> Generalization bounds based on the splitting and connectivity properties of a set of classifiers

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Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Learning with binary loss

$$\mathbb{X}^{L} = \{x_{1}, \dots, x_{L}\} - \text{a finite universe set of objects;} \\ A = \{a_{1}, \dots, a_{D}\} - \text{a finite set of classifiers;} \\ I(a, x) = [classifier a makes an error on object x] - bipar$$

I(a, x) = [classifier *a* makes an error on object x] — binary loss;

 a_1 a_2 a_4 a_5 a_3 aя . . . a_D X - observable1 1 0 0 0 1 . . . 1 X_1 0 0 1 1 (training) sample 0 0 . . . 1 . . . 1 0 0 of size ℓ 0 0 0 0 . . . Xρ \bar{X} — hidden 1 0 0 0 1 1 . . . 0 $x_{\ell+1}$ 0 0 1 0 (testing) sample 0 0 . . . 1 . . . od size $k = L - \ell$ 1 1 1 1 1 0 . . . 0 XL

Loss matrix of size $L \times D$, all columns are distinct:

n(a) — number of errors of a classifier *a* on the set \mathbb{X}^L ; n(a, X) — number of errors of a classifier *a* on a sample $X \subset \mathbb{X}^L$; $\nu(a, X) = n(a, X)/|X|$ — error rate of *a* on a sample $X \subset \mathbb{X}^L$;

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Example. The loss matrix for a set of linear classifiers



1 vector having no errors

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Example. The loss matrix for a set of linear classifiers



1 vector having no errors 5 vectors having 1 error

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

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Example. The loss matrix for a set of linear classifiers



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Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Probability of overfitting

Def. The *learning algorithm* $\mu \colon X \mapsto a$ takes a training sample $X \subset \mathbb{X}^{L}$ and returns a classifier $a \equiv \mu X \in A$.

Def. Algorithm μ overfits on a given partition $X \sqcup \overline{X} = \mathbb{X}^{L}$ if

$$\delta(\mu, X) \equiv \nu(\mu X, \bar{X}) - \nu(\mu X, X) \ge \varepsilon.$$

Def. Probability of overfitting

$$Q_{\varepsilon}(\mu, \mathbb{X}^{L}) = \mathsf{P}[\delta(\mu, X) \ge \varepsilon].$$

Def. Exact bound: $Q_{\varepsilon} = \eta(\varepsilon)$. **Def.** Upper bound: $Q_{\varepsilon} \leq \eta(\varepsilon)$.

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Weak (permutational) probabilistic assumptions

Axiom

All partitions $\mathbb{X}^{L} = \{x_{1}, \dots, x_{L}\} = X \sqcup \overline{X}$ are equiprobable, where X — observable training sample of size ℓ ; \overline{X} — hidden testing sample of size $k = L - \ell$;

Probability is defined as a fraction of partitions:

$$egin{aligned} \mathcal{Q}_arepsilon &= \mathsf{P}ig[\delta(\mu,X) \geqslant arepsilonig] = rac{1}{\mathcal{C}_L^\ell} \sum_{\substack{X,ar{X} \ X \sqcup ar{X} = \mathbb{X}^L}} ig[\delta(\mu,X) \geqslant arepsilonig]. \end{aligned}$$

Interpretation: Only *independence* of observations is postulated. Continuous measures, infinite sets, and limits $|X| \rightarrow \infty$ are illegal.

Nevertheless, tight generalization bounds can be obtained!

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

One-classifier bound (OC-bound)

Let
$$A = \{a\}$$
, $m = n(a)$. Obviously, $\mu X = a$ for all $X \subset \mathbb{X}^{L}$.

Definition

Hypergeometric distribution function:

$$PDF: h_{L}^{\ell, m}(s) = P[n(a, X) = s] = \frac{C_{m}^{s} C_{L-m}^{\ell, m}}{C_{L}^{\ell}};$$

$$CDF: H_{L}^{\ell, m}(z) = P[n(a, X) \leq z] = \sum_{s=0}^{\lfloor z \rfloor} h_{L}^{\ell, m}(s)$$

Theorem (exact OC-bound)

For one-classifier set $A = \{a\}$, m = n(a), and any $\varepsilon \in (0, 1)$

$$Q_{\varepsilon} = H_{L}^{\ell, m}(s_{m}(\varepsilon)), \quad s_{m}(\varepsilon) = \frac{\ell}{L}(m-\varepsilon k).$$

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Hypergeometric distribution, PDF $h_L^{\ell,m}(s) = C_m^s C_{L-m}^{\ell-s} / C_L^{\ell}$



Distribution is concentrated along diagonal $s \approx \frac{\ell}{L}m$, thus allowing to predict both n(a) = m and $n(a, \bar{X}) = \frac{m-s}{k}$ from n(a, X) = s. Law of Large Numbers: $\nu(a, X) \rightarrow \nu(a)$ with $\ell, k \rightarrow \infty$.

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Vapnik-Chervonenkis bound (VC-bound), 1971

For any
$$\mathbb{X}^L$$
, A, μ , and $arepsilon\in(0,1)$

$$\mathcal{Q}_{\varepsilon} = \mathsf{P} \big[\nu \big(\mu X, \bar{X} \big) - \nu \big(\mu X, X \big) \geqslant \varepsilon \big] \leqslant$$

STEP 1: *uniform bound* makes the result independent on μ :

$$\leqslant \widetilde{Q}_{\varepsilon} = \mathsf{P}\max_{a\in A} [\nu(a, \overline{X}) - \nu(a, X) \geqslant \varepsilon] \leqslant$$

STEP 2: *union bound* (wich is usually higly overestimated):

$$\leq \mathsf{P}\sum_{\mathbf{a}\in A} \left[\nu\left(\mathbf{a},\bar{X}
ight) - \nu\left(\mathbf{a},X
ight) \geqslant \varepsilon
ight] =$$

exact one-classifier bound:

$$=\sum_{a\in A}H_L^{\ell,m}\left(s_m(\varepsilon)\right),\quad m=n(a).$$

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

OC-bound vs. VC-bound

The VC-bound [Vapnik and Chervonenkis, 1971] can be represented as a sum of OC-bounds over all classifiers $a \in A$:

Theorem (OC-bound)

$$Q_{\varepsilon} = H_L^{\ell, m}(s_m(\varepsilon)), \quad m = n(a).$$

Theorem (VC-bound)

$$Q_{\varepsilon} \leqslant \widetilde{Q}_{\varepsilon} \leqslant \sum_{a \in A} H_{L}^{\ell, m}(s_{m}(\varepsilon)), \quad m = n(a).$$

VC-bound is highly overestimated because of union bound, which discards the *splitting* and *similarity* properties of *A*.

Probability of overfitting Weak (permutational) probabilistic assumptions OC-bound and VC-bound

Paradigms of COLT not using union bound

- Uniform convergence bounds [Vapnik, Chervonenkis, 1968]
- Theory of learnable (PAC-learning) [Valiant, 1982]
- Data-dependent bounds [Haussler, 1992]
- Concentration inequalities [Talagrand, 1995]
- Connected function classes [Sill, 1995]
- Similar classifiers VC bounds [Bax, 1997]
- Margin based bounds [Bartlett, 1998]
- Self-bounding learning algorithms [Freund, 1998]
- Rademacher complexity [Koltchinskii, 1998]
- Adaptive microchoice bounds [Langford, Blum, 2001]
- Algorithmic stability [Bousquet, Elisseeff, 2002]
- Algorithmic luckiness [Herbrich, Williamson, 2002]
- Shell bounds [Langford, 2002]
- PAC-Bayes bounds [McAllester, 1999; Langford, 2005]
- Splitting and connectivity bounds [Vorontsov, 2010]

SC-graph, UC-bound and SC-bound SC-bound is exact for some model sets of classifiers Proofs technique: generating and inhibiting subsets

Splitting and Connectivity graph

Define two binary relations on classifiers: partial order $a \leq b$: $I(a, x) \leq I(b, x)$ for all $x \in \mathbb{X}^{L}$; precedence $a \prec b$: $a \leq b$ and Hamming distance ||b - a|| = 1.

Definition (SC-graph)

Splitting and Connectivity (SC-) graph $\langle A, E \rangle$: A - a set of classifiers with distinct binary loss vectors; $E = \{(a, b): a \prec b\}.$

Properties of the SC-graph:

- each edge (a, b) is labeled by an object $x_{ab} \in \mathbb{X}^{L}$ such that $0 = I(a, x_{ab}) < I(b, x_{ab}) = 1$;
- multipartite graph with layers $A_m = \{a \in A : n(a) = m\}, m = 0, \dots, L + 1;$

SC-graph, UC-bound and SC-bound

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Example. Loss matrix and SC-graph for a set of linear classifiers



SC-graph, UC-bound and SC-bound

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Example. Loss matrix and SC-graph for a set of linear classifiers



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Connectivity and inferiority of a classifier

Def. Connectivity of a classifier
$$a \in A$$

 $p(a) = \# \{ x_{ba} \in \mathbb{X}^{L} : b \prec a \}$ — low-connectivity.
 $q(a) = \# \{ x_{ab} \in \mathbb{X}^{L} : a \prec b \}$ — up-connectivity;

Def. Inferiority of a classifier $a \in A$ $r(a) = \# \{ x_{cb} \in \mathbb{X}^L : c \prec b \leq a \} \in \{ p(a), \dots, n(a) \}.$

Example:



SC-graph, UC-bound and SC-bound

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Uniform Connectivity (UC-) bound

Theorem (UC-bound)

For all
$$\mathbb{X}^{L}$$
, μ , A and $\varepsilon \in (0, 1)$
 $\widetilde{Q}_{\varepsilon} \leq \sum_{a \in A} [p \leq k] \left(\frac{C_{L-q-p}^{\ell-q}}{C_{L}^{\ell}} \right) H_{L-q-p}^{\ell-q, m-p}(s_{m}(\varepsilon))$
where $m = n(a)$, $q = q(a)$, $p = p(a)$

• UC-bound improves the VC-bound, even if $p(a) \equiv q(a) \equiv 0$: $\widetilde{Q}_{\varepsilon} \leq \sum H_{L}^{\ell, m}(s_{m}(\varepsilon)).$

- Provide the contribution of a ∈ A decreases exponentially by p(a)
 ⇒ connected sets are less subjected to overfitting.
- OC-bound relies on connectivity, but disregards splitting.

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Pessimistic Empirical Risk Minimization

Definition (ERM)

Learning algorithm μ is Empirical Risk Minimization if

$$\mu X \in A(X), \qquad A(X) = \operatorname{Arg\,min}_{a \in A} n(a, X);$$

A choice of a classifier a from A(X) is ambiguous. Pessimistic choice will result in modestly inflated upper bound.

Definition (pessimistic ERM)

Learning algorithm μ is pessimistic ERM if

$$\mu X = \arg \max_{a \in A(X)} n(a, \bar{X});$$

SC-graph, UC-bound and SC-bound

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The Splitting and Connectivity (SC-) bound

Theorem (SC-bound)

For pessimistic ERM μ , any \mathbb{X}^L , A and $\varepsilon \in (0, 1)$

$$Q_{\varepsilon} \leqslant \sum_{a \in A} [r \leqslant k] \left(\frac{C_{L-q-r}^{\ell-q}}{C_{L}^{\ell}} \right) H_{L-q-r}^{\ell-q, m-r} (s_m(\varepsilon))$$

where m = n(a), q = q(a), r = r(a).

If $q(a) \equiv r(a) \equiv 0$ then SC-bound transforms to VC-bound:

$$Q_{\varepsilon} \leq \sum_{a \in A} H_{L}^{\varepsilon, m}(s_{m}(\varepsilon)).$$

The contribution of a ∈ A decreases exponentially by:
 q(a) ⇒ connected sets are less subjected to overfitting;
 r(a) ⇒ only lower layers contribute significantly to Q_ε.

SC-graph, UC-bound and SC-bound SC-bound is exact for some model sets of classifiers Proofs technique: generating and inhibiting subsets

Experiment on model data: SC-bound vs. Monte Carlo estimate

Separable two-dimensional task, L = 100, two classes.



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Experiment on model data: UC-bound vs. Monte Carlo estimate

Separable two-dimensional task, L = 100, two classes.



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Experiment on model data: SC-bounds vs. VC-bound

Two-dimensional task, L = 100, two classes.

Correct — 0% errors; Noise20 — 20% errors; Random — 50% errors; Vapnik — data-independent VC-bound.



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Monotone chain of classifiers

Def. Monotone chain of classifiers: $a_0 \prec a_1 \prec \cdots \prec a_D$.

Example: 1-dimensional threshold classifiers $a_j(x) = [x - \theta_j]$;



SC-graph:

Loss matrix:

m=3 m=2 m=2 m=1 m=1 m=1 m=0 m=0 m=1

	a_0	a_1	a_2	a 3
<i>x</i> ₁	0	1	1	1
<i>x</i> ₂	0	0	1	1
<i>x</i> 3	0	0	0	1
<i>X</i> 4	0	0	0	0
X_5	0	0	0	0
x_6	0	0	0	0

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Two-dimensional monotone lattice of classifiers

Example:

2-dimensional linear classifiers,
2 classes {●, ○},
6 objects



SC-graph:



Loss matrix:

	a_{00}	a_{01}	a_{10}	a_{02}	a_{11}	a_{20}	a 03	a_{12}	a_{21}	a ₃₀
<i>x</i> ₁	0	1	0	1	1	0	1	1	1	0
<i>x</i> ₂	0	0	1	0	1	1	0	1	1	1
<i>X</i> 3	0	0	0	1	0	0	1	1	0	0
<i>x</i> ₄	0	0	0	0	0	1	0	0	1	1
X_5	0	0	0	0	0	0	1	0	0	0
<i>x</i> 6	0	0	0	0	0	0	0	0	0	1

SC-bound is exact(!) for multidimensional(!) lattices of classifiers

Denote $\mathbf{d} = (d_1, \dots, d_h)$ an *h*-dimensional index vector, $d_j = 0, 1, \dots$ Denote $|\mathbf{d}| = d_1 + \dots + d_h$.

Definition

Monotone h-dimensional lattice of classifiers of height D:

$$A = \left\{ a_{\mathbf{d}}, \ |\mathbf{d}| \leqslant D \ \middle| \begin{array}{l} \mathbf{c} < \mathbf{d} \ \Rightarrow \ a_{\mathbf{c}} < a_{\mathbf{d}} \\ n(a_{\mathbf{d}}) = m_0 + |\mathbf{d}| \end{array} \right\}$$

Theorem (exact SC-bound)

If A is monotone h-dimensional lattice of height D, $D \ge k$, and μ is pessimistic ERM then for any $\varepsilon \in (0, 1)$

$$Q_{\varepsilon} = \sum_{t=0}^{k} C_{h+t-1}^{t} \frac{C_{L-h-t}^{\ell-h}}{C_{L}^{\ell}} H_{L-h-t}^{\ell-h, m_{0}} \left(s_{m_{0}+t}(\varepsilon)\right).$$

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Sets of classifiers with known SC-bound

Model sets of classifiers with known exact SC-bound:

- monotone chains and multidimensional lattices;
- unimodal chains and multidimensional lattices;
- pencils of monotone chains;
- layers and intervals of boolean cube;
- hamming balls and their lower layers;
- some sparse subsets of multidimensional lattices;
- some sparse subsets of hamming balls;

Real sets of classifiers with known tight SC-bound:

• conjunction rules (see further);

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Generating and inhibiting subsets of objects

Conjecture

For any $a \in A$ generating set $X_a \subset \mathbb{X}^L$ and inhibiting set $X'_a \subset \mathbb{X}^L$ exist such that if classifier $a \in A$ is a result of learning then all objects X_a lie in the training set and all objects X'_a lie in the testing set:

 $[\mathbf{v} \mathbf{v} \mathbf{v}] < [\mathbf{v} \subset \mathbf{v}] [\mathbf{v}' \subset \mathbf{v}]$

$$[\mu \land -a] \approx [\Lambda_a \subseteq \land] [\Lambda_a \subseteq \land].$$

$$X_a$$

$$X_a$$

$$X_a$$

$$X - \text{training}$$

$$X - \text{testing}$$

$$X^L$$

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Bounds based on generating and inhibiting subsets

Lemma (Probability of obtaining each of classifiers)

If **Conjecture** is true then for any μ , X, $a \in A$

$$\mathsf{P}[\mu X = a] \leqslant P_a = C_{L_a}^{\ell_a} / C_L^{\ell}.$$

where $L_a = L - |X_a| - |X'_a|$, $\ell_a = \ell - |X_a|$.

Theorem (Probability of overfitting)

If **Conjecture** is true then for any \mathbb{X}^L , μ , A and $\varepsilon \in (0, 1)$

$$Q_{\varepsilon} \leqslant \sum_{a \in A} P_a H_{L_a}^{\ell_a, m_a} \left(s_a(\varepsilon) \right),$$

where $m_a = n(a, \mathbb{X}^L) - n(a, X_a) - n(a, X'_a),$ $s_a(\varepsilon) = \frac{\ell}{L}(n(a, \mathbb{X}^L) - \varepsilon k) - n(a, X_a).$

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Correspondence between SC-graph and generating/inhibiting subsets

Upper connectivity of a classifier $a \in A$ $q(a) = |X_a|, X_a = \{x_{ab} \in \mathbb{X}^L : a \prec b\}$ — generating subset.

Inferiority of a classifier $a \in A$ $r(a) = |X'_a|, X'_a = \{x_{cb} \in \mathbb{X}^L : c \prec b \leq a\}$ — inhibiting subset.



SC-bound for conjunctive rules induction SC-modification of rule evaluation heuristics Experiments and conclusions

Classifier — weighted voting of conjunctive rules

Rule-based classifier (weighted voting of rules):

$$a(x) = \arg \max_{y \in Y} \sum_{r \in R_y} w_r r(x),$$

where Y — set of class labels, R_y — set of rules that votes for the class y, $r: X \rightarrow \{0, 1\}$ — rule, and w_r — its weight.

Conjunctive rule:

$$r(x) = \bigwedge_{j\in J} [f_j(x) \leqslant \theta_j],$$

where $f_j(x)$ — real features, θ_j — thresholds, j = 1, ..., n; $J \subseteq \{1, ..., n\}$ — subset of features, usually $|J| \leq 7$;

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Rule evaluation heuristics

Intrinsically the rule learning is a two-criteria optimization problem:

$$N(r,X) = \frac{1}{|X|} \# \{ x_i \in X : r(x_i) = 1, y_i \neq y \} \rightarrow \min_r;$$

$$P(r,X) = \frac{1}{|X|} \# \{ x_i \in X : r(x_i) = 1, y_i = y \} \rightarrow \max_r;$$

Practically one-criterion heuristics $H(P, N) \rightarrow \max_{r}$ are used:

- Information gain;
- Gini Index;
- $\bullet\,$ Fisher exact test, χ^2 or ω^2 statistical tests, etc.

A common drawback of all these criteria:

Ignoring an overfitting that results from thresholds θ_j learning: $N(r, \bar{X})$ will be greater than expected; $P(r, \bar{X})$ will be less than expected.

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Problem: rules are typically overfitted in real applications



Real task: predicting the result of atherosclerosis surgical treatment, L = 98.

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SC-modification of rule evaluation heuristics

Problem:

Estimate $N(r, \overline{X})$ and $P(r, \overline{X})$ to select rules more carefully.

Solution:

1. Calculate data-dependent SC-bounds:

$$\mathsf{P}\big[\mathsf{N}(\mathsf{r},\bar{\mathsf{X}}) - \mathsf{N}(\mathsf{r},\mathsf{X}) \ge \varepsilon\big] \leqslant \eta_{\mathsf{N}}(\varepsilon); \\ \mathsf{P}\big[\mathsf{P}(\mathsf{r},\mathsf{X}) - \mathsf{P}(\mathsf{r},\bar{\mathsf{X}}) \ge \varepsilon\big] \leqslant \eta_{\mathsf{P}}(\varepsilon);$$

2. Invert SC-bounds: with probability at least $1-\eta$

$$N(r, \overline{X}) \leq \hat{N}(r, \overline{X}) = N(r, X) + \varepsilon_{N}(\eta);$$

$$P(r, \overline{X}) \geq \hat{P}(r, \overline{X}) = P(r, X) - \varepsilon_{P}(\eta).$$

3. Substitute \hat{P} , \hat{N} in a one-criterion heuristic: $H(\hat{P}, \hat{N}) \to \max_{r}$.

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Classes of equivalent rules: one point per rule

Example: separable 2-dimensional task, L = 10, two classes. rules: $r(x) = [f_1(x) \leq \theta_1 \text{ and } f_2(x) \leq \theta_2].$



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Classes of equivalent rules: one point per class

Example: the same classification task. One point per class. rules: $r(x) = [f_1(x) \leq \theta_1 \text{ and } f_2(x) \leq \theta_2].$



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Classes of equivalent rules: SC-graph

Example: SC-graph isomorphic to the graph at previous slide.



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Experiment on real data sets

Data sets from UCI repository:

Task	Objects	Features
australian	690	14
echo cardiogram	74	10
heart disease	294	13
hepatitis	155	19
labor relations	40	16
liver	345	6

Learning algorithms:

- WV weighted voting (boosting);
- DL decision list;
- LR logistic regression.

Testing method: 10-fold cross validation.

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Experiment on real data sets. Results

	tasks					
Algorithm	austr	echo	heart	hepa	labor	liver
RIPPER-opt	15.5	2.97	19.7	20.7	18.0	32.7
RIPPER+opt	15.2	5.53	20.1	23.2	18.0	31.3
C4.5(Tree)	14.2	5.51	20.8	18.8	14.7	37.7
C4.5(Rules)	15.5	6.87	20.0	18.8	14.7	37.5
C5.0	14.0	4.30	21.8	20.1	18.4	31.9
SLIPPER	15.7	4.34	19.4	17.4	12.3	32.2
LR	14.8	4.30	19.9	18.8	14.2	32.0
WV	14.9	4.37	20.1	19.0	14.0	32.3
DL	15.1	4.51	20.5	19.5	14.7	35.8
WV+CS	14.1	3.2	19.3	18.1	13.4	30.2
DL+CS	14.4	3.6	19.5	18.6	13.6	32.3

Two top results are highlighted for each task.

SC-bound for conjunctive rules induction SC-modification of rule evaluation heuristics Experiments and conclusions

Conclusions

- Combinatorial framework can give tight and sometimes exact generalization bounds.
- OC (one-classifier) bound is exact.
- UC (uniform connectivity) bound rely on *connectivity* but neglect *splitting*.
- SC (splitting and connectivity) bound is most tight and even *exact* for monotone chains and lattices of classifiers.
- SC-bound being applied to rule induction reduces testing error of classifiers by 1–2%.

Questions, please

SC-bound for conjunctive rules induction SC-modification of rule evaluation heuristics Experiments and conclusions

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