Recent Advances on Generalization Bounds
Part II: Combinatorial Bounds

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Learning with binary loss

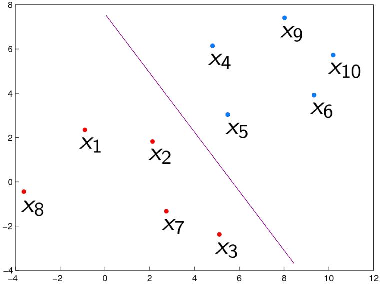
$\mathbb{X}^L = \{x_1, \dots, x_L\}$ — a finite universe set of objects;
$A = \{a_1, \dots, a_D\}$ — a finite set of classifiers;
$I(a, x) = [\text{classifier } a \text{ makes an error on object } x]$ — binary loss;

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

	a_1	a_2	a_3	a_4	a_5	a_6	$\cdots$	a_D	
x_1	1	1	0	**0**	0	1	$\cdots$	1	X — observable
$\dots$	0	0	0	**0**	1	1	$\cdots$	1	(training) sample
x_ℓ	0	0	1	**0**	0	0	$\cdots$	0	of size ℓ
$x_{\ell+1}$	0	0	0	**1**	1	1	$\cdots$	0	$\bar{X}$ — hidden
$\dots$	0	0	0	**1**	0	0	$\cdots$	1	(testing) sample
x_L	0	1	1	**1**	1	1	$\cdots$	0	od size $k = L - \ell$

$n(a)$ — *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 $X \subset \mathbb{X}^L$;

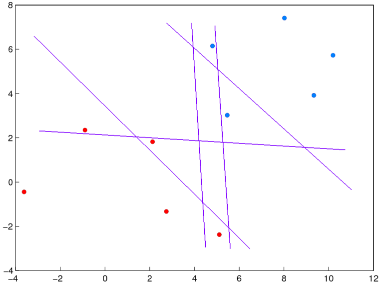
Example. The loss matrix for a set of linear classifiers



1 vector having no errors

	no errors
x_1	0
x_2	0
x_3	0
x_4	0
x_5	0
x_6	0
x_7	0
x_8	0
x_9	0
x_{10}	0

Example. The loss matrix for a set of linear classifiers

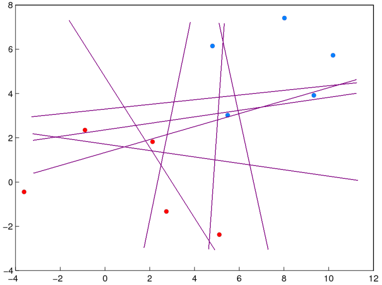


1 vector having no errors

5 vectors having 1 error

	no errors	1 error				
x_1	0	1	0	0	0	0
x_2	0	0	1	0	0	0
x_3	0	0	0	1	0	0
x_4	0	0	0	0	1	0
x_5	0	0	0	0	0	1
x_6	0	0	0	0	0	0
x_7	0	0	0	0	0	0
x_8	0	0	0	0	0	0
x_9	0	0	0	0	0	0
x_{10}	0	0	0	0	0	0

Example. The loss matrix for a set of linear classifiers



1 vector having no errors
5 vectors having 1 error
8 vectors having 2 errors

	no errors	1 error					2 errors								
x_1	0	1	0	0	0	0	1	0	0	0	0	1	1	0	...
x_2	0	0	1	0	0	0	1	1	0	0	0	0	0	0	...
x_3	0	0	0	1	0	0	0	1	1	0	0	0	0	1	...
x_4	0	0	0	0	1	0	0	0	1	1	0	0	0	0	...
x_5	0	0	0	0	0	1	0	0	0	1	1	1	0	0	...
x_6	0	0	0	0	0	0	0	0	0	0	1	0	1	0	...
x_7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	...
x_8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...
x_9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...
x_{10}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...

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 $X \sqcup \bar{X} = \mathbb{X}^L$ if

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

Def. ***Probability of overfitting***

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

Def. *Exact bound*: $Q_\varepsilon = \eta(\varepsilon)$.

Def. *Upper bound*: $Q_\varepsilon \leqslant \eta(\varepsilon)$.

Weak (permutational) probabilistic assumptions

Axiom

All partitions $\mathbb{X}^L = \{x_1, \ldots, x_L\} = X \sqcup \bar{X}$ are equiprobable, where
X — observable training sample of size ℓ;
$\bar{X}$ — hidden testing sample of size $k = L - \ell$;

Probability is defined as a *fraction of partitions*:

$$Q_\varepsilon = \mathsf{P}\bigl[\delta(\mu, X) \geqslant \varepsilon\bigr] = \frac{1}{C_L^\ell} \sum_{\substack{X, \bar{X} \\ X \sqcup \bar{X} = \mathbb{X}^L}} \bigl[\delta(\mu, X) \geqslant \varepsilon\bigr].$$

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

Nevertheless, tight generalization bounds can be obtained!

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:

$$\text{PDF:} \quad h_L^{\ell,m}(s) = \mathsf{P}\big[n(a,X) = s\big] = \frac{C_m^s C_{L-m}^{\ell-s}}{C_L^\ell};$$

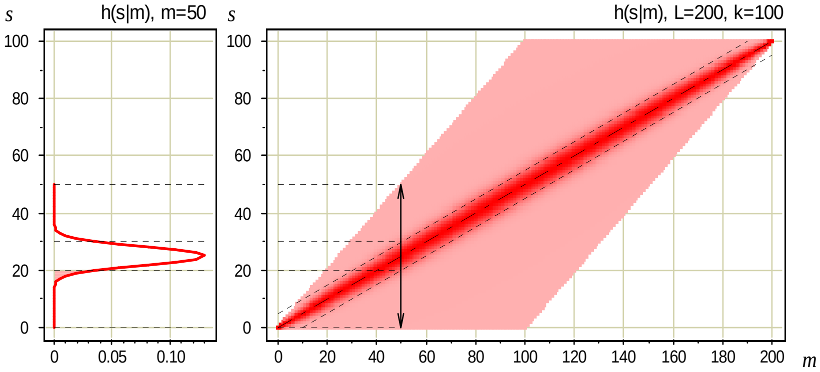
$$\text{CDF:} \quad H_L^{\ell,m}(z) = \mathsf{P}\big[n(a,X) \leqslant z\big] = \sum_{s=0}^{\lfloor z \rfloor} h_L^{\ell,m}(s).$$

Theorem (exact OC-bound)

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

$$Q_\varepsilon = H_L^{\ell,m}\big(s_m(\varepsilon)\big), \quad s_m(\varepsilon) = \tfrac{\ell}{L}(m - \varepsilon k).$$

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: $\nu(a, X) \to \nu(a)$ with $\ell, k \to \infty$.

Vapnik-Chervonenkis bound (VC-bound), 1971

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

$$Q_\varepsilon = \mathsf{P}\bigl[\nu(\mu X, \bar{X}) - \nu(\mu X, X) \geqslant \varepsilon\bigr] \leqslant$$

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

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

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

$$\leqslant \mathsf{P}\sum_{a\in A}\bigl[\nu(a, \bar{X}) - \nu(a, X) \geqslant \varepsilon\bigr] =$$

exact one-classifier bound:

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

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)

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

Theorem (VC-bound)

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

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

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]

Splitting and Connectivity graph

Define two binary relations on classifiers:

partial order $a \leqslant b$: $I(a,x) \leqslant I(b,x)$ for all $x \in \mathbb{X}^L$;

precedence $a \prec b$: $a \leqslant b$ and Hamming distance $\|b - a\| = 1$.

Definition (SC-graph)

Splitting and Connectivity (SC-) graph $\langle A, E\rangle$*:*

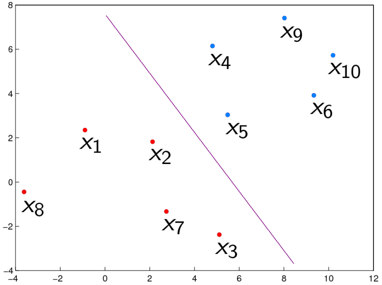
A *— a set of classifiers with distinct binary loss vectors;*

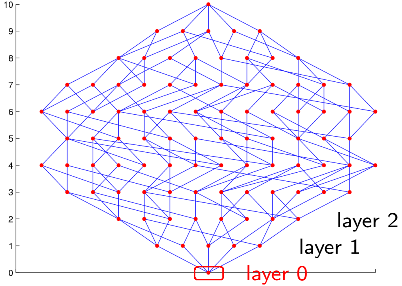
$E = \bigl\{(a,b)\colon a \prec b\bigr\}$.

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 $A_m = \bigl\{a \in A\colon n(a) = m\bigr\}$, $m = 0, \dots, L+1$;

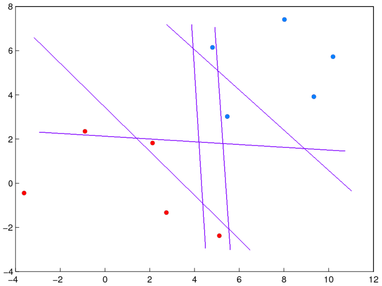
Example. Loss matrix and SC-graph for a set of linear classifiers

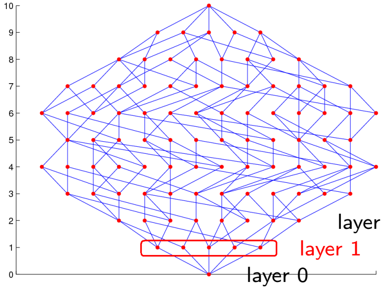




	layer 0
x_1	0
x_2	0
x_3	0
x_4	0
x_5	0
x_6	0
x_7	0
x_8	0
x_9	0
x_{10}	0

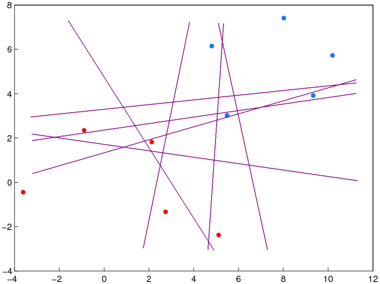
Example. Loss matrix and SC-graph for a set of linear classifiers

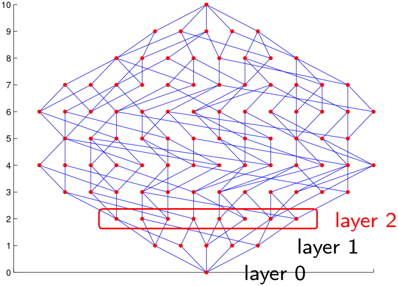




	layer 0	layer 1				
x_1	0	1	0	0	0	0
x_2	0	0	1	0	0	0
x_3	0	0	0	1	0	0
x_4	0	0	0	0	1	0
x_5	0	0	0	0	0	1
x_6	0	0	0	0	0	0
x_7	0	0	0	0	0	0
x_8	0	0	0	0	0	0
x_9	0	0	0	0	0	0
x_{10}	0	0	0	0	0	0

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





	layer 0	layer 1					layer 2								
x_1	0	1	0	0	0	0	1	0	0	0	0	1	1	0	...
x_2	0	0	1	0	0	0	1	1	0	0	0	0	0	0	...
x_3	0	0	0	1	0	0	0	1	1	0	0	0	0	1	...
x_4	0	0	0	0	1	0	0	0	1	1	0	0	0	0	...
x_5	0	0	0	0	0	1	0	0	0	1	1	1	0	0	...
x_6	0	0	0	0	0	0	0	0	0	0	1	0	1	0	...
x_7	0	0	0	0	0	0	0	0	0	0	0	0	0	1	...
x_8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...
x_9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...
x_{10}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	...

Connectivity and inferiority of a classifier

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

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

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

Def. *Inferiority* of a classifier $a \in A$

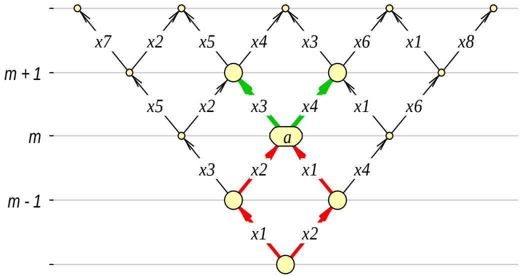
$r(a) = \#\{x_{cb} \in \mathbb{X}^L\colon c \prec b \leqslant a\} \in \{p(a), \dots, n(a)\}.$

Example:

$p(a) = \#\{x1, x2\} = 2,$

$q(a) = \#\{x3, x4\} = 2,$

$r(a) = \#\{x1, x2\} = 2.$



Uniform Connectivity (UC-) bound

Theorem (UC-bound)

For all $\mathbb{X}^L$, μ, A *and* $\varepsilon \in (0,1)$

$$\widetilde{Q}_\varepsilon \leqslant \sum_{a\in A} \left(\frac{C_{L-q-p}^{\ell-q}}{C_L^\ell} \right) H_{L-q-p}^{\ell-q,\; m-p}\left(s_m(\varepsilon)\right)$$

where $m = n(a)$, $q = q(a)$, $p = p(a)$.

1. UC-bound improves the VC-bound, even if $p(a) \equiv q(a) \equiv 0$: $\widetilde{Q}_\varepsilon \leqslant \sum\limits_{a\in A} H_L^{\ell,\, m}\left(s_m(\varepsilon)\right)$.
2. The contribution of $a \in A$ decreases exponentially by $p(a)$ $\Rightarrow$ **connected sets are less subjected to overfitting**.
3. UC-bound relies on connectivity, but disregards splitting.

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

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

The Splitting and Connectivity (SC-) bound

Theorem (SC-bound)

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

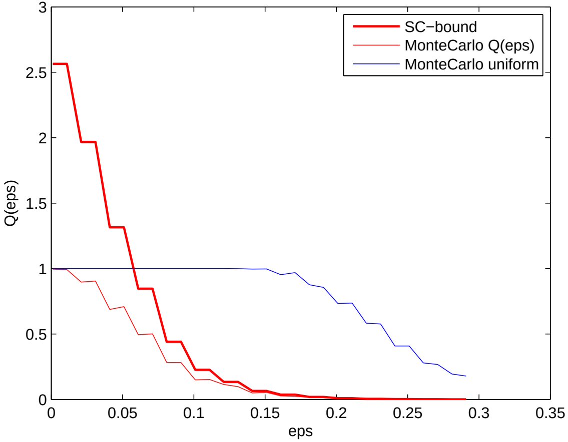
$$Q_\varepsilon \leqslant \sum_{a \in A} \left(\frac{C_{L-q-r}^{\ell-q}}{C_L^\ell} \right) H_{L-q-r}^{\ell-q,\, m-r}\left(s_m(\varepsilon)\right),$$

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

1. If $q(a) \equiv r(a) \equiv 0$ then SC-bound transforms to VC-bound:
   $Q_\varepsilon \leqslant \sum\limits_{a \in A} H_L^{\ell,\, m}\left(s_m(\varepsilon)\right)$.
2. The contribution of $a \in A$ decreases exponentially by:
   $q(a) \Rightarrow$ **connected sets are less subjected to overfitting**;
   $r(a) \Rightarrow$ **only lower layers contribute significantly to Q_ε.**

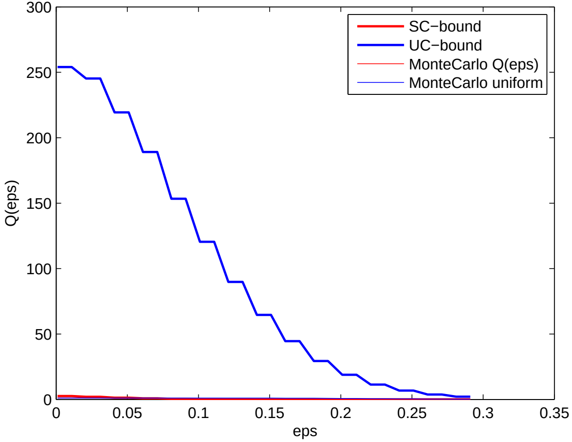
Experiment on model data: SC-bound vs. Monte Carlo estimate

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



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

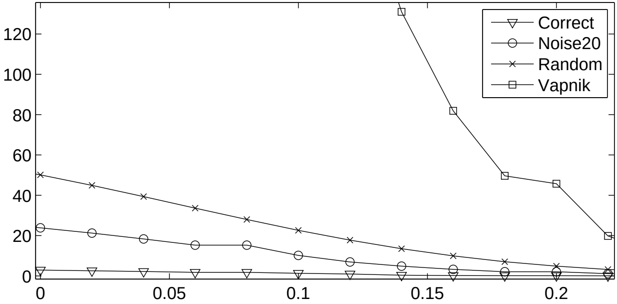
Separable two-dimensional task, $L = 100$, two classes.



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.

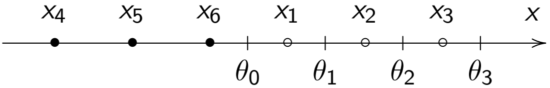


Monotone chain of classifiers

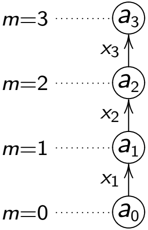
Def. *Monotone chain* of classifiers: $a_0 \prec a_1 \prec \cdots \prec a_D$.

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

2 classes $\{\bullet, \circ\}$
6 objects



SC-graph:



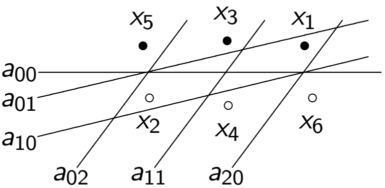
Loss matrix:

	a_0	a_1	a_2	a_3
x_1	0	1	1	1
x_2	0	0	1	1
x_3	0	0	0	1
x_4	0	0	0	0
x_5	0	0	0	0
x_6	0	0	0	0

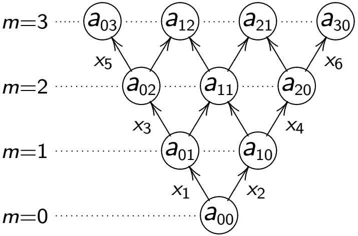
Two-dimensional monotone lattice of classifiers

Example:

2-dimensional linear classifiers,
2 classes $\{\bullet, \circ\}$,
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}
x_1	0	1	0	1	1	0	1	1	1	0
x_2	0	0	1	0	1	1	0	1	1	1
x_3	0	0	0	1	0	0	1	1	0	0
x_4	0	0	0	0	0	1	0	0	1	1
x_5	0	0	0	0	0	0	1	0	0	0
x_6	0	0	0	0	0	0	0	0	0	1

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

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

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, $D \geqslant k$, and μ is pessimistic ERM then for any $\varepsilon \in (0,1)$

$$Q_\varepsilon = \sum_{t=0}^{k} C_{h+t-1}^{t} \frac{C_{L-h-t}^{\ell-h}}{C_L^\ell} H_{L-h-t}^{\ell-h,\ m_0}\left(s_{m_0+t}(\varepsilon)\right).$$

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);
- linear classifiers (under construction now).

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%.

Further: thee appendix slides about underlying combinatorial technique for SC-bounds.

Generating and inhibiting subsets of objects

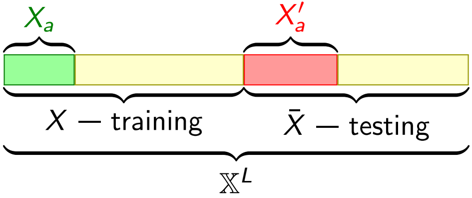
Conjecture

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:

$$[\mu X = a] \leqslant [X_a \subseteq X]\,[X'_a \subseteq \bar{X}].$$



Bounds based on generating and inhibiting subsets

Lemma (Probability of obtaining each of classifiers)

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

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

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

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 $m_a = n(a, \mathbb{X}^L) - n(a, X_a) - n(a, X'_a)$,

$$s_a(\varepsilon) = \tfrac{\ell}{L}\bigl(n(a, \mathbb{X}^L) - \varepsilon k\bigr) - n(a, X_a).$$

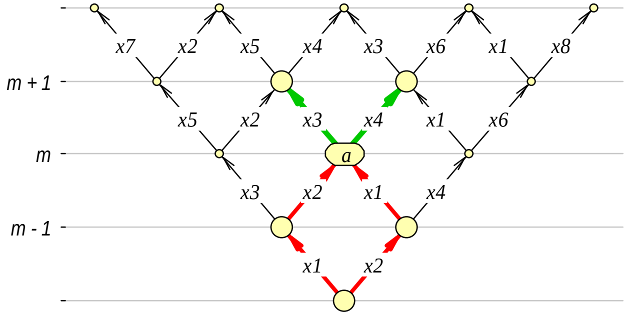
Correspondence between SC-graph and generating/inhibiting subsets

Upper connectivity of a classifier $a \in A$

$q(a) = |X_a|, \;\; X_a = \{x_{ab} \in \mathbb{X}^L \colon a \prec b\}$ — generating subset.

Inferiority of a classifier $a \in A$

$r(a) = |X'_a|, \;\; X'_a = \{x_{cb} \in \mathbb{X}^L \colon c \prec b \leqslant a\}$ — inhibiting subset.



Questions?

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www.MachineLearning.ru/wiki (in Russian):

- Участник:Vokov
- Слабая вероятностная аксиоматика
- Расслоение и сходство алгоритмов (виртуальный семинар)