Data-dependent Generalization Bounds for Multi-class Classification

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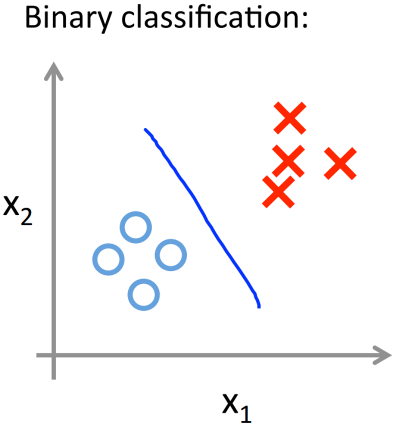
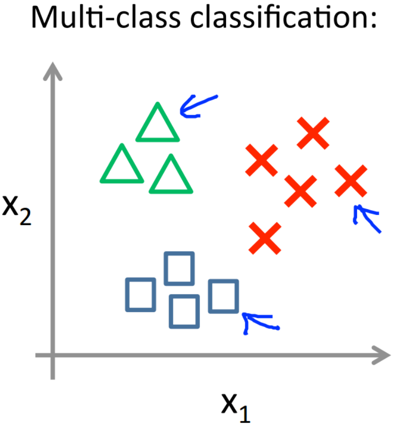
Joint work with Ürün Dogan, Alexander Binder, Ding-Xuan Zhou and Marius Kloft

Outline

Multi-class Classification (MCC): Classic Problem in ML

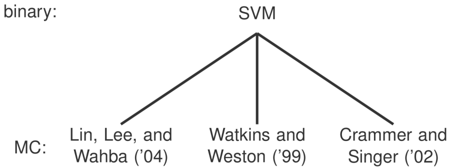


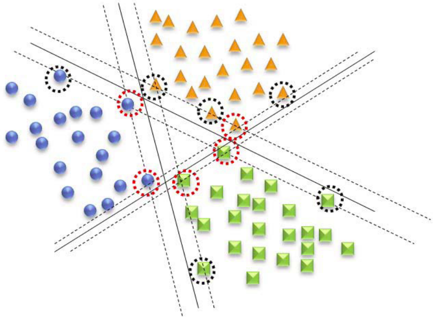


Many MCC **Algorithms** out there...

E.g.:

- Multinomial logistic regression
- Multi-class SVMs





In this talk: **Theory** for MCC

Koltchinskii and Panchenko (2002); Mohri et al. (2012); Kuznetsov et al. (2014)

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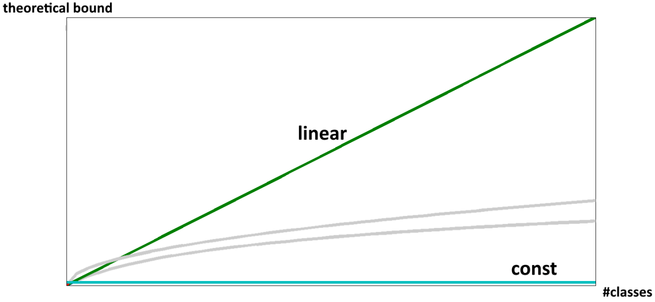
Especially interesting in XC:

What is the **scaling** of generalization bounds for MCC in the **number of classes**?



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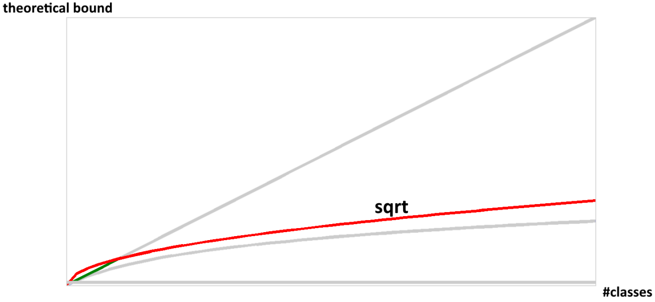

Lei et al. (2015); Maurer (2016); Cortes et al. (2016)

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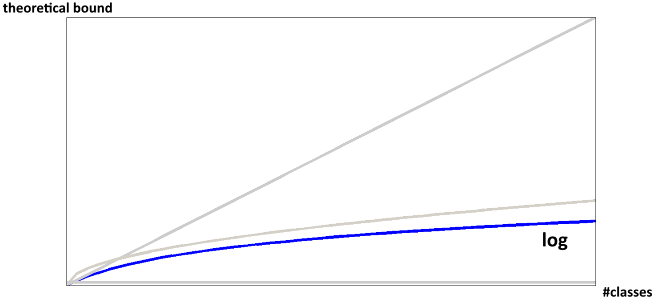


Lei et al. (2019)

Outline

Problem Setting

Multi-class Classification

Given training data:

- (,`dog`), (,`car`), (,`airplane`), ...

Multi-class Classification

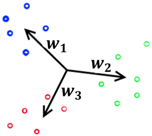
Given training data:

- (,`dog`), (,`car`), (,`airplane`), ...
- Formally $\underbrace{z_1 = (x_1, y_1), \ldots, z_n = (x_n, y_n)}_{\in \mathcal{X} \times \mathcal{Y}} \overset{\text{i.i.d.}}{\sim} P$
  - $\mathcal{Y} := \{1, 2, \ldots, \mathbf{c}\}$
  - $\mathbf{c}$ = number of classes

Multi-class Classification

Aim:

- Define a hypothesis class H of functions $h = (h_1, \ldots, h_c)$
  - e.g., $h_y(x) = \langle \mathbf{w}_y, \phi(x) \rangle \in H_K$



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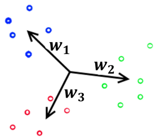

- Find an $h \in H$ that "predicts well" via

$$\hat{y} := \boxed{\arg\max}_{y \in \mathcal{Y}} h_y(x)$$

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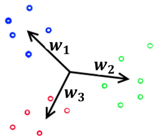

- Find an $h \in H$ that "predicts well" via

$$\hat{y} := \boxed{\arg\max}_{y \in \mathcal{Y}} h_y(x)$$

- Want $h_{y_i}(x_i)$ being larger than all other $h_y(x_i)$
  - otherwise loss incurred through loss function $\Psi_y : \mathbb{R}^c \to \mathbb{R}_+$

Want: small generalization error $\mathbb{E}_{\mathbf{X},\mathbf{Y}} \Psi_Y(h_Y(X))$.

Types of Generalization bounds for MCC

Data-independent bounds

- based on covering numbers
  (Guermeur, 2002; Zhang, 2004a,b; Hill and Doucet, 2007)
- unable to adapt to data

Data-dependent bounds

- based on Rademacher complexity
  (Koltchinskii and Panchenko, 2002; Mohri et al., 2012; Cortes et al., 2013; Kuznetsov et al., 2014)
- computable from the data

In this talk: **data-dependent bounds**

Generalization Error Bounds

Data-dependent bounds based on **Rademacher Complexity** (RC)

Definition (RC)

$$\mathfrak{R}_S(H) := \mathbb{E}_{\boldsymbol{\sigma}}\Big[\sup_{h\in H} \frac{1}{n}\sum_{i=1}^{n} \boxed{\epsilon_i}\, h(z_i)\Big]$$

where $\epsilon_1, \ldots, \epsilon_n$ are random signs ("Rademacher variables")

Interpretation: RC measures how much **the hypothesis class can correlate with random noise**.

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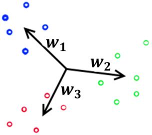
$$\forall h \in H_K^c:\ \underbrace{\mathbb{E}_Y \Psi_Y(h(X))}_{\text{expectation}} - \underbrace{\frac{1}{n}\sum_{i=1}^{n}\Psi_{y_i}(h(x_i))}_{\text{empirical}} \le 2\mathfrak{R}_S\Big(\Psi_y(h(x)) : h \in H_K^c\Big)$$

Data-dependent bounds based on **RC**

Example (Crammer & Singer):

$$H = \{ h^{\mathbf{w}} = (\langle \mathbf{w}_1, \phi(x) \rangle, \ldots, \langle \mathbf{w}_c, \phi(x) \rangle) : \mathbf{w} = (\mathbf{w}_j)_{j=1}^{c}, \boxed{\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2} \leq 1 \}$$



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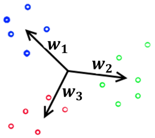

Multi-class margin: for any $h : \mathcal{X} \mapsto \mathbb{R}^c$, we denote by

$$\rho_h(\mathbf{x}, y) := h_y(\mathbf{x}) - \max_{y' : y' \neq y} h_{y'}(\mathbf{x}) \tag{1}$$

Multi-class margin loss:

$$\Psi_y(h(\mathbf{x})) = \max\left(1 - \rho_h(\mathbf{x}, y), 0\right)$$

Key step is to estimate

$$\mathfrak{R}_S\Big(\Psi_y(h) : h \in H\Big) \Leftarrow \mathfrak{R}_S\Big(\rho_h(\mathbf{x}, y) : h \in H\Big) \Leftarrow \mathfrak{R}_S\Big(\max_{j=1,\ldots,c}(h(\mathbf{x})) : h \in H\Big)$$

linear dependency on #classes

Classic analysis based on:

$$\mathfrak{R}_S(\max\{h_1, \ldots, h_c\} : h_j \in H_j, j = 1, \ldots, c) \leq \boxed{\sum_{j=1}^{c} \mathfrak{R}_S(H_j)} \tag{2}$$

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Implies linear dependence on number of classes

Koltchinskii and Panchenko (2002); Mohri et al. (2012); Cortes et al. (2013); Kuznetsov et al. (2014)

From **linear** to **sqrt** dependency on #classes

Key is to use the Lipschitz continuity of loss function:

A function $f : \mathbb{R}^c \to \mathbb{R}$ is L-Lips. cont. w.r.t. a norm $\|\cdot\|$ in $\mathbb{R}^c$ if

$$|f(\mathbf{t}) - f(\mathbf{t}')| \leq L\|(t_1 - t'_1, \ldots, t_c - t'_c)\|, \quad \forall \mathbf{t}, \mathbf{t}' \in \mathbb{R}^c.$$

- e.g., ℓ_∞-norm: $\|\mathbf{t}\|_\infty = \max_{j=1,\ldots,c} |t_j|$ (Crammer & Singer)

Y. Lei, U. Dogan, A. Binder, and M. Kloft. Multi-class svms: From tighter data-dependent generalization bounds to novel algorithms.
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From **linear** to **sqrt** dependency on #classes

Key is to use the **Lipschitz** continuity of loss function:

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Key result

If $f_1, \ldots, f_n$ are L-Lips. cont. w.r.t. $\|\cdot\|_2$, then

$$\mathbb{E}_\epsilon \sup_{h=(h_1,\ldots,h_c)\in H} \sum_{i=1}^n \epsilon_i f_i(h(x_i)) \leq \sqrt{2} L \mathbb{E}_\epsilon \sup_{h=(h_1,\ldots,h_c)\in H} \sum_{i=1}^n \sum_{j=1}^c \epsilon_{ij} h_j(x_i) \tag{3}$$

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Crammer & Singer

The function $f_i(\mathbf{t}) = \max_{j=1,\ldots,c} t_j$ is 1-Lipschitz continuous w.r.t. ℓ_2-norm:

$$\Big|\max_{j=1,\ldots,c} t_j - \max_{j=1,\ldots,c} \tilde{t}_j\Big| \leq \|\mathbf{t} - \tilde{\mathbf{t}}\|_2 = \Big(\sum_{j=1}^{c} |t_j - \tilde{t}_j|^2\Big)^{1/2}$$

We have the **constraint**: $\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2 \leq 1$

- by (2),

$$\mathfrak{R}_S\Big(\max_{j=1,\ldots,c}(h(\mathbf{x})) : h \in H\Big) \leq \sum_{j=1}^{c} \mathbb{E}_{\boldsymbol{\sigma}} \sup_{\|\mathbf{w}_j\|_2 \leq 1} \frac{1}{n} \sum_{i=1}^{n} g_i \langle \mathbf{w}_j, \mathbf{x}_i \rangle$$

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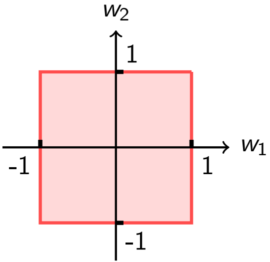
Result Preserves Correlation

classic result (2):

$$\sup_{\|w_1\|_2 \le 1} \sum_{i=1}^{n} \epsilon_i \langle w_1, x_i \rangle + \sup_{\|w_2\|_2 \le 1} \sum_{i=1}^{n} \epsilon_i \langle w_2, x_i \rangle$$

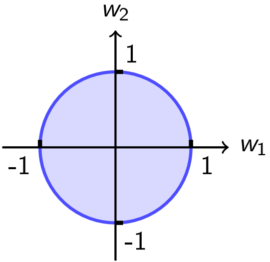
supremum taken **separately**



Lipschitz result (3):

$$\sup_{\|(w_1, w_2)\|_2 \le 1} \sum_{i=1}^{n} [\epsilon_{i1} \langle w_1, x_i \rangle + \epsilon_{i2} \langle w_2, x_i \rangle]$$

supremum taken **jointly**



Preserving the coupling means supremum in a smaller space!

Overview

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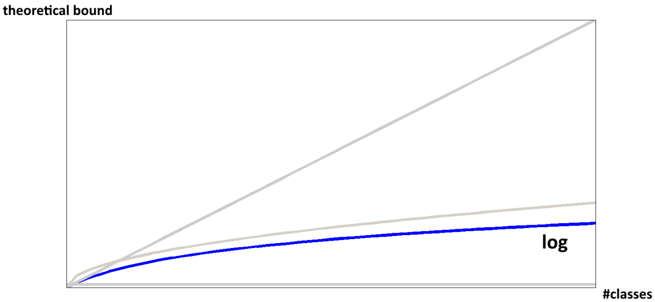

Key observation

- Structural result (3) uses **lipschitz continuity** of maximum w.r.t. $\|\cdot\|_2$

$$\Big|\max_{j=1,\dots,c} t_j - \max_{j=1,\dots,c} \tilde{t}_j\Big| \le \|\mathbf{t}-\tilde{\mathbf{t}}\|_2 = \Big(\sum_{j=1}^{c} |t_j - \tilde{t}_j|^2\Big)^{1/2}$$

- However, maximum is 1-Lipschitz continuous w.r.t. $\|\cdot\|_\infty$

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- the same Lipschitz constant but ℓ_∞-norm is much milder:

$$\|\mathbf{t}\|_2 = \sqrt{c}\|\mathbf{t}\|_\infty \quad \text{if elements of } \mathbf{t} \text{ are the same}$$

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Can we directly use ℓ_∞ Lipschitz continuity?

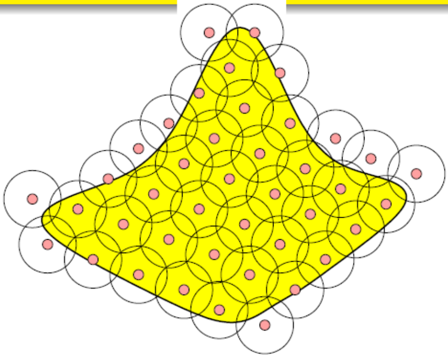
Background: Covering numbers

- F is a class of scalar-valued functions defined over a space $\tilde{\mathcal{Z}}$
- $S := \{\mathbf{z}_1, \ldots, \mathbf{z}_n\} \subset \tilde{\mathcal{Z}}$ is a set of cardinality n

$\{\mathbf{v}^1, \ldots, \mathbf{v}^m\} \subset \mathbb{R}^n$ is an (ϵ, ℓ_∞)-cover of F w.r.t. S if

$$\sup_{f \in F} \min_{j=1,\ldots,m} \max_{i=1,\ldots,n} |f(\mathbf{z}_i) - \mathbf{v}_i^j| \leq \epsilon.$$

$\mathcal{N}_\infty(\epsilon, F, n)$: the smallest cardinality m of such an (ϵ, ℓ_∞)-cover



Core Idea

Introduce the **linear** and scalar-valued function class

$$\widetilde{H} := \{\mathbf{v} \to \langle \mathbf{w}, \mathbf{v} \rangle : \|\mathbf{w}\| \leq 1, \mathbf{v} \in \widetilde{S}\},$$

$$\widetilde{S} := \{\underbrace{\tilde{\phi}_1(x_1), \tilde{\phi}_2(x_1), \ldots, \tilde{\phi}_c(x_1)}_{\text{induced by } \mathbf{x}_1}, \ldots, \underbrace{\tilde{\phi}_1(x_n), \tilde{\phi}_2(x_n), \ldots, \tilde{\phi}_c(x_n)}_{\text{induced by } \mathbf{x}_n}\},$$

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Key identity:

$$\langle \mathbf{w}, \tilde{\phi}_j(\mathbf{x}_i) \rangle = \Big\langle (\mathbf{w}_1, \ldots, \mathbf{w}_c), \big(\underbrace{0, \ldots, 0}_{j-1}, \phi(\mathbf{x}_i), \underbrace{0, \ldots, 0}_{c-j}\big) \Big\rangle = \langle \mathbf{w}_j, \phi(\mathbf{x}_i) \rangle.$$

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Traversing all i, j means
extracting all components $\mathbf{w}_j$ over all examples $\mathbf{x}_i$

New Structural Result based on Covering Numbers

$$\mathcal{N}_\infty(\epsilon, \{\Psi_y(h(\mathbf{x})) : h \in H\}, n) \leq \mathcal{N}_\infty(\epsilon/L, \widetilde{H}, \boxed{nc}). \quad (4)$$

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- Complexity of $\widetilde{H}$ is readily tackled (Zhang, 2002; Srebro et al., 2010)

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Main result

Theorem (Lei, Dogan, Zhou, and Kloft, 2019)

If Ψ_y is L-Lipschitz continuous w.r.t. $\|\cdot\|_\infty$, then

$$\mathfrak{R}_S(F) \leq 27L\sqrt{c}\,\boxed{\mathfrak{R}_{nc}(\widetilde{H})}.$$

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Proof?

$\mathfrak{R}_S(F)$ $\mathcal{N}_\infty(\epsilon, F, n)$ $\mathcal{N}_\infty(\epsilon, \widetilde{H}, nc)$ $\mathfrak{R}_{nc}(\widetilde{H})$

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Proof?

$\mathfrak{R}_S(F)$ $\quad\quad$ $\mathcal{N}_\infty(\epsilon, F, n)$ $\quad\quad$ $\mathcal{N}_\infty(\epsilon, \widetilde{H}, nc)$ $\quad\quad$ $\mathfrak{R}_{nc}(\widetilde{H})$

Example

If $\|\mathbf{w}\| = \|\mathbf{w}\|_2$, then

$$\max_{i\in\mathbb{N}_n} \|\phi(\mathbf{x}_i)\|_2 (2nc)^{-\frac{1}{2}} \leq \mathfrak{R}_{nc}(\widetilde{H}) \leq \max_{i\in\mathbb{N}_n} \|\phi(\mathbf{x}_i)\|_2 (nc)^{-\frac{1}{2}}.$$

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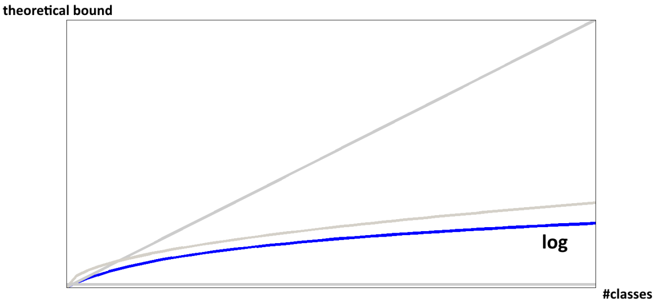

Applications & Discussions

Applications–classic MC-SVMs

MC-SVM in Cramer & Singer (2002): Crammer and Singer (2002)

$$\min_{\mathbf{w}} \ \frac{1}{2}\Big[\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2\Big] + C\sum_{i=1}^{n} \max_{y':y'\neq y_i} \big(1 - \langle \mathbf{w}_{y_i} - \mathbf{w}_{y'}, \phi(x_i)\rangle\big)_+$$

Multinomial logistic regression: Bishop (2006)

$$\min_{\mathbf{w}} \ \frac{1}{2}\Big[\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2\Big] + C\sum_{i=1}^{n} \log\Big(\sum_{y'=1}^{c} \exp\big(\langle \mathbf{w}_{y'} - \mathbf{w}_{y_i}, \phi(x_i)\rangle\big)\Big)$$

Applications–**classic MC-SVMs**

MC-SVM in Cramer & Singer (2002): Crammer and Singer (2002)

$$\min_{\mathbf{w}} \frac{1}{2}\left[\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2\right] + C\sum_{i=1}^{n} \max_{y': y' \neq y_i} \left(1 - \langle \mathbf{w}_{y_i} - \mathbf{w}_{y'}, \phi(x_i)\rangle\right)_+$$

Multinomial logistic regression: Bishop (2006)

$$\min_{\mathbf{w}} \frac{1}{2}\left[\sum_{j=1}^{c} \|\mathbf{w}_j\|_2^2\right] + C\sum_{i=1}^{n} \log\left(\sum_{y'=1}^{c} \exp\left(\langle \mathbf{w}_{y'} - \mathbf{w}_{y_i}, \phi(x_i)\rangle\right)\right)$$

Classic bound by (2)	$O\left(n^{-1}\boxed{c}\sqrt{\sum_{i=1}^{n}\langle\phi(x_i),\phi(x_i)\rangle}\right)$
Lipschitz bound by (3)	$O\left(n^{-1}\sqrt{\boxed{c}\sum_{i=1}^{n}\langle\phi(x_i),\phi(x_i)\rangle}\right)$
Covering no. bound by (4)	$O\left(n^{-\frac{1}{2}}\boxed{\log c}\max_{i\in\mathbb{N}_n}\|\phi(x_i)\|_2\right)$

Applications–ℓ_p-norm MC-SVM

ℓ_p-norm MC-SVM (Lei, Dogan, Binder, and Kloft, 2015)

$$\min_{\mathbf{w}} \ \frac{1}{2}\Big[\sum_{j=1}^{c}\|\mathbf{w}_j\|_2^p\Big]^{\frac{2}{p}} + C\sum_{i=1}^{n}\max_{y':y'\neq y_i}\big(1-\langle \mathbf{w}_{y_i}-\mathbf{w}_{y'},\phi(x_i)\rangle\big)_+$$

Applications–ℓ_p-norm MC-SVM

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$$\min_{\mathbf{w}} \ \frac{1}{2}\Big[\sum_{j=1}^{c}\|\mathbf{w}_j\|_2^p\Big]^{\frac{2}{p}} + C\sum_{i=1}^{n}\max_{y':y'\neq y_i}\big(1-\langle \mathbf{w}_{y_i}-\mathbf{w}_{y'},\phi(x_i)\rangle\big)_+$$

Classic bound by (2)	$O\Big(n^{-1}\boxed{c}\sqrt{\sum_{i=1}^n\langle\phi(x_i),\phi(x_i)\rangle}\Big)$
Lipschitz bound by (3)	$O\Big(n^{-1}\boxed{c^{1-\frac{1}{p}}}\sqrt{\sum_{i=1}^n\langle\phi(x_i),\phi(x_i)\rangle}\Big)$
Covering no. bound by (4)	$O\Big(n^{-\frac{1}{2}}\boxed{c^{\frac{1}{2}-\frac{1}{\max(2,p)}}\log c}\max_{i\in\mathbb{N}_n}\|\phi(x_i)\|_2\Big)$

- Bound by (3) enjoys **logarithmic** dependency if $p \approx 1$ and sublinear dependency $c^{1-\frac{1}{p}}$ otherwise — Lei et al. (2015)
- Bound by (4) enjoys **logarithmic** dependency if $p \leq 2$ and sublinear dependency $c^{\frac{1}{2}-\frac{1}{p}}$ otherwise — Lei et al. (2019)

Empirical Verification

- We consider two datasets **ALOI** and **Sector**
- Vary the number of classes by grouping class labels
- **Approximation of the Empirical Rademacher Complexity** (AERC) defined by

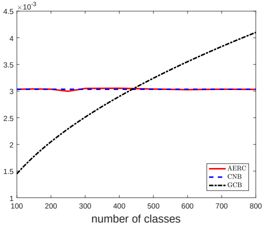
$$\mathrm{AERC}(F) := \frac{1}{50}\sum_{t=1}^{50}\widetilde{\mathfrak{R}}_S(\boldsymbol{\epsilon}^{(t)}, F),$$

where (Monte Carlo approximation)

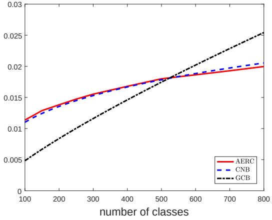
$$\widetilde{\mathfrak{R}}_S(\boldsymbol{\epsilon}, F) := \frac{1}{n}\sup_{\substack{\mathbf{w}\in\mathbb{R}^{d\times c}\\ \|\mathbf{w}\|_{2,p}\leq\Lambda}}\sum_{i=1}^{n}\epsilon_i\Psi_{y_i}\big(\langle\mathbf{w}_1,\mathbf{x}_i\rangle,\ldots,\langle\mathbf{w}_c,\mathbf{x}_i\rangle\big). \tag{5}$$

AERC w.r.t. #classes

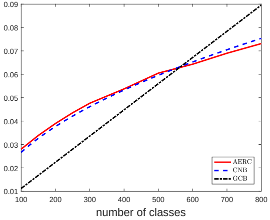
ALOI



$p = 2$



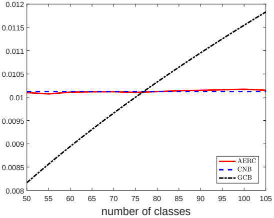
$p = 5$



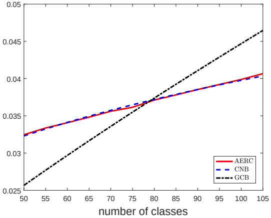
$p = \infty$

AERC w.r.t. #classes

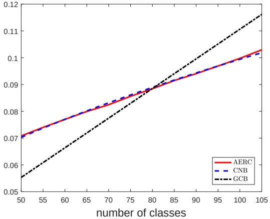
Sector



$p = 2$



$p = 5$



$p = \infty$

Conclusions & Future Directions

Conclusions:

- New data-dependent bound with **mild** dependency on c
  - logarithmic for Cramer & Singer MC-SVM
  - logarithmic for Multinomial logistic regression
  - sublinear for ℓ_p-norm MC-SVM
- Key is **structural result** (4) using lips. cont. w.r.t. $\|\cdot\|_\infty$

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Directions:

- Extension to multi-label
- A data-dependent bound **independent** of the class size?

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