Multiclass Universum SVM

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Abstract
We introduce Universum learning for multiclass problems and propose a novel formulation for multiclass universum SVM (MU-SVM). We also propose an analytic span bound for model selection with $\sim 2 - 4 \times$ faster computation times than standard resampling techniques. We empirically demonstrate the efficacy of the proposed MU-SVM formulation on several real world datasets achieving $> 20\%$ improvement in test accuracies compared to multi-class SVM.

1. Introduction

Many applications of machine learning involve analysis of sparse high-dimensional data, where the number of input features is larger than the number of data samples. Such settings are typically seen in several real life applications in domains such as, healthcare, autonomous driving, prognostics and health management etc. (Cherkassky & Mulier, 2007). Such high-dimensional data sets present new challenges for most learning problems. Novel data intensive deep architectures are naturally not suited for such scenarios (Goodfellow et al., 2016). Recent studies have shown Universum learning to be particularly effective for such high-dimensional low sample size data settings (Sinz et al., 2008; Chen & Zhang, 2009; Dhar & Cherkassky, 2015; Lu & Tong, 2014; Qi et al., 2014; Shen et al., 2012; Wang et al., 2014; Zhang et al., 2008; Xu et al., 2015; 2016; Zhu, 2016; Chen et al., 2017; Dhar & Cherkassky, 2017). However, most such studies are limited to binary classification problems. On the other hand, many practical applications involve classification of more than two categories. In order to incorporate a priori knowledge (in the form of universum data) for such applications, there is a need to extend universum learning for multiclass problems.

In this paper we focus on formulating the universum learning for multiclass SVM under balanced settings with equal misclassification costs. Researchers have proposed several methods to solve a multiclass SVM problem. Typically these methods follow two basic approaches (Hsu & Lin, 2002; Wang & Xue, 2014). The first approach follows an Error Correcting Output Code (ECOC) based setting (Dietterich & Bakiri, 1995), where several binary classifiers are combined to solve the multiclass problem viz., one-vs-one, one-vs-all, directed acyclic graph SVM (Platt et al., 1999). Previous works, such as (Sinz, 2007; Chen & Zhang, 2009) which follow this setting, focus on the binary universum learning paradigm and only provide “some hints” for their extensions to the multiclass problems. An alternative to the ECOC based setting is the direct approach, where the entire multiclass problem is solved through a single larger optimization formulation (Vapnik, 1998; Crammer & Singer, 2002; Weston & Watkins, 1998). Recently, (Zhang & LeCun, 2017) adopted such a direct approach for universum learning under a probabilistic framework using a logistic loss function. This paper also adopts such a direct approach, but proposes an alternate universum learning framework that utilizes an SVM like loss function following (Crammer & Singer, 2002), and introduces the Multiclass Universum SVM (MU-SVM) formulation. The proposed framework allows for: a) an efficient implementation for MU-SVM using existing multiclass SVM solvers (Section 3.2), and b) deriving practical analytic error bounds for model selection (Section 3.3). Further, compared to ECOC based approaches, we provide a unified framework for multiclass learning under universum settings, with similar (or better) performance accuracies (see Appendix B.1).

The main contributions of this paper are as follows:

1. We formalize the notion of universum learning for SVM under multiclass settings, and propose a novel direct formulation called Multiclass Universum SVM (MU-SVM) (in Section 3.1). The proposed MU-SVM formulation has the neat property that it reduces to: i) standard (C&S) multiclass SVM in absence of universum data and ii) binary U-SVM formulation (Weston et al., 2006) for two-class problems (Section 3.1, Proposition 1). This consolidates the propriety of MU-SVM as the apt extension for multiclass SVM under universum settings.

2. The proposed formulation has a desirable structure that renders the MU-SVM formulation solvable through
any state-of-art multiclass SVM solvers (Section 3.2, Proposition 2).

3. We provide a new Span definition for multiclass formulations, and derive a leave-one-out bound for MU-SVM (Section 3.3, Theorem 1). Under additional assumptions, we provide a computationally efficient version of the leave-one-out error bound (Section 3.3, Theorem 2), which presents a practical mechanism for model selection.

4. Empirical results are provided in support of the proposed strategy (Section 4).

Finally, conclusions are presented in Section 5.

Note that, a shorter version of this work is available in (Dhar et al., 2016). Compared to (Dhar et al., 2016), this paper includes additional proofs and results as highlighted below,

- This paper provides the new Propositions 1, 2 & 3.
- We provide a new leave-one-out bound in Theorem 1 without any assumptions.
- Under the assumptions in Section 3.3, we provide a stricter leave-one-out error bound, which holds for both Type 1 & 2 support vectors.
- Exhaustive results for all the claims are provided for additional data sets.

2. Multiclass SVM

This section provides a brief description of the multiclass SVM formulation following (Crammer & Singer, 2002). Given i.i.d training samples \((x_i, y_i)_{i=1}^n\), with \(x \in \mathbb{R}^d\) and \(y \in \{1, \ldots, L\}\); where \(n\) is the number of training samples, \(d\) is the dimensionality of the input space and \(L\) is the total number of classes, the task of a multiclass classifier is to estimate a vector valued function \(f = [f_1, \ldots, f_L]\) for predicting the class labels for future unseen samples \((x, y)\) using the decision rule \(\hat{y} = \arg\max_{l=1,\ldots, L} f_l(x)\). The C&S multiclass SVM is a widely used formulation which generalizes the concept of large margin classifier for multiclass problems. This multiclass SVM setting employs a special margin-based loss (similar to the hinge loss),

\[
\mathcal{L}(y, f(x)) = [\max_l(f_l(x) + 1 - \delta_{yl}) - f_y(x)]_+ \text{ where } [a+] = \max(a, 0) \text{ and } \delta_{yl} = \begin{cases} 1; & y = l \\ 0; & y \neq l \end{cases}
\text{ (see Fig 1)}.
\]

Here, for any sample \((x, y = k)\), having \(\mathcal{L}(y, f(x)) = 0\) ensures a margin-distance of ‘+1’ for the correct prediction i.e. \(f_k(x) - f_l(x) \geq 1; \forall l \neq k\). The SVM multiclass formulation (for linear parameterization) is provided below:

\[
\min_{w_1, \ldots, w_L, \xi} \frac{1}{2} \sum_{l=1}^L ||w_l||^2 + C \sum_{i=1}^n \xi_i \\
\text{s.t.} \quad (w_y - w_l)\top x_i \geq e_{il} - \xi_i; \quad e_{il} = 1 - \delta_{il}
\]

\(i = 1 \ldots n, \quad l = 1 \ldots L\)

here, \(f_l(x) = w_l\top x\). Note that training samples falling inside the margin border (‘+1’) are linearly penalized using the slack variables \(\xi_i \geq 0, \quad i = 1 \ldots n\) (as shown in Fig 1). These slack variables contribute to the empirical risk for the multiclass SVM formulation \(R_{emp}(w) = \sum_{i=1}^n \xi_i\). The SVM formulation attempts to strike a balance between minimization of the empirical risk and the regularization term. This is controlled through the user-defined parameter \(C \geq 0\).

3. Multiclass Universum SVM

3.1. Multiclass U-SVM formulation

The idea of Universum learning was introduced by (Vapnik, 1998; 2006) to incorporate a priori knowledge about admissible data samples. The Universum learning was introduced for binary classification, where in addition to labeled training data we are also given a set of unlabeled samples from the Universum. The Universum contains data that belongs to the same application domain as the training data. However, these samples are known not to belong to either class. In fact, this idea can also be extended to multiclass problems. For multiclass problems in addition to the labeled training data we are also given a set of unlabeled examples from the Universum. These Universum samples are known not to belong to any of the classes in the training.

\footnote{We refer to the C & S formulation in (1) as SVM throughout.}
data. For example, if the goal of learning is to discriminate between handwritten digits 0, 1, 2,...,9; one can introduce additional ‘knowledge’ in the form of handwritten letters A, B, C,...,Z. These examples from the Universum contain certain information about handwriting styles, but they cannot be assigned to any of the classes (0 to 9). Also note that, Universum samples do not have the same distribution as labeled training samples. These unlabeled Universum samples are introduced into the learning as contradictions and hence should lie close to the decision boundaries of all the classes 1...L. This argument follows from (Vapnik, 2006; Weston et al., 2006), where the universum samples lying close to the decision boundaries are more likely to falsify the classifier. To ensure this, we incorporate a Δ-insensitive loss function for the universum samples (shown in Fig 2). This Δ-insensitive loss forces the universum samples to lie close to the decision boundaries (‘0’ in Fig. 2). Note that, this idea of using a Δ-insensitive loss for Universum samples has been previously introduced in (Weston et al., 2006) for binary classification. However, different from (Weston et al., 2006), here the Δ-insensitive loss is introduced for the decision boundary for all the classes i.e. \( w_i^T x^* - \max_{l=1...L} w_l^T x^* = 0; \forall k = 1...L \). This reasoning motivates the new multiclass Universum-SVM (MU-SVM) formulation where:

- Standard hinge loss is used for the training samples (shown in Fig. 1). This loss forces the training samples to lie outside the ‘+1’ margin border.

- The universum samples are penalized by a Δ-insensitive loss (see Fig. 2) for the decision functions of all the classes \( f = [f_1,...,f_L] \).

This leads to the MU-SVM formulation. Given training samples \( T := (x_i, y_i)_{i=1}^n \), where \( y_i \in \{1,...,L\} \) and additional unlabeled universum samples \( U := (x_i^u)_{i=1}^m \). Solve:

\[
\min_{w_1,...,w_L,\xi,\xi} \sum_{i=1}^n \frac{1}{2} \|w_i\|^2 + C \sum_{i=1}^n \xi_i + C^* \sum_{i'=1}^m \sum_{k=1}^L \xi_{i'k}\]
\[s.t. \ \forall i = 1...n, \ i' = 1...m \]
\[
(w_i - w_i^T x_i) \geq \xi_i; \ e_{il} = 1 - \delta_{il}; \ l = 1...L
\]
\[
(w_i^T x_i^u - \max_{l=1...L} w_l^T x_i^u) \leq \Delta + \xi_{i'k}; \ k = 1...L
\]
\[
\xi_{i'k} \geq 0, \ \delta_{il} = \begin{cases} 1; & y_i = l \\ 0; & y_i \neq l \end{cases}
\]

Here, for the \( k^{th} \) class decision boundary the universum samples \( (x_i^u)_{i=1}^m \) that lie outside the Δ-insensitive zone are linearly penalized using the slack variables \( \xi_{i'k} \geq 0, \ i' = 1...m \). The user-defined parameters \( C, C^* \geq 0 \)

Proposition 1. For binary classification \( L = 2 \), \( 2 \) reduces to the standard U-SVM formulation in (Weston et al., 2006) with \( w = w_1 - w_2 \) and \( b = 0 \).

3.2. Computational Implementation of MU-SVM

This section describes computational implementation of the MU-SVM formulation (2). Here, for every universum sample \( x_i^u \) we create \( L \) artificial samples belonging to all the classes, i.e. \( (x_i^u, y_i^u_1 = 1),...,(x_i^u, y_i^u_L = L) \) as below,

\[
(x_i, y_i) = \begin{cases} (x_i^u, y_i^u_1) & i = 1...n \\ (x_i^u, y_i^u_L) & i = n + 1...n + mL; \ i' = 1...m; \ l = 1...L \end{cases}
\]

Proposition 2. Under transformation (3), the MU-SVM formulation in eq. (2) can be exactly solved using,

\[
\min_{w_1,...,w_L,\xi} \frac{1}{2} \sum_{l=1}^L \|w_l\|^2 + \sum_{i=1}^{n+mL} C_i \xi_i
\]
\[s.t. \ (w_{y_i} - w_l)^T x_i \geq e_{il} - \xi_i \]
\[
i = 1...n + mL, \ l = 1...L
\]

The formulation (4) has the same form as (1) except that the former has additional \( mL \) constraints for the universum samples. Like most other SVM solvers, the MU-SVM formulation in (4) is also solved in its dual form as shown in Algorithm 1 see (Hsu & Lin, 2002). Hence, the computational complexity is same as solving a multiclass SVM formulation (in (1)) with \( n + mL \) samples. Most off-the-shelf multiclass SVM solvers can be used for solving the proposed MU-SVM.

3.3. Model Selection

As presented in (5), the current MU-SVM algorithm has four tunable parameters: \( C, C^* \), kernel parameter, and \( \Delta \). So in practice, multiclass SVM may yield better results than MU-SVM, simply because it has an inherently simpler model selection. Successful application of the proposed MU-SVM heavily depends on the optimal tuning of its model parameters. This paper adopts a simplified strategy
Algorithm 1 MU-SVM (dual form)
1. Given training \((x_i, y_i)_{i=1}^n\) and universum \((x'_i)_{j=1}^m\)
2. Transform (3) and solve (5),
\[
\max_{\alpha} \quad W(\alpha) = -\frac{1}{2} \sum_{i,j} \sum_l \alpha_{il} \alpha_{jl} K(x_i, x_j) - \sum_i \alpha_{il} e_{il}
\]
s.t. \(\sum_i \alpha_{il} = 0\) \(\alpha_{il} \leq C_l\) if \(l = y_i\); \(\alpha_{il} \leq 0\) if \(l \neq y_i\)
\(i, j = 1 \ldots n + mL\), \(l = 1 \ldots L\)
3. Obtain the class label using the following decision rule:
\[
y = \arg\max_i \sum_l \alpha_{il} K(x_i, x)
\]
for model selection previously used in (Cherkassky et al., 2011). This mainly involves two steps,

a. First, perform optimal tuning of the \(C\) and kernel parameters for multiclass SVM classifier. This step equivalently performs model selection for the parameters specific only to the training samples in the MU-SVM formulation (2).

b. Second, tune the parameter \(\Delta\) while keeping \(C\) and kernel parameters fixed (as selected in step a). Parameter \(C^*/C = \frac{n}{m^T}\) is kept fixed throughout the paper to ensure equal contribution of training and universum samples in the optimization formulation.

This strategy selects an MU-SVM solution (in step b) close to a given SVM solution (selected in step a). The model parameters in Steps (a) & (b) are typically selected through resampling techniques such as, leave one out (l.o.o) or stratified cross-validation approaches (Japkowicz & Shah, 2011). Of these approaches, l.o.o provides an almost unbiased estimate of the test error (Luntz, 1969; Scholkopf & Smola, 2001). However, on the downside it is very computationally intensive. In this paper, we propose a new analytic bound for the leave-one-out error for MU-SVM formulation. The proposed bound can be used for model selection in Steps (a) & (b) and provides a computational edge over standard resampling techniques. Detailed discussion regarding this new l.o.o error bound is provided next.

Note that, the l.o.o formulation with the \(t^{th}\) training sample dropped is the same as in (5) with an additional constraint \(\alpha_{il} = 0\); \(\forall l\). Then, the l.o.o error is given as: \(R_{l.o.o} = \frac{1}{n} \sum_{i=1}^n I[y_i \neq \hat{y}_i]\), where \(\hat{y}_i = \arg\max_i \sum_l \alpha_{il}^t K(x_i, x_t)\) is the predicted class label for the \(t^{th}\) sample and \(\alpha^t = [\alpha^t_1, \ldots, \alpha^t_{i}, \ldots, 0, \ldots, 0] = 0, \ldots, \alpha^t_L = 0, \ldots\) is the l.o.o solution. In this paper, we follow a strategy very similar to the one used in (Vapnik & Chapelle, 2000), and derive the new l.o.o bound for the MU-SVM formulation in (5). The necessary prerequisites are presented next.

Definition 1. (Support vector categories)
1. A support vector obtained from eq. (5) is called a Type 1 support vector if \(0 < \alpha_{iy} < C_i\). This is represented as, \(SV_1 = \{ i \mid 0 < \alpha_{iy} < C_i\}\)
2. A support vector obtained from eq. (5) is called a Type 2 support vector if \(\alpha_{iy} = C_i\). This is represented as, \(SV_2 = \{ i \mid \alpha_{iy} = C_i\}\)

The set of all support vectors are represented as, \(SV = SV_1 \cup SV_2\). Similarly, the set of support vectors for l.o.o solution is given as \(SV^t\). Under definition (1) we have,

Lemma 1. If in leave-one-out procedure a Type 1 support vector \(x_i\) is classified incorrectly, then we have,
\[
S_t \ max(\sqrt{2D}, \frac{1}{\sqrt{C}}) \geq 1
\]

where,
\[
S_i^2 = \min_{\beta_i} \sum_{i,j} \left(\sum_{l} \beta_{il} \beta_{jl}\right) K(x_i, x_j)
\]
s.t. \(\alpha_{il} - \beta_{il} \leq C_l\); \(\forall\{i \neq t, l\} 0 < \alpha_{il} < C_l\); \(l = y_i\)
\(\alpha_{il} - \beta_{il} \leq 0\); \(\forall\{i \neq t, l\} \alpha_{il} < 0\); \(l \neq y_i\)
\(\beta_{il} = 0\); \(\forall i \notin SV_1 \{t\} \forall l = 1 \ldots L\)
\(\beta_{il} = \alpha_{il}\); \(\forall l = 1 \ldots L\)
\(\sum_{l} \beta_{il} = 0\)

\(S_t := \text{Span of the Type 1 support vector} x_i\)
\(D := \text{Diameter of the smallest hypersphere containing all training samples}\).

This leads to the following upper bound on the l.o.o error.

Theorem 1. The leave-one-out error is upper bounded as:
\[
R_{l.o.o} \leq \frac{1}{n} (|\Psi_1| + |\Psi_2|)
\]

\(\Psi_2 := \{ t \in SV_1 \cap T \mid S_t \ max(\sqrt{2D}, \frac{1}{\sqrt{C}}) \geq 1 \}\)

\(\Psi_1 := \{ t \in SV_2 \cap T \}; \mid 
\mid := \text{Cardinality of a set} \text{ and } T := \text{Training Set}\).

Following Theorem 1, it is desirable to select a model with a) lower number of Type 2 training support vectors and, b) smaller span for the type 1 training support vectors. Roughly, for a fixed number of type 2 support vectors a solution with smaller span value (for the type 1 training support vectors) could yield lower test error. The following proposition shows how the universum samples influence these span values in (6).
**Proposition 3.** If the Type 1 training support vectors i.e. \( t \in SV_1 \cap T \) for SVM and MU-SVM solutions remain same, then \( S_{SV}^M \geq S_{SV}^I ; \forall t \in SV_1 \cap T \).

Loosely speaking, for cases where the type of training support vectors remain same, introducing universum samples through the MU-SVM formulation could result in smaller span values and better generalization for future test data compared to standard SVM solution.

Now, Theorem 1 provides an analytic tool for model selection with small l.o.o error. Here, the right hand side of (7) serves as a leave-one-out error estimate, and the goal is to select a model parameter which minimizes this value. However, the practical utility of (7) is limited due to the significant computational complexity involved in estimating the span of the type 1 training support vectors \( \sim O(n + mL)^4 \) (worst case). Next, we provide a more computationally attractive alternative to the above l.o.o bound.

**Assumption:** For the MU-SVM solution,

1. The set of support vectors of the Type1 and Type2 categories remain the same during the leave-one-out procedure.
2. The dual variables of the Type1 support vectors have only two active elements i.e. \( \forall x_i \) s.t. \( \{0 < \alpha_{iy_i} < C_i\} \exists k \neq y_i \) s.t. \( \alpha_{ik} = -\alpha_{iy_i} \).

**Lemma 2.** Under the above assumptions the following equality holds for both Type 1 & 2 support vectors,

\[
S_{t}^2 = \left[ \alpha_t^T \sum_{i \in SV_1} \sum_l \alpha_{il} K(x_i, x_l) \right] - \alpha_{ty_i} g_{yik}^T \sum_{i \in SV} \sum_l \alpha_{il} K(x_i, x_l)]
\]

with, \( S_{t}^2 = \{ \min \beta \sum_{i,j} (\sum_{l} \beta_{il} \beta_{jl}) K(x_i, x_j) \} \beta_t = \alpha_t ; \sum_{l} \beta_{il} = 0 \); \( i,j \in SV_1 \) and \( g_{yik} = [0, \ldots, 1, \ldots, -1, \ldots, 0] ; k = \arg\max_j \sum_q \alpha_{jq} K(x_j, x_l) \)

Now \( S_t \) can be efficiently computed using lemma (3).

**Lemma 3.** Under Assumptions (i) & (ii)

\[
S_{t}^2 = \begin{cases} 
\alpha_t^T \left[ (H^{-1})_{tt} \right]^{-1} \alpha_t & t \in SV_1 \cap T \\
\alpha_t^T \left[ K(x_t, x_t) \otimes I_L - (2H)^{-1} K_{L} \right] \alpha_t & t \in SV_2 \cap T 
\end{cases}
\]

where, \( H := \begin{bmatrix} K_{SV} \otimes I_L & A^T \\ A & 0 \end{bmatrix} \)

\[
A := I_{|SV_1|} \otimes (1_L)^T; \quad 1_L = \left[ \frac{1}{L} \ldots \frac{1}{L} \right]
\]

\((H^{-1})_{tt} := \text{sub-matrix of } H^{-1} \text{ for indices } i = (t-1)L + 1 \ldots tL
\)

\(K_{SV} := \text{Kernel matrix of Type 1 support vectors.}
\)

\(K_t = [(k_t^T \otimes 1_L) 0_{L \times |SV_1|}]^T \)

where, \( k_t = n_{|SV_1|} \) dim vector where ith element is \( K(x_i, x_t) \), \( \forall x_t \in SV_1 \); and \( \otimes \) is the Kronecker product.

Finally, we have,

**Theorem 2.** Under the Assumptions (i) & (ii) the leave-one-out error is upper bounded as:

\[
R_{l.o.o} \leq \frac{1}{n} \left| \Psi_3 \right|
\]

\[\Psi_3 = \left\{ t \in SV \cap T | S_{t}^2 \geq \alpha_t^T \sum_{i \in SV} \sum_l \alpha_{il} K(x_i, x_t) \right\} \]

and \( T := \text{Training Set} \) and \( S_t := \text{defined in Lemma 3} \)

Note that, similar to (Vapnik & Chapelle, 2000), the assumptions (i) & (ii) are not satisfied in most cases. Nevertheless, Theorem 2 provides a good approximation of the l.o.o procedure (see Section 4.2.2). In addition, compared to Theorem 1, it provides the following advantages,

- Eq. (9) is valid for both type 1 & 2 training support vectors and typically results in a stricter bound.
- Span computation for all support vectors requires inverting the \( H \) - matrix only once (Lemma 3). This results to an overall cost of \( O(n + mL)^3 \) for computing (9) and provides a computation edge over (7) which involves a cost of \( O(n + mL)^4 \).

Empirical results for model selection using Theorem 2 are provided in Section 4.2.2.

### 4. Empirical Results

#### 4.1. Datasets and Experimental settings

Our empirical results use three real life datasets:

- **German Traffic Sign Recognition Benchmark** (GTSRB) (Stallkamp et al., 2012): The goal here is to identify the traffic signs for the speed-zones ‘30’, ‘70’ and ‘80’. Here, the images are represented by their histogram of gradient (HOG 1) features. The experimental setting is provided in Table 1. For this data we use three kinds of Universum:
  - Random Averaging: synthetically created by first selecting a random traffic sign from each class (‘30’, ‘70’ and ‘80’) in the training set and averaging them.
Table 1: Real-life datasets.

| DATASET | TRAIN/TEST SIZE | DIMENSION |
|---------|-----------------|-----------|
| GTSRB   | 300 / 1500      | 1568      |
|         | (100 / 500 PER CLASS) (HOG FEATURES) |          |
| ABCDETC | 600 / 400       | 10000     |
|         | (150 / 100 PER CLASS) (100 x 100 PIXEL) |          |
| ISOLET  | 500 / 500       | 617       |
|         | (100 / 100 PER CLASS) |      |

- **Non-Speed**: all other non-speed zone traffic signs.
- **Sign 'priority-road'**: An exhaustive search over several non-speed zone traffic signs showed this universum to provide the best performance (Appendix B.3)

**Handwritten characters (ABCDETC)** (Weston et al., 2006): The data consists images of handwritten digits ‘0-9’, uppercase ‘A-Z’, lowercase letters ‘a-z’ and some additional symbols: ! ? , . ; : = - + / ( ) $ % ` @. The goal here is to identify the handwritten digits ‘0’ - ‘3’ based on their pixel values. We use four different types of universum: **Upper**: ‘A - Z’, **Lower**: ‘a - z’, **Symbols**: all additional symbols and **Random Averaging (RA)** obtained by randomly averaging the training samples.

**Speech-based Isolated Letter Recognition** (ISOLET) (Fanty & Cole, 1991): This is a speech recognition dataset where 150 subjects spoke the name of each letter ‘a - z’ twice. The goal is to identify the spoken letters ‘a’ - ‘e’ using the spectral coefficients, contour features, sonorant features, presonorant features, and post-sonorant features. We use two different types of universum: **Others**, which consists of all other speech i.e. ‘f’ - ‘z’ and **Random Averaging (RA)**.

Note that, to simplify our analysis (in Section 4.2.1) we used a subset of the training classes. However, similar results can be expected using all the training classes (Appendix B.2). Our initial experiments suggest that linear parameterization is optimal for the GTSRB dataset; hence only linear kernel has been used for it. For the ABCDETC and ISOLET datasets an RBF kernel of the form $K(x_i, x_j) = \exp(-\gamma\|x_i - x_j\|^2)$ with $\gamma = 2^{-7}$ provided optimal results for SVM. For all the experiments model selection is done over the range of parameters, $C = [10^{-4}, \ldots, 10^3]$, $C^*/C = \frac{n}{mL}$ and $\Delta = [0, 0.01, 0.05, 0.1]$ using stratified 5-Fold cross validation.

4.2. Results

4.2.1. COMPARISON BETWEEN SVM vs. MU-SVM

Performance comparisons between SVM and MU-SVM for the different types of Universum are shown in Table 2. The table shows the average test error over 10 random training/test partitioning of the data in similar proportions as shown in Table 1. As seen from Table 2, MU-SVM provides better generalization than SVM. In fact, for certain universum types, like **Priority-Road** for GTSRB, **RA** for ABCDETC and ISOLET; MU-SVM significantly outperforms the multiclass SVM model. In such cases, the performance gains improve significantly up to $20 - 25\%$ with the increase in number of universum samples, and stagnates for a significantly large universum set size. This indicates that for sufficiently large universum set size the effectiveness of MU-SVM depends mostly on the type (statistical characteristics) of the universum data. For a better understanding of such statistical characteristics, we adopt the technique of ‘histogram of projections’ originally introduced for binary classification in (Cherkassky & Dhar, 2010). However, different from binary classification, here we project a training sample $(x, y = k)$ onto the decision space for that class i.e. $w_k^T x - \max_{l \neq k} w_l^T x = 0$ and the universum samples onto the decision spaces of all the classes. Finally, we generate the histograms of the projection values for our analysis. Further, in addition to the histograms, we also generate the frequency plot of the predicted labels for the universum samples.

Figs. 3 shows the typical histograms and frequency plots for the SVM and MU-SVM models for the GTSRB dataset using the ‘priority-road’ sign (as universum). As seen from Fig. 3, the optimal SVM model has high separability for
the training samples i.e., most of the training samples lie outside the margin borders. In fact, similar to binary SVM (Cherkassky & Dhar, 2010), we see data-piling effects for the training samples near the ‘+1’ - margin borders of the decision functions for all the classes. This is typically seen under high-dimensional low sample size settings. However, the universum samples (‘priority-road’) are widely spread about the margin-borders. Moreover, here the universum samples are biased towards the positive side of the decision boundary of the sign ‘30’ (Fig. 3(a)) and hence predominantly gets classified as sign ‘30’ (Fig. 3(d)). As seen from Figs 3. (e)-(h), applying the MU-SVM model preserves the separability of the training samples and additionally reduces the spread of the universum samples. Such a model exhibits uncertainty on the universum samples’ class membership, and uniformly assigns them over all the classes i.e. signs ‘30’, ‘70’ and ‘80’ (Fig. 3(h)). This shows that, the resulting MU-SVM model has higher contradiction (uncertainty) on the universum samples and hence provides better generalization compared to SVM.

Fig 4 shows the histograms and the frequency plots for SVM and MU-SVM models for RA universum. As shown in Fig 4 (a), the SVM model already results in a narrow distribution of the universum samples and in turn provides near random prediction on the universum samples (Fig. 4(d)). Applying MU-SVM for this case provides no significant change to the multiclass SVM solution and hence no additional improvement in generalization (see Table 2 and Fig.4 (e)-(h)).

Finally, we provide the histograms and the frequency plots for SVM and MU-SVM models for the Non-Speed Univer-
Table 3: Performance comparisons for model selection using cross validation vs. analytic bound in Theorem 2. Train/Test partitioning follows Table 1. No. of universum samples \((m = 1000)\). Model parameters used \(C^*/C = \frac{n}{mL}, \Delta = [0, 0.01, 0.05, 0.1]\)

|            | 5-Fold CV | Theorem 2 |
|------------|-----------|-----------|
|            | Test Error | Time | Test Error | Time |
| **MU-SVM** |           |       |            |      |
| Priority Road | 5.5 ± 0.6 | 3.5 ± 0.3 | 5.2 ± 0.4 | 0.9 ± 0.1 |
| GTSRB      | 6.9 ± 0.9 | 3.7 ± 0.5 | 6.9 ± 0.9 | 0.8 ± 0.3 |
| Non-Speed  | 6.9 ± 0.9 | 3.7 ± 0.7 | 6.8 ± 0.8 | 1.0 ± 0.5 |
| **ABC/LET** |           |       |            |      |
| Upper      | 26.1 ± 4.0 | 2.8 ± 0.1 | 26.1 ± 3.7 | 1.1 ± 0.1 |
| Lower      | 24.2 ± 3.1 | 2.8 ± 0.1 | 24.4 ± 3.2 | 1.3 ± 0.1 |
| Symbols    | 23.3 ± 3.2 | 2.6 ± 0.2 | 24.1 ± 3.8 | 0.9 ± 0.09 |
| RA         | 22.1 ± 3.2 | 2.6 ± 0.1 | 22.0 ± 2.8 | 0.9 ± 0.1 |
| **OTHERS** |           |       |            |      |
| RA         | 2.8 ± 0.3 | 3.1 ± 0.6 | 2.6 ± 0.3 | 1.9 ± 0.7 |
| Others     | 3.3 ± 0.3 | 4.8 ± 0.9 | 3.3 ± 0.3 | 2.1 ± 0.5 |

4.2.2. Effectiveness using Analytic Bound in Theorem 2

Next we illustrate the practical utility of the bound in Theorem 2 for model selection.

First, we provide a comparison between the error estimates using 5-Fold cross validation (CV) vs. Theorem 2\(^3\). For illustration we use the GTSRB dataset under the experimental setting provided in Table 1. Fig. 6 (a) shows the average error estimates using 5-Fold CV and Theorem 2 as well as the true test error for the MU-SVM model using \(\text{priority-road}\) over the range of parameters \(C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]\) with fixed \(\Delta = 0\). The results are obtained over 10 random partitioning of the training/test dataset. Fig. 6 (a) shows that the error estimates using Theorem 2 follows a very similar pattern as 5-Fold CV and test error. This shows that the model parameter \(C^*/C = 10^{-1}\) that minimizes the \(\text{loo}\) error estimate in Theorem 2, also minimizes the test error and 5 Fold CV. Hence, Theorem 2 provides a practical alternative to model selection using resampling techniques.

Throughout our results we observe that the error estimates using Theorem 2 are uniformly lower than the 5-Fold CV and test error. This can be attributed to two main reasons. First, for high-dimensional low sample size settings, majority of the training samples lie outside the margin borders (see Figs. 3-5). This results in a significantly low proportion of training SVs, and hence low \(\text{loo}\) error in general. Secondly, Theorem 2 holds under additional assumptions (i) & (ii), and is further constrained compared to Theorem 1. Hence, Theorem 2 is an under estimator of the \(\text{loo}\) bound in Theorem 1. Of course, for the purpose of model selection we are only interested in the pattern, rather than the scale of the error estimates. Hence, such a difference in scale will not impact the model selection. However, to further simplify our illustrations, we also provide a scale invariant ranking curve of the model parameters in Fig. 6(b). The figure shows the average rankings of the model parameters based on the error estimate values over each experiments. Here, for each experiment we rank the model parameter with the smallest error estimate as \(\sim 1\), and the parameter with the largest estimate as \(\sim 4\), and average these rank values over the 10 experiments. The parameter with the smallest rank value \(\sim 1\) (in Fig. 6(b)) is typically selected through the model selection strategy. Finally, as seen from

\(^3\)Note that, Theorem 2 approximates Theorem 1 to provide an upper bound on the \(\text{loo}\) error. Hence, a good comparison would be between Theorem 2 vs. Theorem 1 and \(\text{loo}\) error. However, results using \(\text{loo}\) and Theorem 1 were prohibitively slow and hence could not be reported in this paper. As an alternative, we compare the error estimates from Theorem 2 with 5-Fold cross validation (CV) and test error. The objective is to illustrate that similar to 5-Fold CV, using Theorem 2 we can obtain the optimal model parameters providing smallest test error.

Appendix B.4
Figure 6: Performance of MU-SVM with priority-road universum for the GTSRB dataset. Here, no. of training samples \((n = 300)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0] \), \(C = 1\), \(\Delta = 0\). (b) Ranking of the model parameters based on the error estimate values over each experiments.

Figs. 6 (a) - (b), although different in scale, the error estimates using Theorem 2 correctly captures the pattern of the test error and selects the model parameter with the smallest test error (i.e. \(C^*/C = 10^{-1}\)). A similar comparison over the range of parameters \(\Delta = [0.001, 0.01, 0.1, 1]\) with fixed \(C^*/C = \frac{n}{mnL} = 0.3\) is also provided in Fig. 7. Here, compared to 5-Fold CV , Theorem 2 correctly selects the optimal parameter \(\Delta = 0.01\) with the smallest test error (Fig. 7 (b)).

As seen from Figs. 6 and 7, the model parameters minimizing the error estimates in Theorem 2 also minimizes the true test error. This can be also seen for all other datasets in Table 1 (Appendix B.5). Hence, Theorem 2 provides a practical alternative to resampling techniques for model selection. This is further confirmed from the results in Table 3. Table 3 shows the average test error over 10 random training/test partitioning of the data in similar proportions as shown in Table 1. Here, the MU-SVM models selected using Theorem 2 provides similar generalization error compared to the models selected through 5-Fold CV . Further, the proposed model selection strategy using Theorem 2 involves an \(O(n + mL)^3\) operation, and provides a computational edge over standard resampling techniques. Table 3 provides the average time (in seconds) for the MU-SVM model selection using Theorem 2 vs. 5-fold CV for 10 runs over the entire range of parameters. The experiments were run on a desktop with 12 core Intel Xeon @3.5 Ghz and 32 GB RAM. As seen from Table 3, the bound based model selection is \(\sim 2-4\) times faster than the standard 5-fold resampling technique.

5. Conclusions
We introduced a new universum-based formulation for multiclass SVM (MU-SVM). The proposed formulation embodies several useful mathematical properties amenable to: a) an efficient implementation of the MU-SVM formulation using existing multiclass SVM solvers, and b) deriving practical analytic bounds for model selection. We empirically demonstrated the effectiveness of the proposed formulation as well as the bound on real-world datasets. In addition, we also provided insights into the underlying behavior of universum learning and its dependence on the choice of universum samples using the proposed histogram-of-projections method.

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Multiclass Universum SVM

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Appendix

Contents

A Proofs
A.1 Proof of Proposition 1
A.2 Proof of Proposition 2
A.3 Derivation of Algorithm 1
A.4 Proof of Lemma 1
A.5 Proof of Theorem 1
A.6 Proof of Proposition 3
A.7 Proof of Lemma 2
A.8 Proof of Lemma 3
A.9 Proof of Theorem 2

B Additional Results
B.1 ECOC vs. Direct Approach
B.2 SVM vs. MU-SVM using all training classes
B.3 Performance comparisons for several Universum types with varying Training set size for GTSRB dataset
B.4 Additional Histogram of Projections
B.5 Comparison of the error estimates using 5-Fold CV vs. Theorem 2

A Proofs

The references cited in this document follow the numbering used in the main paper.

A.1 Proof of Proposition 1

Such a proposition is available for multiclass SVMs (Crammer & Singer, 2002). Here, we provide a proof for the MU-SVM formulation. Formulation (2) for binary classification becomes,

\[
\min_{w_1, w_2, \xi, \zeta} \frac{1}{2}(\|w_1\|^2 + \|w_2\|^2) + C \sum_{i=1}^{n} \xi_i + C^* \sum_{i'=1}^{m} (\zeta_{i'1} + \zeta_{i'2})
\]

\[
\text{s.t.} \quad (w_{y_i} - w_l)^T x_i \geq e_{il} - \xi_i; \quad e_{il} = 1 - \delta_{il}, \quad l = 1, 2
\]

\[
|\langle w_k, x_i^* \rangle - \max_{l=1,2} \langle w_l, x_i^* \rangle | \leq \Delta + \zeta_{i'k}; \quad \zeta_{i'k}, \quad k = 1, 2
\]

\[
i = 1 \ldots n, \quad i' = 1 \ldots m, \quad \delta_{il} = \begin{cases} 1; & y_i = l \\ 0; & y_i \neq l \end{cases}
\]

The constraints become,

Training samples (\forall i = 1 \ldots n)
For any $x_i \in \text{class 1}$ labeled as $y_i = +1$; we have
\[(w_1 - w_1)\top x_i \geq -\xi_i \Rightarrow \xi_i \geq 0\]
\[(w_1 - w_2)\top x_i \geq 1 - \xi_i \Rightarrow y_i(w_1 - w_2)\top x_i \geq 1 - \xi_i\]

Similarly, for any $x_i \in \text{class 2}$ labeled as $y_i = -1$; we have,
\[(w_2 - w_1)\top x_i \geq 1 - \xi_i \Rightarrow y_i(w_1 - w_2)\top x_i \geq 1 - \xi_i\]
\[(w_2 - w_2)\top x_i \geq -\xi_i \Rightarrow \xi_i \geq 0\]

Univem samples ($\forall i' = 1\ldots m$)

For any universum sample $x^*_i$, WLOG we assume $w_1 x^*_i \geq w_2 x^*_i$. Then,
When $k = 1$ we have $|w_1 x^*_i - \max_{i=1\ldots L} w_i x^*_i| \leq \Delta + \zeta_i ^{k} \Rightarrow \zeta_i ^{k} \geq -\Delta$ (true i.e. $\zeta_i ^{k} \geq 0$).

When $k = 2$ we have $|w_2 x^*_i - \max_{i=1\ldots L} w_i x^*_i| \leq \Delta + \zeta_i ^{k} \Rightarrow |w_2 x^*_i - w_1 x^*_i| \leq \Delta + \zeta_i ^{k}$, $\zeta_i ^{k} \geq 0$.

Hence, eq. (10) can be re-written as,
\[
\min_{w_1, w_2, \xi, \zeta} \frac{1}{2} (\|w_1\|_2^2 + \|w_2\|_2^2) + C \sum_{i=1}^n \xi_i + C^* \sum_{i'=1}^m \zeta_i ^{k} \tag{11}
\]
\[\text{s.t. } y_i(w_1 - w_2)\top x_i \geq 1 - \xi_i; \quad \xi_i \geq 0, \quad i = 1 \ldots n \]
\[|w_1 - w_2|\top x_i^* \leq \Delta + \zeta_i ^{k}; \quad \zeta_i ^{k} \geq 0, \quad i' = 1 \ldots m \]

The solution to the KKT system of (11) satisfies $w_1 = -w_2$. Hence replacing $w = w_1 - w_2$ in (11) still solves (10). This is the U-SVM formulation in (Weston et. al, 2006) with $b = 0$.

A.2 Proof of Proposition 2

The contribution due to the universum samples are same for both (2) and (3). For any universum sample ($x^*_i$) we identify the active constraints and its overall contribution to the objective function through slack variables i.e.

Equation (2), the overall contribution of the universum sample $x^*_i$ is,
\[
C^* \sum_{k=1}^L \zeta_i ^{k} \text{ s.t. } |w_k \top x^*_i - \max_{i' \neq k} w_i \top x^*_i| \leq \Delta + \zeta_i ^{k} \quad \zeta_i ^{k} \geq 0, \quad k = 1 \ldots L
\]

Case 1: If $k = \arg \max_{i' \neq k} w_i \top x^*_i$. The constraint is inactive and $\zeta_i ^{k} = 0$.

Case 2: Let $k \neq \arg \max_{i' \neq k} w_i \top x^*_i$. Since, $\zeta_i ^{k} \geq 0$ the constraint is active if, $-(w_k \top x^*_i - \max_{i' \neq k} w_i \top x^*_i) > \Delta$. Then, $\zeta_i ^{k} = -[\Delta + (w_k \top x^*_i - \max_{i' \neq k} w_i \top x^*_i)]$.

Hence, keeping only the active constraints the overall contribution of the sample $x^*_i$ is,
\[
C^* \sum_{k \in K_{i'}} -[\Delta + w_k \top x^*_i - \max_{i' \neq k} w_i \top x^*_i] \quad \text{where, } K_{i'} = \{k | -(w_k \top x^*_i - \max_{i' \neq k} w_i \top x^*_i) > \Delta\}
\]

Equation (3), Following eq. (3) for the universum sample $x^*_i$ we have $L$ artificial samples as $(x^*_i, y_i = 1), \ldots, (x^*_i, y_i = L')$ stacked at indices $i = n + (i' - 1)L + 1 \ldots n + i'L$. Hence for $x^*_i$ we have the overall contribution as,
\[
C^* \sum_{i=n+(i'-1)L+1}^{n+i'L} \xi_i \text{ s.t. } (w_{y_i} - w_i) \geq -\Delta (1 - \delta_{ii}) - \xi_i
\]
Now, for \( i = n + (i' - 1) + k \), we have \( x_i = x^*_i, y_i = k \). The constraints are,
\[
(w_k - w_1)^T x^*_i - \xi_i \geq -\Delta - \eta_l (C_j \delta_{jl} - \eta_{jl})K(x_i, x_j) + \sum_{l \neq k} \eta_{il} e_{il} (16)
\]
s.t.
\[
\sum_{l \neq k} \eta_{il} = C_i
\]
\[
\eta_{il} \geq 0
\]
\[
\text{Setting } \alpha_{il} = C_i \delta_{il} - \eta_{il} \text{ we get (5).}
\]

The proof is available in (Crammer & Singer, 2002), (Hsu & Lin, 2002a). We reproduce it for completeness and for better readability of the subsequent proofs. The Lagrangian of the MU-SVM formulation is given as,
\[
\text{Lagrangian, } \mathcal{L} = \frac{1}{2} \sum_l \| w_l \|^2 + \sum_{i=1}^{n+mL} C_i \xi_i - \sum_{i \neq l} \eta_{il}[(w_{yi} - w_l)^T x_i - e_{il} + \xi_l] (14)
\]

**KKT System**
\[
\nabla_{w_i} \mathcal{L} = 0 \quad \Rightarrow \quad w_i = \sum_i (C_i \delta_{il} - \eta_{il}) x_i (15)
\]
\[
\nabla_{\xi_i} \mathcal{L} = 0 \quad \Rightarrow \quad \sum_{l \neq i} \eta_{il} = C_i
\]

Complimentary Slackness
\[
\eta_{il}[(w_{yi} - w_l)^T x_i - e_{il} + \xi_l] = 0 \quad \forall (i, l)
\]

Constraints,
\[
(w_{yi} - w_l)^T x_i \geq e_{il} + \xi_i \quad \forall (i, l)
\]
\[
\eta_{il} \geq 0
\]

Finally the dual problem is,
\[
\max_{\eta} \quad -\frac{1}{2} \sum_{i,j \neq l} \sum_{l} (C_i \delta_{il} - \eta_{il})(C_j \delta_{jl} - \eta_{jl})K(x_i, x_j) + \sum_{i,l} \eta_{il} e_{il} (16)
\]
s.t.
\[
\sum_{l \neq i} \eta_{il} = C_i
\]
\[
\eta_{il} \geq 0
\]

Setting \( \alpha_{il} = C_i \delta_{il} - \eta_{il} \) we get (5).
A.4 Proof of Lemma 1

First we prove some interesting properties specific to the MU-SVM solution.

Lemma A.1. \[ \forall \alpha_i \in SV_1 = \{ i | 0 < \alpha_i < C_i; y_i = l \}, \]

\[ i. \sum_k \alpha_{ik} \sum_j \alpha_{jk} K(x_i, x_j) + e_{ik} = 0 ; \quad k = 1 \ldots L \]

\[ ii. \forall k \neq y_i with \alpha_{ik} < 0 (strict) ; \sum_j \alpha_{jk} K(x_i, x_j) + e_{ik} = \sum_j \alpha_{jy_i} K(x_i, x_j) + e_{iy_i} , i.e. \]

the projection values for the type 1 support vectors for such classes are equal.

\[ iii. For any \gamma_i \in \{ \gamma_i \sum_k \gamma_{ik} = 0 ; \gamma_{ik} = 0 if \alpha_i \in SV_1 and \alpha_{ik} = 0 \} we have \]

\[ \sum_k \gamma_{ik} \sum_j \alpha_{jk} K(x_i, x_j) + e_{ik} = 0 \]

Proof

For simplicity we provide the proof for linear kernel. The same proof applies for non-linear transformations. The proof uses the KKT system for (4). (Appendix A.3)

\[ i. \sum_k \gamma_{ik} (w_{yi} - w_k)^T x_i \quad [\text{From (15)}] \]

\[ = \sum_k \gamma_{ik} (\sum_l \delta_{il} w_l)^T x_i - \sum_k \gamma_{ik} w_k^T x_i \]

\[ = \sum_l C_l \delta_{il} w_l^T x_i - \sum_k \gamma_{ik} w_k^T x_i = \sum_k (C_l \delta_{ik} - \gamma_{ik}) w_k^T x_i \]

\[ = \sum_k \alpha_{ik} \sum_j \alpha_{jk} K(x_i, x_j) \]

From complimentary slackness, if \( \alpha_{il} < C_i \) with \( y_i = l \) \( \Rightarrow \eta_{il} = (C_i \delta_{il} - \alpha_{il}) > 0 \). This gives, \( (w_{yi} - w_{k=l})^T x_i - e_{ik} + \xi_i = 0 \Rightarrow \xi_i = 0 \) (i.e. lies on margin). Now, from complimentary slackness in (15),

\[ \sum_k \eta_{ik} [(w_{yi} - w_k)^T x_i - e_{ik}] = 0 \]

\[ \Rightarrow \sum_k \alpha_{ik} [\sum_j \alpha_{jk} K(x_i, x_j) + e_{ik}] = 0 \quad [\therefore \eta_{ik} e_{ik} = (C_i \delta_{ik} - \alpha_{ik}) e_{ik} = -\alpha_{ik} e_{ik}] \]

\[ ii. From complimentary slackness (15) \]

\[ \eta_{ik} [(w_{yi} - w_k)^T x_i - e_{ik}] = 0 \quad (\forall k \neq y_i ; \alpha_{ik} < 0 , \therefore \xi_i = 0) \]

\[ \Rightarrow (w_{yi} - w_k)^T x_i - e_{ik} = 0 \quad (\therefore \eta_{ik} > 0) \]

\[ \Rightarrow w_{yi}^T x_i - w_k^T x_i + e_{ik} \]

\[ \Rightarrow \sum_j \alpha_{jy_i} K(x_i, x_j) + e_{iy_i} = \sum_j \alpha_{j\neq y_i} K(x_i, x_j) + e_{ik \neq y_i} \]

\[ iii. For any such \gamma_i, \]

\[ \sum_k \gamma_{ik} [\sum_j \alpha_{jk} K(x_i, x_j) + e_{ik}] \]

\[ = \gamma_{iy_i} \sum_j \alpha_{jy_i} K(x_i, x_j) + \sum_{k \neq y_i, \alpha_{ik} < 0} \gamma_{ik} [\sum_j \alpha_{j\neq y_i} K(x_i, x_j) + e_{ik \neq y_i}] \]

\[ = (\gamma_{iy_i} + \sum_{k \neq y_i} \gamma_{ik}) \sum_j \alpha_{jy_i} K(x_i, x_j) \quad (\text{from ii above and } \therefore e_{iy_i} = 1 - \delta_{iy_i} = 0) \]

\[ = 0 \quad (\therefore \sum_k \gamma_{ik} = 0 by construction) \]
With the above properties for the MU-SVM solution we provide the proof for Lemma 1 following similar lines as in (Vapnik & Chapelle, 2000). We restate the lemma here for better readability.

**Lemma 1.** If in leave-one-out procedure a Type 1 (training) support vector \( x_t \in SV_1 \cap T \) is recognized incorrectly, then we have,

\[
S_t \max(\sqrt{2}D, \frac{1}{\sqrt{C}}) > 1
\]

where,

\[
S_t^2 = \min_{\beta} \sum_{i,j,l} (\sum_{i,l} \beta_{il} \beta_{jl}) K(x_i, x_j)
\]

s.t. \( \alpha_{il} - \beta_{il} \leq C_i; \forall \{(i \neq t, l) | \alpha_{il} < C_i; l = y_i\} \)

\( \alpha_{il} - \beta_{il} \leq 0; \forall \{(i \neq t, l) | \alpha_{il} > 0; l \neq y_i\} \)

\( \beta_{il} = 0; \forall (i, l) \notin SV_1 - \{t\} \)

\( \beta_{il} = \alpha_{il}; \forall l \)

\( \sum_l \beta_{il} = 0 \)

\( D = \text{Diameter of the smallest hypersphere containing all training samples, and } T = \text{Training set} \)

**Proof**

The leave-one-out formulation for MU-SVM with the \( t \in T \) sample dropped is,

\[
\max_{\alpha} W(\alpha) = -\frac{1}{2} \sum_{i,j} \sum_{l} \alpha_{il} \alpha_{jl} K(x_i, x_j) - \sum_{i,l} \alpha_{il} c_{il}
\]

s.t. \( \sum_l \alpha_{il} = 0 \) \hspace{1cm} (17)

\( \alpha_{il} \leq C_i \text{ if } l = y_i; \alpha_{il} \leq 0 \text{ if } l \neq y_i; \alpha_{il} = 0; \forall l \text{ (additional constraint)} \)

Then, the leave-one-out (l.o.o) error is given as: \( R_{l.o.o} = \frac{1}{n} \sum_{t=1}^{n} [y_t \neq \hat{y}_t] \) where, \( \alpha^t = [\alpha_{11}^t, \ldots, \alpha_{1L}^t, \ldots, \alpha_{L1}^t, 0, \ldots, \alpha_{L1}^t = 0, \ldots] \) is the solution for (17) and \( \hat{y}_t = \arg \max_i \sum_i \alpha_{il}^t K(x_i, x_t) \) (estimated class label for the \( t^{th} \) sample). The overall proof for the bound on the l.o.o error follows three major steps.

**First.** we construct a feasible solution for (5) using the optimal leave-one-out solution \( \alpha^t \). i.e., construct \( \alpha^t + \gamma \) as shown below,

\[
\alpha_{il}^t + \gamma_{il} \leq C_i; \forall (i, l) \in \{(i, l) | 0 < \alpha_{il}^t < C_i; l = y_i\} := A_1^t
\]

\( \alpha_{il}^t + \gamma_{il} \leq 0; \forall (i, l) \in \{(i, l) | \alpha_{il}^t < 0; l \neq y_i\} := A_2^t \)

\( \gamma_{il} = 0; \forall (i, l) \notin SV_1^t [SV_1^t = A_1^t \cup A_2^t] \)

\( \sum_l \gamma_{il} = 0 \) \hspace{1cm} (18)
Now,
\[
I_1 = W(\alpha^t + \gamma) - W(\alpha^t)
= -\frac{1}{2} \sum_{i,j} \sum_{l} (\alpha_{il}^t + \gamma_{il}) (\alpha_{jl}^t + \gamma_{jl}) K(x_i, x_j) - \sum_i \sum_{l} (\alpha_{il}^t + \gamma_{il}) e_{il} + \frac{1}{2} \sum_{i,j} \sum_{l} \alpha_{jl}^t \alpha_{jl}^t K(x_i, x_j) + \sum_i \sum_{l} \alpha_{il}^t e_{il}
= -\frac{1}{2} \sum_{i,j} \sum_{l} \gamma_{il} \gamma_{jl} K(x_i, x_j) - \sum_i \sum_{l} \gamma_{il} e_{il}
= -\frac{1}{2} \sum_{i,j} \sum_{l} \gamma_{il} \gamma_{jl} K(x_i, x_j) - \sum_i \gamma_{il} \sum_j \alpha_{jl}^t K(x_i, x_j) + e_{il}
= -\frac{1}{2} \sum_{i,j} \sum_{l} \gamma_{il} \gamma_{jl} K(x_i, x_j) - \sum_i \gamma_{il} \sum_j \alpha_{jl}^t K(x_i, x_j) + e_{il} \quad (\text{Lemma A.1 (iii)})
\]
(19)

As a special case we set,
\[
\gamma_t = \ldots [a_{1t}, \ldots, -a_{yt}, \ldots] = -a_{g_t k}; \quad (k = \arg \max_{q \neq y_t} \sum_j \alpha_{jq}^t K(x_j, x_t); \quad g_{yk} = \ldots [1, \ldots, -1])
\]

Further, we select another \(p \in SV_1\) where \(\gamma_{p \neq t} = -a_{g_{yk}}\). Finally, we set, \(\gamma_i = 0 \forall i \notin \{t, p\}\). For such a case,
\[
I_1 = -\alpha^2||x_t - x_p||^2 + a[1 - \left(\sum_j \alpha_{jyt}^t K(x_j, x_t) - \sum_j \alpha_{jkt}^t K(x_j, x_i)\right)] \\
\geq -\hat{a}^2 D^2 + \hat{a}[1 - \left(\sum_j \alpha_{jyt}^t K(x_j, x_t) - \sum_j \alpha_{jkt}^t K(x_j, x_i)\right)] \quad (20)
\]

with, \(\hat{a} = \frac{1}{2D^2} [1 - \left(\sum_j \alpha_{jyt}^t K(x_j, x_t) - \sum_j \alpha_{jkt}^t K(x_j, x_i)\right)]\) (the value that maximizes the R.H.S in (20)) and \(D\) = Diameter of the smallest hypersphere containing all training samples.

Now, if: \(\hat{a} \leq C \Rightarrow I_1 \geq \frac{1}{4D^2} [1 - \left(\sum_j \alpha_{jyt}^t K(x_j, x_t) - \sum_j \alpha_{jkt}^t K(x_j, x_i)\right)] = \frac{1}{2} \hat{a}\)

else, \(I_1 \geq -C^2 D^2 + C[1 - \left(\sum_j \alpha_{jyt}^t K(x_j, x_t) - \sum_j \alpha_{jkt}^t K(x_j, x_i)\right)] = 2CD^2[\hat{a} - \frac{C}{2}] \geq 2CD^2 \frac{\hat{a}}{2}\)

If there is an error due to leave one out procedure, then \(\max_{q \neq y_t} \sum_j \alpha_{jm}^t K(x_j, x_t) > \sum_j \alpha_{jyt}^t K(x_j, x_t)\).

This gives, \(I_1 > \frac{1}{2} \min(C, \frac{1}{2D^2})\) (for l.o.o error) \quad (21)

**Second**, we construct a feasible solution for the leave-one-out formulation (17) using the optimal solution for (5). i.e., construct \(\alpha - \beta\) as shown below,
\[
\alpha_{il} - \beta_{il} \leq C_t; \quad \forall (i, l) \in A_1 - \{t\}; \quad A_1 = \{(i, l) | 0 < \alpha_{il} < C_t; \; l = y_t\}
\]
\[
\alpha_{il} - \beta_{il} \leq 0; \quad \forall (i, l) \in A_2 - \{t\}; \quad A_2 = \{(i, l) | \alpha_{il} < 0; \; l \neq y_t\}
\]
\[
\sum_l \beta_{il} = 0;
\]
\[
\beta_{it} = 0 \quad \forall (i, l) \notin SV_1 - \{t\}
\]
\[
\beta_t = \alpha_t \quad (22)
\]
with $SV_1 = A_1 \cup A_2 = \{i \mid 0 < \alpha_i y_i < C_i\}$ such that, it is a feasible solution for (17). As before, define

$$I_2 = W(\alpha) - W(\alpha - \beta)$$

$$= -\frac{1}{2} \sum_{i,j} \sum_{k} \alpha_i \alpha_j K(x_i, x_j) - \sum_i \sum_l \alpha_i \epsilon_{il} + \frac{1}{2} \sum_{i,j} \sum_l (\alpha_i - \beta_i)(\alpha_j - \beta_j)K(x_i, x_j)$$

$$+ \sum_i \sum_l (\alpha_i - \beta_i)e_{il}$$

$$= \frac{1}{2} \sum_{i,j} (\sum_l \beta_i \beta_j)K(x_i, x_j) - \sum_l \beta_l [\sum_j \alpha_j K(x_j, x_i) + e_{il}]$$

$$= \frac{1}{2} \sum_{i,j} (\sum_l \beta_i \beta_j)K(x_i, x_j) \quad \text{(Lemma A.1 (iii))}$$

$$= \frac{1}{2} \sum_{i,j} (\sum_l \beta_i \beta_j)K(x_i, x_j)$$

(23)

**Third**, as the final step define,

$$S_t^2 = \min_{\beta} \sum_{i,j} (\sum_l \beta_i \beta_j)K(x_i, x_j)$$

s.t. $\alpha_{il} - \beta_{il} \leq C_i; \quad (i, l) \in A_1 - \{t\}$

$\alpha_{il} - \beta_{il} \leq 0; \quad (i, l) \in A_2 - \{t\}$

$\beta_{il} = 0; \quad \forall (i, l) \notin SV_1 - \{t\}$

$\sum_l \beta_{il} = 0$; $\forall l$

Now, let $\beta'$ be the minimizer for (24). For such a $\beta'$

$$I_2(= \frac{1}{2} S_t^2)$$

$$\geq I_1 \quad [:: W(\alpha) \geq W(\alpha + \gamma) \forall \gamma; \quad -W(\alpha - \beta) \geq -W(\alpha) \forall \beta]$$

$$> \frac{1}{2} \min(C, \frac{1}{2D^2}) \quad \text{(from (21))}$$

\[\square\]

**A.5 Proof of Theorem 1**

**Theorem 1.** The leave-one-out error is upper bounded as:

$$R_{l.o.o} \leq \frac{1}{n} (|\Psi_1| + |\Psi_2|)$$

$$\Psi_2 := \{ t \in SV_1 \cap T \mid S_t \max(\sqrt{2D}, \frac{1}{\sqrt{C}}) \geq 1 \}$$

$$\Psi_1 := \{ t \in SV_2 \cap T \}; \quad |\cdot| := \text{Cardinality of a set}$$

where $T := \text{Training Set}$.

**Proof**

The proof depends on the contribution of a sample to the leave-one-out error,

**First**, for a sample $(x_t, y_t)$ which is not a support vector, i.e. $t \notin SV$ and $t \in T$ (Training set); it lies outside margin borders. Dropping such a sample does not change the original solution of (5). Hence, it does not contribute to an error.

**Secondly**, for a sample $(x_t, y_t) \in SV_1 \cap T$ contributing to leave-one-out error, Lemma 1 holds i.e.

$$S_t \max(\sqrt{2D}, \frac{1}{\sqrt{C}}) > 1.$$

**Finally**, for a sample $(x_t, y_t)$ with $t \in SV_2 \cap T$ we add to the leave-one-out error. \[\square\]
A.6 Proof of Proposition 3

Remark 2. If the Type 1 training support vectors i.e. \( \{ t | t \in SV_1 \cap T \} \) for SVM and MU-SVM solutions remain same, then we have \( S_{i}^{SV,M} \geq S_{i}^{MU-SVM} \).

Proof By definition in Lemma 1,

\[
S_{i}^{2} = \min_{\beta} \sum_{i,j} (\sum l \beta_{il} \beta_{jl}) K(x_i, x_j) \\
\text{s.t.} \\
\beta_{MU-SVM} := \left\{ \begin{array}{l}
\alpha_{il} - \beta_{il} \leq C_i; \quad (i,l) \in A_1 - \{ t \} \\
\alpha_{il} - \beta_{il} \leq 0; \quad (i,l) \in A_2 - \{ t \} \\
\beta_{ul} = 0; \\
\forall (i,l) \notin SV_1 - \{ t \} \\
\sum l \beta_{il} = 0
\end{array} \right.
\]

If the Type 1 (training) support vectors for SVM and MU-SVM solutions remain same, we get the same relation as Lemma 1 for C&S SVM with,

\[
\beta_{SV,M} = \{ \beta_{il} \in \beta_{MU-SVM} | \beta_{il} = \alpha_{il} \; \forall i \in SV_1 \cap U \} ,
\]

where \( U \) = Universum samples.

i.e. \( \beta_{SV,M} \subseteq \beta_{MU-SVM} \Rightarrow S_{i}(\beta_{SV,M}) \geq S_{i}(\beta_{MU-SVM}) \)

A.7 Proof of Lemma 2

Lemma 2. Under the assumptions (i) and (ii) in Section 3.3 the following equality holds for both Type 1 & 2 training support vectors, i.e. \( x_i \in SV \cap T \)

\[
S_{i}^{2} = [\alpha_{i}^{T} \sum_{i \in SV} \sum_{l} \alpha_{il} K(x_i, x_i) - \alpha_{yil} g_{yik} \sum_{i \in SV} \sum_{l} \alpha_{il}^l K(x_i, x_i)]
\]

with, \( S_{i}^{2} = \min_{\beta} \sum_{i,j} (\sum_{l} \beta_{il} \beta_{jl}) K(x_i, x_j) | \beta_{il} = \alpha_{il}; \sum_{l} \beta_{il} = 0; (i,j) \in SV_1 \) and \( g_{yik} = [0, \ldots, 1, \ldots, -1, \ldots, 0] \ldots \)

Proof

Under the Assumption (i) we set \( \beta = \gamma = (\alpha - \alpha^t) \). Then \( I_1 = W(\alpha) - W(\alpha^t) = I_2 \)

A similar analysis as in (19) gives,

\[
I_1 = -\frac{1}{2} \sum_{(i,j) \in SV_1} (\sum_{l} \gamma_{il} \gamma_{jl}) K(x_i, x_j) - \sum_{l} \alpha_{il} \sum_{j \in SV} \alpha_{jl}^l K(x_j, x_i) + e_{it}
\]

Note the difference in form compared to (19). This is because now the analysis applies for both type 1 & 2 support vectors. Similarly,

\[
I_2 = \frac{1}{2} \sum_{i,j} (\sum_{l} \beta_{il} \beta_{jl}) K(x_i, x_j) - \sum_{l} \alpha_{il} \sum_{j \in SV} \alpha_{jl} K(x_j, x_i) + e_{it}
\]

Combining, (26) and (27)

\[
\sum_{(i,j) \in SV_1} \sum_{l} \beta_{il} \beta_{jl} K(x_i, x_j) = \sum_{l} \alpha_{il} \sum_{j \in SV} \alpha_{jl} K(x_j, x_i) + e_{it} - \sum_{l} \alpha_{il} \sum_{j \in SV} \alpha_{jl}^l K(x_j, x_i) + e_{it}
\]
Next, let \( \beta' \) be the minimizer for (24). Then, \( (\alpha - \beta') \) is a feasible solution for (17). Hence,
\[
W(\alpha') \geq W(\alpha - \beta') \\
\Rightarrow W(\alpha) - W(\alpha') \leq W(\alpha) - W(\alpha - \beta') \\
\Rightarrow \sum_{i,j,l} (\sum \beta_{il} \beta_{jl}) K(x_i, x_j) \leq S_t^2
\]

However, from Assumption (i), \( \beta = (\alpha - \alpha') \) is a feasible solution for (24). Hence for such a \( \beta \) we have :
\[
S_t^2 \leq \sum_{i,j,l} (\sum \beta_{il} \beta_{jl}) K(x_i, x_j). 
\]
Combining the above inequality,
\[
S_t^2 = \sum_{i,j,l} (\sum \beta_{il} \beta_{jl}) K(x_i, x_j) \tag{29}
\]

Further, under Assumption (i) the inequality constraints in (24) are not activated. Hence, \( S_t^2 = \{ \min_{\beta} \sum_{i,j,l} (\sum \beta_{il} \beta_{jl}) K(x_i, x_j) | \beta_t = \alpha_t; \sum_{l} \beta_{il} = 0 ; (i, j) \in SV_1 \} \).

Finally combining (28) and (29) we get,
\[
S_t^2 = \sum_{l} \alpha_{tl} - \sum_{j \in SV} \left( \sum \alpha_{jl} K(x_j, x_t) + \varepsilon_t \right) - \sum_{l} \alpha_{tl} - \sum_{j \in SV} \alpha_{jl} K(x_j, x_t) + \varepsilon_t \tag{30}
\]

For leave one out error (under Assumption (ii)),
\[
- \sum_{l} \alpha_{tl} \left( \sum_{j \in SV} \alpha_{jl} K(x_j, x_t) \right) = \alpha_{t\nu} \left( \sum_{j \in SV} \alpha_{jl} K(x_j, x_t) - \sum_{j \in SV} \alpha_{jl} K(x_j, x_t) \right) \geq 0 \quad (k = \arg \max_{m \neq \nu} \sum_{j \in SV} \alpha_{jm} K(x_j, x_t))
\]
\[\therefore S_t^2 \geq \sum_{l} \alpha_{tl} \left( \sum_{j \in SV} \alpha_{jl} K(x_j, x_t) \right) \]
\[\square\]

A.8 Proof of Lemma 3

Lemma 3. The span \( S_t^2 \) can be efficiently computed as
\[
S_t^2 = \begin{cases} 
\alpha_t^T (H^{-1})_{tt}^{-1} \alpha_t & t \in SV_1 \cap T \\
\alpha_t^T K(x_t, x_t) \otimes I_L - K_t^T H^{-1} K_t | \alpha_t & t \in SV_2 \cap T
\end{cases}
\]
here, \( H := \begin{bmatrix} K_{SV_1} \otimes I_L & A^T \\ A & 0 \end{bmatrix} ; \quad A := I_{|SV_1|} \otimes (1_L)^T ; \quad 1_L = \begin{bmatrix} \frac{1}{L} \ldots \frac{1}{L} \end{bmatrix} \text{L elements}
\]
\( (H^{-1})_{tt} := \text{sub-matrix of } H^{-1} \text{for indices } i = (t-1)L + 1 \ldots tL \)
\( K_{SV_1} := \text{Kernel matrix of Type 1 support vectors. } \quad K_t = \left( k_t^T \otimes 1_L \right) 0_{L \times |SV_1|}^T \)

where, \( k_t = n_{|SV_1| \times 1} \) dim vector where \( t^{th} \) element is \( K(x_t, x_i), \forall x_i \in SV_1 \); and \( \otimes \) is the Kronecker product.

Proof

The Span is defined as:
\[
S_t^2 = \min_{\beta} \sum_{i,j,l} (\sum \beta_{il} \beta_{jl}) K(x_i, x_j) \tag{31}
\]
\[s.t. \quad \beta_{il} = \alpha_{tl} ; \quad \forall l = 1, \ldots, L \\
\sum_{l} \beta_{il} = 0 ; \quad \forall (i, j) \in SV_1
\]
Case \( t \in SV_1 \)

\[
\begin{align*}
\text{Case}(t \in SV_1) &= \min_{\beta} \sum_{t} (\alpha_l \alpha_{tl}) K(x_t, x_t) + 2 \sum_{i \in SV_1 - \{t\}} \sum_l \alpha_l \beta_{il} K(x_t, x_i) + \sum_{(i,j) \in SV_1 - \{t\}} (\sum_r \beta_{il} \beta_{jl}) K(x_t, x_j) \\
\text{s.t.} & \quad (I_{|SV_1 - \{t\}|} \otimes 1_L) \beta = 0 \\
& = \min \max_{\beta} \alpha_t^T [K(x_t, x_t) \otimes I_L] \alpha_t + 2 \sum_{i \in SV_1 - \{t\}} \sum_l \alpha_l \beta_{il} K(x_t, x_i) + \sum_{(i,j) \in SV_1 - \{t\}} (\sum_r \beta_{il} \beta_{jl}) K(x_t, x_j) \\
& \quad + 2\mu^T A \beta + 2\alpha^T A_l \mu \quad (\mu := \text{Lagrange Multiplier}, \quad \sum_l \alpha_l = 0 \Rightarrow \alpha^T A_l \mu = 0) \\
& = \alpha_t^T [K(x_t, x_t) \otimes I_L] \alpha_t + \min \max_{\beta} 2\alpha_t^T (H_t(-t)^T \lambda + \lambda H_t(-t) \lambda) \quad (\text{with } \lambda = [\beta; \mu])
\end{align*}
\]

where, 
\( I_{|SV_1 - \{t\}|} := \text{Identity Matrix of size } |SV_1 - \{t\}|, \)
\( A_l := \text{submatrix of } A \text{ for indices } (t-1)L + 1, \ldots, tL \)
\( H_t(-t) := (t-1)L + 1, \ldots, tL \) rows/columns of matrix \( H \) (in Lemma ???) removed; and
\( H_t(-t)^T := (t-1)L + 1, \ldots, tL \) columns of \( H \).

Further, at saddle point : \( \nabla_\lambda L(\lambda) = 0 \Rightarrow \lambda^* = -[H(-t)]^{-1} H_t(-t) \alpha_t. \)

Hence,

\[
\begin{align*}
S_t^2 &= \alpha_t^T [K(x_t, x_t) \otimes I_L] - (H_t(-t))^T (H(-t))^{-1} H_t(-t) \alpha_t \\
& = \alpha_t^T (H^{-1})_{tt} \alpha_t
\end{align*}
\]

where, \( (H^{-1})_{tt} := \text{sub-matrix of } H^{-1} \text{ for index } i = (t-1)L + 1, \ldots, tL. \)

Case \( t \in SV_2 \)

A similar analysis as above gives,

\[
S_t^2 = \alpha_t^T [K(x_t, x_t) \otimes I_L - K_t^T H^{-1} K_t] \alpha_t
\]

(33)

where, \( K_t := [(k_t^T \otimes 1_L) 0_L \times |SV_1|]^T \) and \( k_t = n_{|SV_1| \times 1} \) dim vector where ith element is \( K(x_t, x_t), \forall x_t \in SV_1. \)

\( \square \)

A.9 Proof of Theorem 2

The proof has two steps.

- \textit{First}, a sample \((x_t, y_t)\) which is not a support vector does not contribute to an error.
- \textit{Secondly}, for a sample \((x_t, y_t)\) with \( t \in SV \cap T \) Theorem 2 holds. Finally, combining the form of \( S_t^2 \) in Lemma 3 completes the proof.

\( \square \)

B Additional Results

B.1 ECOC vs. Direct Approach for MU-SVM

This section provides the performance comparisons between two major ECOC based approaches: one-vs-all (OVA) and one-vs-one (OVO) vs. the direct formulation (C & S based MU-SVM in (2)).

For the ECOC based approaches we use standard U-SVM formulation (in Weston et. al 2006) to solve the binary problems. Further, we use the same datasets and experimental settings as discussed in Section 4. For all the datasets we show the results for Universum types which provided the best performance in Table 2.

As shown above, for the datasets and experimental settings used in this paper, the C&S based direct formulation (MU-SVM) performs as good as (or better) than the ensemble based methods.
Table 4: Mean (± standard deviation) test error in % over 10 runs.

| DATA SET | METHOD       | ONE VS ALL   | ONE VS ALL | C&S (MU-SVM) |
|----------|--------------|--------------|------------|--------------|
| GTSRB    | SVM          | 7.07 ± 1.08  | 7.16 ± 1.92| 7.24 ± 1.16  |
|          | U-SVM (PRIORITY-ROAD) | 6.05 ± 0.61  | 5.97 ± 0.63| 5.67 ± 0.32  |
| ABCDETC  | SVM          | 28.1 ± 4.74  | 29.05 ± 4.16| 27.50 ± 3.34|
|          | U-SVM (RA)   | 26.05 ± 4.93 | 26.90 ± 4.51| 22.20 ± 2.89|
| ISOLET   | SVM          | 3.72 ± 0.59  | 3.88 ± 0.44| 3.60 ± 0.31  |
|          | U-SVM (RA)   | 3.56 ± 0.55  | 3.88 ± 0.63| 2.83 ± 0.32  |

B.2 SVM vs MU-SVM using all training classes

Table 5: Performance comparisons between SVM vs. MU-SVM using all training classes

| DATA SETS | # TRAIN / TEST = 700 / 3500 (100 / 500 PER CLASS), # UNIVERSUM (M) = 500 |
|-----------|-------------------------------------------------------------------------|
| GTSRB     | MU-SVM (PRIORITY-ROAD) 9.77 ± 0.43                                   |
| SVM = 11.75 ± 0.77 | MU-SVM (RA) 11.29 ± 0.48                              |
|           | MU-SVM (NON-SPEED) 11.82 ± 0.93                                     |
|           |                                                                      |
| ABCDETC   | U-PRIORITY 41.1 ± 2.6          | L-PRIORITY 40.2 ± 3.2 | S-PRIORITY 39.3 ± 3.2 | R-PRIORITY 38.8 ± 2.1 |
| SVM = 42.1 ± 1.9 |                                                                      |
B.3 Performance comparisons for several Universum types with varying Training set size for GTSRB dataset

The experiments follow the same setting as in Table 2. However in this case we vary the number of training samples. The universum set size is fixed to $m = 500$ following Table 2 i.e. Further, increase in universum samples does not provide significant performance gains. Table 6 provides the mean and std. deviation of the test errors for the SVM and MU-SVM models over 10 random training/test partitioning of the dataset.

Table 6: Mean (± standard deviation) of the test errors (in %) over 10 runs for the GTSRB dataset.

| METHODS       | NO. OF TRAINING SAMPLES (PER CLASS) |            |            |            |
|---------------|-------------------------------------|------------|------------|------------|
|               |                                     | 300 (100)  | 750 (250)  | 1500 (500) |
| C&S SVM       |                                     | 7.54 ± 0.82| 4.23 ± 0.49| 3.61 ± 0.38|
| (No Passing)  |                                     | 6.98 ± 0.93| 4.64 ± 0.42| 3.49 ± 0.42|
| (No Passing for Trucks) |     | 6.07 ± 0.68| 4.37 ± 0.9 | 3.56 ± 0.41|
| (Right of Way) |                                   | 6.17 ± 0.67| 4.03 ± 0.2 | 3.12 ± 0.42|
| (Priority Road) |                               | 5.52 ± 0.68| 3.52 ± 0.37| 3.15 ± 0.44|
| (Yield Right of Way) |                     | 6.2 ± 0.7  | 3.83 ± 0.24| 3.11 ± 0.4 |
| (Stop)        |                                     | 6.5 ± 0.66 | 4.24 ± 0.45| 3.21 ± 0.5 |
| (No Vehicles) |                                     | 6.24 ± 0.39| 4.29 ± 0.33| 3.16 ± 0.24|
| (No Entry)    |                                     | 6.17 ± 0.86| 3.95 ± 0.47| 3.31 ± 0.65|
| (Danger)      |                                     | 6.01 ± 0.74| 3.92 ± 0.55| 3.49 ± 0.62|
| (Slippery Road) |                               | 6.03 ± 0.64| 3.85 ± 0.28| 3.45 ± 0.62|
| RA            |                                     | 6.98 ± 0.93| 4.12 ± 0.5  | 3.44 ± 0.54|
| Non Speed     |                                     | 7.46 ± 0.64| 4.32 ± 0.47| 3.65 ± 0.4 |
Table 6 shows that MU-SVM with priority-road universum provides the best performance. Further, the performance gains due to MU-SVM reduces with the increase in the number of training samples. For further analysis of this result we use the histogram of projections method. The histogram of projections for the priority-road universum with increased training samples \( n = 750 \), 1500 are provided in Figs. 9 and 10 respectively. As seen from the figures when the number of training samples is large, the estimation problem becomes well-posed and SVM model does not exhibit a huge data-piling effect about the +1 margin borders (compared to Fig. 3). In such cases, application of MU-SVM does not provide a significant improvement over the SVM solution. This is consistent with the results reported in (Cherkassky et al., 2011) for binary U-SVM. This shows that MU-SVM is typically effective for (ill-conditioned) high dimension low sample size settings.
B.4 Additional Histogram of Projections

This section provides the histogram of projections on the modeling results for the ABCDETC and ISOLET datasets. The experimental settings are discussed in Section 4.1.

B.4.1 ABCDETC Dataset

As seen from Figs 11 - 14,
• **Upper**: the SVM model results in a narrow distribution of the universum samples and in turn provides near random prediction on the universum samples. Applying MU-SVM for this case provides no significant change to multiclass SVM solution and hence no additional improvement in generalization (see Table 2).

• **Lower**: the SVM model results in a relatively wider distribution of the universum samples (compared to **Upper**). Applying MU-SVM for this case provides some improvement to the multiclass SVM (see Table 2).

• **Symbol and RA**: the SVM model results in a wide distribution of the universum samples. Further, in both the cases the universum samples are mostly predicted as digit ‘1’. Applying MU-SVM for this case results to a narrow distribution of the universum samples and increases the uncertainty on the universum samples. This results to a significant improvement to the multiclass SVM solution (see Table 2).
B.4.2 ISOLET Dataset

Figure 15: Typical histogram of projection of training samples \((n = 500)\) (shown in blue) and universum samples ‘Others’ \((m = 1000)\) (shown in red). SVM decision functions (with \(C = 1, \gamma = 2^{-7}\)) for (a) letter ‘a’. (b) letter ‘b’. (c) letter ‘c’. (d) letter ‘d’. (e) letter ‘e’. (f) frequency plot of predicted labels for universum samples using SVM model. MU-SVM decision functions (with \(C^*/C = 0.1, \Delta = 0.05\)) for (g) letter ‘a’. (h) letter ‘b’. (i) letter ‘c’. (j) letter ‘d’. (k) letter ‘e’. (l) frequency plot of predicted labels for universum samples using MU-SVM model.

Figure 16: Typical histogram of projection of training samples \((n = 500)\) (shown in blue) and universum samples ‘RA’ \((m = 1000)\) (shown in red). SVM decision functions (with \(C = 1, \gamma = 2^{-7}\)) for (a) letter ‘a’. (b) letter ‘b’. (c) letter ‘c’. (d) letter ‘d’. (e) letter ‘e’. (f) frequency plot of predicted labels for universum samples using SVM model. MU-SVM decision functions (with \(C^*/C = 0.1, \Delta = 0.1\)) for (g) letter ‘a’. (h) letter ‘b’. (i) letter ‘c’. (j) letter ‘d’. (k) letter ‘e’. (l) frequency plot of predicted labels for universum samples using MU-SVM model.

As seen from Figs 15-16,

- **Others**: the SVM model results in a near random prediction on the universum samples. Applying MU-SVM for this case reduces the projection of the universum samples but does not result to a significant increase in the uncertainty of the universum samples, and hence no additional improvement in generalization (see Table 2).
- **RA**: the SVM model results in a wide distribution of the universum samples. Further, the universum samples are mostly predicted as letter ‘d’. Applying MU-SVM for this case results to a narrow distribution of the universum samples and increases the uncertainty on the universum samples. This results to a significant improvement to the multiclass SVM solution (see Table 2).
B.5 Comparison of the error estimates using 5-Fold CV vs. Theorem 2

This section provides the error estimates curves for the different model parameters for the datasets in Table 1.

B.5.1 GTSRB dataset

WITH VARYING $C^*/C$

Figure 17: Performance of MU-SVM with RA universum for the GTSRB dataset. Here, no. of training samples ($n = 300$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]$, $C = 1$, $\Delta = 0$. (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 18: Performance of MU-SVM with Non-Speed universum for the GTSRB dataset. Here, no. of training samples ($n = 300$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]$, $C = 1$, $\Delta = 0$. (b) Ranking of the model parameters with the smallest error estimate over each experiments.

WITH VARYING $\Delta$

Figure 19: Performance of MU-SVM with RA universum for the GTSRB dataset. Here, no. of training samples ($n = 300$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $\Delta = [0, 0.01, 0.05, 0.1]$, $C = 1$, $C^*/C = \frac{n}{mL} = 0.1$ (b) Ranking of the model parameters with the smallest error estimate over each experiments.
Figure 20: Performance of MU-SVM with Non-Speed universum for the GTSRB dataset. Here, no. of training samples ($n = 300$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $\Delta = [0, 0.01, 0.05, 0.1]$, $C = 1$, $C^*/C = \frac{n}{m_L} = 0.1$ (b) Ranking of the model parameters with the smallest error estimate over each experiments.

B.5.2 ABCDETC dataset

with Varying $C^*/C$

Figure 21: Performance of MU-SVM with Upper-case universum for the ABCDETC dataset. Here, no. of training samples ($n = 600$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $\Delta = 0$, $C = 1$, $\gamma = 2^{-7}$, $C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]$ (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 22: Performance of MU-SVM with Lower-case universum for the ABCDETC dataset. Here, no. of training samples ($n = 600$), no. of universum samples ($m = 1000$) (a) Error estimates for the model parameters $\Delta = 0$, $C = 1$, $\gamma = 2^{-7}$, $C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]$ (b) Ranking of the model parameters with the smallest error estimate over each experiments.
Figure 23: Performance of MU-SVM with Symbol universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = 0, C = 1, \gamma = 2^{-7}, C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 24: Performance of MU-SVM with RA universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = 0, C = 1, \gamma = 2^{-7}, C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0]\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

WITH VARYING \(\Delta\)

Figure 25: Performance of MU-SVM with Upper universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = [0, 0.01, 0.05, 0.1], C = 1, \gamma = 2^{-7}, C^*/C = \frac{n}{mL} = 0.15\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.
Figure 26: Performance of MU-SVM with Lower universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = [0, 0.01, 0.05, 0.1], C = 1, \gamma = 2^{-7}, C^*/C = \frac{n}{mL} = 0.15\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 27: Performance of MU-SVM with Symbol universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = [0, 0.01, 0.05, 0.1], C = 1, \gamma = 2^{-7}, C^*/C = \frac{n}{mL} = 0.15\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 28: Performance of MU-SVM with RA universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = [0, 0.01, 0.05, 0.1], C = 1, \gamma = 2^{-7}, C^*/C = \frac{n}{mL} = 0.15\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

**B.5.3 ISOLET dataset**

*with Varying \(C^*/C\)*
Figure 29: Performance of MU-SVM with Others universum for the ISOLET dataset. Here, no. of training samples \( n = 500 \), no. of universum samples \( m = 1000 \) (a) Error estimates for the model parameters \( C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0] \), \( C = 1 \), \( \Delta = 0 \) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

Figure 30: Performance of MU-SVM with RA universum for the ISOLET dataset. Here, no. of training samples \( n = 500 \), no. of universum samples \( m = 1000 \) (a) Error estimates for the model parameters \( C^*/C = [10^{-3}, 10^{-2}, 10^{-1}, 10^0] \), \( C = 1 \), \( \Delta = 0 \) (b) Ranking of the model parameters with the smallest error estimate over each experiments.

\( \text{WITH VARYING } \Delta \) 

Figure 31: Performance of MU-SVM with RA universum for the ABCDETC dataset. Here, no. of training samples \( n = 600 \), no. of universum samples \( m = 1000 \) (a) Error estimates for the model parameters \( \Delta = [0, 0.01, 0.05, 0.1] \), \( C = 1 \), \( C^*/C = \frac{n}{mL} = 0.1 \) (b) Ranking of the model parameters with the smallest error estimate over each experiments.
Figure 32: Performance of MU-SVM with Others universum for the ABCDETC dataset. Here, no. of training samples \((n = 600)\), no. of universum samples \((m = 1000)\) (a) Error estimates for the model parameters \(\Delta = [0, 0.01, 0.05, 0.1]\), \(C = 1, C^*/C = \frac{n}{mL} = 0.1\) (b) Ranking of the model parameters with the smallest error estimate over each experiments.