself and computing a displacement vector \( n \), with \( p_k^* = p_k^{in} + n \). Since \( p_k^* \) must fulfill \( A^W p_k^* = 0 \) \( 17 \) (i.e. \( p_k^* \) is in \( N(A^W) \)), we can see that \( n \) can too be (i.e. like \( p_k^{in} \)) in \( N(A^W) \) and thus \( n = Z^k n_z \) (and may be 0 or nonzero) for some column-vector \( n_z \). Finding \( n_z \) takes almost no computation because \((Z^k^T G Z^k)n_z = -Z^k^T r_k \) \(^ {10} \) where both \( Z^k^T G Z^k \) (which is \((|w|^2)^{-M} z^2 \)) and \( Z^k^T r_k \) are known scalars (and thus so is \( n_z \), i.e. \( n_z = n_z \); here, \( r_k \equiv h_k + G p^{in}_k = (|w|^2)^{-M}(q_k + p^{in}_k G) 0 C11xN)^T \). Thus when \( p^{in}_k \) is set to \( Z^k \) itself (as mentioned above) the \( p_k^* \) can be found by simply multiplying \( Z^k \) by the scalar

\[-(\frac{q_k}{z_1} + \frac{C}{(|w|^2)^{-M} z_1^2} \sum_{i=3}^{N+2} \sum_{i=3}^{N+2} z_i) \].

We have thus reduced, as mentioned above, the \( p_k^* \) computation to only \( N \) additions and 3 multiplications, given \( Z^k \). We have thus reduced, as mentioned above, the complexity of the \( p_k^* \) computation to the complexity of finding the single basis vector \( Z^k \) for iteration \( k \). After finding \( p_k^* \), one can compute \( \delta_k \), determine \( j \equiv \arg \min_{i \in B} (R_i) \) and associated

\(^{28}\) Because in the \( N + 2 \) case \( Z \) (and thus \( p_k^* \)) is \( 0 \); cf. proof of Theorem 1.

\(^{29}\) \( Z^k^T G Z^k \) may seem computationally costly but it is not, because, due to \( Z^k \) being one-column, \( Z^k^T G Z^k \) is given by the scalar \((|w|^2)^{-M} z^2 \) which is not computationally costly.

\(^{30}\) Subscript \( i \) as used here on \( q \) and \( p^{in}_k \) for \( i = 1 \) denotes \( i \)-th coordinate.
sample \( n_j \), upon which two cases need to be considered. In the first case, defined as \( \delta_k \) being 1, there is no blocking constraint (i.e. one can move from \( q_k \) to \( q_k + 1p_k^* \) without interruption); accordingly the sample currently designated “doubly-active” can maintain that designation and \( W \) can remain the same. In the second case, defined as \( 0 < \delta_k < 1 \), there is a blocking constraint, which is a constraint associated with \( n_j \), and thus \( n_j \) can become the newly designated doubly-active sample; i.e. \( W \) can be modified by placing \( j \) into \( W \) to replace in \( W \) a constraint of the previous doubly-active sample. At any setting, or designation, of a sample as “doubly-active” sample, slackness may need to be computed for the remaining \( N - 1 \) samples to ensure that all slackness values are consistent with the contents of \( W \).

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