Machine Learning and Data Analysis
Learning Logic Formulas

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PAC Learning

So far our PAC-learning framework considered *sample complexity*

- how fast m grows with $1/\epsilon$, $1/\delta$, and n
- we requested m to grow polynomially

Note about PAC-learning: inability to produce a consistent hypothesis implies inability to PAC-learn

- Fix a finite $X' \subseteq X$, set $P_X(x) = 1/|X'|$ for all $x \in X'$, set $\epsilon < \frac{1}{|X'|+1}$ and $\delta < 1$ (we are allowed to set any P_X, ϵ, and δ in PAC-learning).
- If hypothesis f is not consistent on an arbitrary example (x, y), then $e(f) \geq 1/|X'| > \epsilon$, violating a PAC-learning condition with probability $1 > \delta$
- Thus if f is not consistent then we did not PAC-learn.

Efficient PAC-Learning

We now also consider *computational complexity*

Efficient PAC Learnability

An algorithm *efficiently PAC-learns* $\mathcal{C}$ by $\mathcal{F}$ if it PAC-learns $\mathcal{C}$ by $\mathcal{F}$ in polynomial time.

Polynomial: again in $1/\epsilon$, $1/\delta$, and the size n of examples

- Learning time grows at least as m does: learner needs at least a unit of time for processing each example
- Efficient PAC-learning thus requires each example to be processed in polynomial time
- Previous slide now implies: if finding a consistent model is NP-hard then we cannot efficiently PAC-learn (unless RP=NP)

Conjunctions and Disjunctions

$X = \{0,1\}^n$, i.e each $x = (x^1, \ldots, x^n)$ where $x^i \in \{0,1\}$, $Y = \{0,1\}$

each f in $\mathcal{F} = \mathcal{C}$ defined by a conjunction ϕ of literals using propositional variables from set $\{p_1 \ldots p_n\}$

$f(x) = 1$ iff ϕ is true under assignment of values x^i to p^i

Generalization algorithm:

$\phi = p_1 \wedge \neg p_1 \wedge \ldots p_n \wedge \neg p_n$ {'most specific hypothesis'}
for each example $(x, 1) \in S$ **do**
  for i = 1 . . . n **do**
    if $x^i = 0$ **then**
      delete p_i from ϕ
    else
      delete $\neg p_i$ from ϕ
return ϕ

Conjunctions and Disjunctions (cont'd)

Algorithm never deletes a literal that must stay in ϕ. Final ϕ is thus consistent or no consistent ϕ exists.

A consistent algorithm exists and $|\mathcal{F}| = 3^n$, therefore conjunctions are PAC-learnable.[1]

Sample complexity: $m \geq \frac{1}{\epsilon}\left(n \ln 3 + \ln \frac{1}{\delta}\right)$

Algorithm makes $m \cdot n$ steps, i.e. time linear in n (size of examples), therefore conjunctions are *efficiently PAC-learnable*.

Same applies for *disjunctions* using a simple transformation:

- run algorithm on 'negated' examples $(x, 1 - c(x))$
- negate its output ϕ ($\neg\phi$ is a disjunction)

[1] $|\mathcal{F}| = 2^{2n}$ if $p_i \wedge \neg p_i$ allowed in the conjunction.

k-Conjunctions and k-Disjunctions

Generalization algorithm produces the most specific (longest) consistent ϕ. Often, small ϕ are wanted.

A *k-conjunction* contains at most k literals. $\mathcal{C}^{k\text{conj}}$ is efficiently PAC-learnable simply by trying the $\mathcal{O}(n^k)$ possible k-conjunctions on n variables.

Heuristic approaches such as best-first search may be employed to speed-up the search within the polynomial bound. Search would start from the empty conjunction, adding a single literal in each step. The heuristic function evaluating the current conjunction ϕ would e.g. be

$$h(\phi) = -|\{(x, 0) \in S \mid x \models \phi\}|$$

while all descendants of any ϕ such that $x \not\models \phi$ for some $(x, 1) \in S$ would be pruned.

k-disjunctions $\mathcal{C}^{k\text{-disj}}$: analogical case, reduce by negating examples and ϕ

k-term DNF and k-clause CNF

A k-term DNF formula: disjunction of at most k conjunctions ('terms').
Example of a 3-term DNF formula:

$$(\neg p_1 \wedge p_3) \vee (p_2 \wedge \neg p_3 \wedge p_4 \wedge \neg p_6) \vee p_2$$

A k-clause CNF formula: conjunction of at most k disjunctions ('clauses').
Example of a 3-clause CNF formula:

$$(p_1 \vee \neg p_3) \wedge (\neg p_2 \vee p_3 \vee \neg p_4 \vee p_6) \wedge \neg p_2$$

Learnability results for the two classes analogical (again reduction by negation), we continue analysis with k-term DNF.

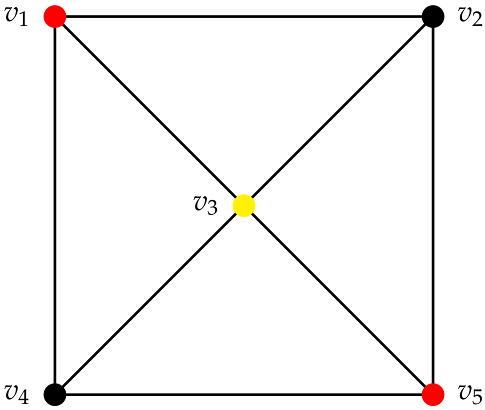
Consistent 3-term DNF as Graph Coloring

Finding a 3-term DNF formula consistent with a sample is as hard graph 3-coloring.

Graph 3-coloring:

- given vertices V and edges E,
- assign one of 3 colors to each vertex $v \in V$ so that no adjacent vertices have same color
- NP-complete problem

Graph Coloring



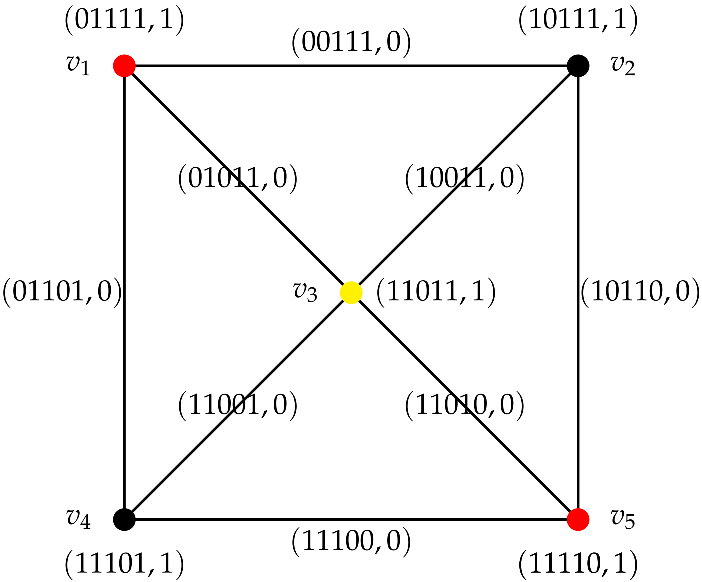
Reduction from a Graph to a Learning Sample

Graph	Sample
vertices $v_1 \ldots v_n$	propositional variables $p_1 \ldots p_n$
vertex v_i	example $(x, 1)$, $x^k = \begin{cases} 0 \text{ if } k = i \\ 1 \text{ otherwise} \end{cases}$
e.g.: vertex v_3	example $(11011, 1)$
edge e_{ij}	example $(x, 0)$, $x^k = \begin{cases} 0 \text{ if } k = i \text{ or } k = j \\ 1 \text{ otherwise} \end{cases}$
e.g.: edge v_{34}	example $(11001, 0)$

Reduction takes time linear in $m = \|V\| + \|E\|$ and n.

Remind: $(x, 1)$ denote positive examples, $(x, 0)$ negative examples.

Reduction from a Graph to a Learning Sample (cont'd)



Consistent 3-term DNF as Graph Coloring (cont'd)

Let S be a sample obtained by reduction of graph (V, E). We will show:

1. If (V, E) is 3-colorable then there is a 3-term DNF formula ϕ consistent with S
2. If there is a 3-term DNF formula ϕ consistent with S then (V, E) is 3-colorable

Colorability $\Rightarrow$ Consistency

Assume vertices V are split in partitions R, B, Y (red, black, yellow) representing a valid coloring.

Consider 3-term DNF formula

$$\phi = T_R \vee T_B \vee T_Y$$

such that

$$T_R = \bigwedge_{v_i \notin R} p_i \qquad T_B = \bigwedge_{v_i \notin B} p_i \qquad T_Y = \bigwedge_{v_i \notin Y} p_i$$

We will show that ϕ is consistent with S reduced from graph (V, E).

Colorability $\Rightarrow$ Consistency (cont'd)

Consistency with positive examples:

1. One positive example $(x, 1)$ for each vertex v_i
2. Assume $v_i \in R$ (B and Y are analogical)
3. T_R does not contain p_i (by definition of T_R)
4. $x^j = 1$ for $i \neq j$ (by reduction)
5. x satisfies T_R (denote $x \models T_R$) (from 3 and 4)
6. Therefore $x \models \phi$

Colorability $\Rightarrow$ Consistency (cont'd)

Consistency with negative examples:

1. One negative example $(x, 0)$ for each edge e_{ij}
2. $x^i = 0$ (by definition)
3. v_i and v_j cannot both be red (because the coloring is valid)
4. Assume v_i is not red
5. $p_i \in T_R$ (by definition of T_R)
6. Therefore $x \not\models T_R$ (from 2 and 5)
7. Analogically $x \not\models T_B$ and $x \not\models T_Y$ (repeat from Step 3 for the remaining colors)
8. Therefore $x \not\models \phi$

Consistency $\Rightarrow$ Colorability

Assume there is a consistent 3-term DNF ϕ, denote the 3 terms T_R, T_B, T_Y:

$$\phi = T_R \vee T_B \vee T_Y$$

This prescribes coloring:

for all positive examples $(x, 1)$ **do**
    Let v_i be the vertex corresponding to x
    if $x \models T_R$ **then**
        color v_i red
    else
        if $x \models T_B$ **then**
            color v_i black
        else
            if $x \models T_Y$ **then**
                color v_i yellow

Consistency ⇒ Colorability (cont'd)

We prove that invalid coloring implies inconsistency of ϕ.

1. Suppose the coloring is not valid.
2. Then there are some adjacent v_i and v_j of same color, say red
3. Let $(x_i, 1)$, $(x_j, 1)$ and $(x_{ij}, 0)$ denote the examples corresponding to v_i, v_j and e_{ij}
4. $x_i, x_j \models T_R$ (by coloring algorithm)
5. $x_i^i = x_j^j = 0$ (by reduction)
6. T_R does not contain p_i or p_j (from 4 and 5)
7. $x_{ij}^k = 1$ for $k \notin \{i, j\}$ (by reduction)
8. $x_{ij} \models T_R$ (from 5 and 7)
9. Therefore $x_{ij} \models \phi$ but then ϕ is not consistent since $(x_{ij}, 0)$ is a negative example

3-term DNF not Efficiently PAC-Learnable

We proved that graph 3-coloring can be solved by linear-time reduction to a learning sample S and learning a 3-term DNF formula ϕ consistent with S.

Since graph 3-coloring is NP-hard, finding a consistent ϕ is also NP-hard.

Therefore $\mathcal{C}^{\text{3-term DNF}}$ is not efficiently PAC-learnable by $\mathcal{C}^{\text{3-term DNF}}$.

- This follows from the fact that inability to find a consistent hypothesis implies inability to PAC-learn (as we have already shown)

Can be also shown for any $\mathcal{C}^{k\text{-term DNF}}$, $k \geq 2$.

k-CNF and k-DNF

$\mathcal{C}^{k\text{-CNF}}$ contains conjunctions of k-disjunctions. Example:

$$(p_1 \vee p_2) \wedge (\neg p_3 \vee p_4 \vee p_5)$$

belongs in $\mathcal{C}^{3\text{-CNF}}$.

$\mathcal{C}^{3\text{-DNF}}$ analogical, we continue with $\mathcal{C}^{3\text{-CNF}}$.

$\mathcal{C}^{k\text{-CNF}}$ is as easy to learn as monotone conjunctions:

- assign a new atom p_i' to each clause that can be written with the original symbols p_i
- there is $\mathcal{O}(n^k)$ (i.e. poly number) of such clauses
- convert all examples into the new representation using symbols p_i' (in poly time)
- learn a monotone conjunction with the new examples using symbols p_i'
- convert it back to the original representation using symbols p_i

k-CNF vs. k-term DNF

Every k-term DNF formula can be written as an equivalent k-CNF formula. Example:

$$(p_1 \wedge p_2) \vee (p_2 \wedge p_3) \equiv (p_1 \vee p_2) \wedge (p_1 \vee p_3) \wedge p_2 \wedge (p_2 \vee p_3)$$

Thus $\mathcal{C}^{k\text{-term DNF}} \subseteq \mathcal{C}^{k\text{-CNF}}$.

$$|\mathcal{C}^{k\text{-term DNF}}| = \mathcal{O}(2^n)$$

$$|\mathcal{C}^{k\text{-CNF}}| = \mathcal{O}(2^{\binom{2n}{k}}) = \mathcal{O}(2^{n^k})$$

So $\mathcal{C}^{k\text{-term DNF}} \subset \mathcal{C}^{k\text{-CNF}}$, thus not every k-CNF formula can be written as an equivalent k-term DNF formula.

Learning k-term DNF by k-CNF

Learning k-term DNF can be reduced to learning k-CNF. Assume examples in sample S contain values for n propositional variables.

- Create a new variable for each possible clause; there are $\mathcal{O}(n^k)$ of them
- Create a new sample S' using the new variables computed from the original variables.
- Learn a monotone conjunction from S'. Translating it back to the original variables yields a k-CNF formula

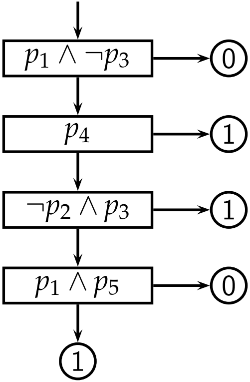
Since conjunctions are efficiently PAC-learnable, k-term DNF are efficiently PAC-learnable *by k-CNF*. (Caveat: Learning may produce a k-CNF formula not rewrittable into a k-term DNF formula.)

In general: a hypothesis class may not be efficiently PAC-learnable by itself, but may be efficiently PAC-learnable by a larger hypothesis class!

k-Decision Lists

A k-Decision list is an ordered set of conjunctive rules with at most k literals in each, and a default value.

Example of a 2-DL:



k-Decision Lists (cont'd)

For $|\mathcal{C}^{k\text{-DL}}|$ we have

$$|\mathcal{C}^{k\text{-DL}}| = \mathcal{O}(3^{|\mathcal{C}^{k\text{-conj}}|}(|\mathcal{C}^{k\text{-conj}}|)!)$$

(each conjunction in in the list can be either be absent, attached to 0, or 1, and the order in the list is arbitrary). Therefore $\log(|\mathcal{C}^{k\text{-DL}}|)$ is polynomial in n, implying polynomial sample complexity.

Every k-DNF formula can be written as a k-Decision List

- every term T of the formula (in any order) forms one rule $\boxed{\text{T}} \rightarrow 1$
- default value is 0

Thus

$$\mathcal{C}^{k\text{-DNF}} \subseteq \mathcal{C}^{k\text{-DL}}$$

For every $c \in \mathcal{C}^{k\text{-DL}}$, also $\neg c \in \mathcal{C}^{k\text{-DL}}$ (revert values in leaves). Therefore also

$$\mathcal{C}^{k\text{-CNF}} \subseteq \mathcal{C}^{k\text{-DL}}$$

k-Decision Lists (cont'd)

$\mathcal{C}^{k\text{-DL}}$ is efficiently PAC-learnable (by $\mathcal{C}^{k\text{-DL}}$) with the *covering algorithm*

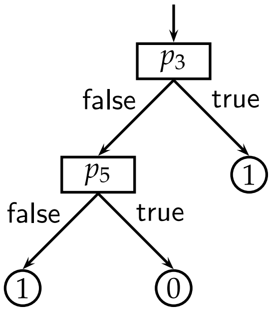
1: $S =$ training sample, $DL =$ empty decision list
2: **while** $S \neq \{\}$ **do**
3: $\quad \phi =$ any k-conjunction such that
$\quad\{(x,0) \in S \,|x \models \phi\} \neq \{\}$ and $\{(x,1) \in S \,|x \models \phi\} = \{\}$ or
$\quad\{(x,0) \in S \,|x \models \phi\} = \{\}$ and $\{(x,1) \in S \,|x \models \phi\} \neq \{\}$
4: $\quad$ add $\boxed{\phi} \rightarrow 0$ or $\boxed{\phi} \rightarrow 1$ (respectively) to DL
5: $\quad S = S \setminus \{(x,y) \in S \mid x \models \phi\}$
6: $\quad$ **if** $S = \{\}$ **then**
7: $\quad\quad$ add default value 1 or 0 (respectively) to DL
8: **return** DL

Note: in Step 3 may go over all $\mathcal{O}(n^k)$ k-conjunctions; heuristic search applicable as in learning k-conjunctions.

k-Decision Trees

A tree in which each path from the root to a leaf has length at most k and represents a rule. Each non-leaf vertex contains one propositional variable, each leaf a class value.

Example of a 3-decision tree:



k-Decision Trees (cont'd)

Any k-DT can be represented by a k-DNF:

- create one term for each path leading to a leaf labelled with "1"

Any k-DT can be represented by a k-CNF:

- create one clause for each path leading to a leaf labelled with "0"

Therefore

$$\mathcal{C}^{k\text{-DT}} \subseteq \mathcal{C}^{k\text{-CNF}} \cap \mathcal{C}^{k\text{-DNF}}$$

Since $\mathcal{C}^{k\text{-CNF}} \neq \mathcal{C}^{k\text{-DNF}}$, we have $\mathcal{C}^{k\text{-DT}} \subset \mathcal{C}^{k\text{-CNF}}$ and $\mathcal{C}^{k\text{-DT}} \subset \mathcal{C}^{k\text{-DNF}}$ and since $\mathcal{C}^{k\text{-CNF}} \subseteq \mathcal{C}^{k\text{-DL}}$ we also have

$$\mathcal{C}^{k\text{-DT}} \subset \mathcal{C}^{k\text{-DL}}$$

k-Decision Trees (cont'd)

It is NP-hard to find a consistent k-Decision tree. $\mathcal{C}^{k\text{-DT}}$ is not efficiently PAC-learnable by $\mathcal{C}^{k\text{-DT}}$.

What is the error bound for an *inconsistent* tree? Remind: if

$$m \geq \frac{1}{2\epsilon^2} \ln \frac{2|\mathcal{F}|}{\delta}$$

then classification error will not exceed training error by more than ϵ with at least $1 - \delta$ probability.

Need to calculate $|\mathcal{F}| = |\mathcal{C}^{k\text{-DT}}|$

k-Decision Trees (cont'd)

$$|\mathcal{C}^{1\text{-DT}}| = 2$$

For depth $k+1$ we have n choices of the root variable, $|\mathcal{C}^{k\text{-DT}}|$ possible left subtrees and $|\mathcal{C}^{(k\text{-DT}}|$ possible right subtrees.

$$|\mathcal{C}^{(k+1)\text{-DT}}| = n \cdot |\mathcal{C}^{k\text{-DT}}|^2$$

Denote $l_k = \log_2 |\mathcal{C}^{k\text{-DT}}|$

$$\begin{aligned} l_1 &= 1 \\ l_{k+1} &= \log_2 n + 2l_k \end{aligned}$$

Solution:

$$l_k = (2^k - 1)(1 + \log_2 n) + 1$$

I.e. $\ln |\mathcal{C}^{k\text{-DT}}|$ polynomial in n (and exponential in k).

k-leave Decision Trees

Altnernatively, we may bound the number of leaves.

$\mathcal{C}^{k\text{-leave DT}}$: trees with at most k leaves.

Finding a consistent k-leave DT still NP-hard. $\mathcal{C}^{k\text{-leave DT}}$ not efficiently PAC-learnable with $\mathcal{C}^{k\text{-leave DT}}$.

Error bound for an inconsistent tree? Size of the concept space:

$$|\mathcal{C}^{k\text{-leave DT}}| \leq n^{k-1}(k+1)^{(2k-1)}$$

Provides better bound than in k-DT: $\ln|\mathcal{C}^{k\text{-leave DT}}|$ polynomial in both n and k.

TDIDT algorithm

A recursive heuristic algorithm for quick (poly-time) construction of a possibly inconsistent DT .

TDIDT(S: sample, $P = \{p_1, \ldots, p_n\}$: propositional variables)

if all examples in S have same class y **then**
  return vertex labeled y
else
  if $P = \{\}$ **then**
    return vertex labeled by the *majority class* in S
  else
    Choose $p_i \in P$ and create a vertex labeled p_i
    for $v \in \{0,1\}$ **do**
      Create an edge from the p_i vertex, label it v
      $S' = \{(x,y) \in S \mid x^i = v\}$
      if $S' = \{\}$ **then**
        add a leaf to edge v, label it by the majority class in S
      else
        add TDIDT(S',$P \setminus p_i$) to edge v

TDIDT algorithm: remarks

- The heuristic in Choose $p_i \in P$

Define $S_i = \{(x, y) \mid x \models p_i\}$. Usually we choose p_i maximizing

$$\Delta H(S, p_i) = H(S) - \frac{|S_i|}{S} H(S_i) - \frac{|S \setminus S_i|}{S} H(S \setminus S_i)$$

where *entropy* $H(S)$ is defined as

$$H(S) = -\sum_{y \in \{0,1\}} \frac{|\{(x, y) \in S\}|}{|S|} \log_2 \frac{|\{(x, y) \in S\}|}{|S|}$$

Remarks

- TDIDT easily adaptable to constructing k-DT

Condition $P = \{\}$ is replaced by $P = \{\}$ or current depth $= k$

- TDIDT and other logic-based learners applicable also non-Boolean classification

TDIDT: No change in code needed. Decision lists: use multiple target values instead of 0 and 1, covering strategy remains same.

- TDIDT and other logic-based learners easily adaptable to nominal features

TDIDT: Instead of going over the Boolean range $v \in \{0,1\}$, we go over all possible values of the nominal feature x^i. Other learners: pre-construct Boolean features from nominal features (similarly to what follows).

Remarks (cont'd)

- TDIDT and other logic-based learners easily adaptable to real-valued features

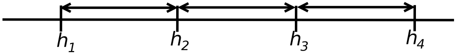
Use pre-constructed Boolean features such as p:

$$p \text{ is true iff } x^i > 153.56$$

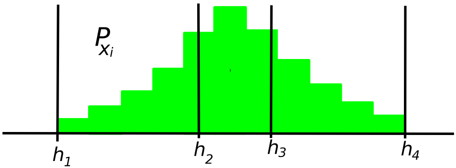
where x^i is an original real-valued feature and the threshold value 153.56 is determined in a preprocessing step. Multiple thresholds for one real-valued feature may be considered and used to define multiple Boolean features.

Discretization: 3 General Approaches

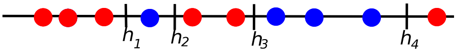
- Equilength intervals



- Equiprobable intervals



- Intervals containing same-class examples (most popular)



Inconsistent Hypotheses

Remind: when $\mathcal{C} \not\subseteq \mathcal{F}$ or $P_{Y|X}$ is not a concept, we must learn inconsistent hypotheses. Then we do not PAC-learn but we still have error bounds:

- Training error vs. classification error bound

$$|e(f) - e(S,f)| \leq \sqrt{\frac{1}{2m} \ln \frac{2|\mathcal{F}|}{\delta}}$$

does not assume the learner minimizes training error, i.e. that it outputs $\arg\min_{f \in \mathcal{F}} e(S,f)$

- Classification error of learned vs. best hypothesis bound

$$e(f) \leq \left(\min_{f \in \mathcal{F}} e(f) \right) + 2\sqrt{\frac{1}{2m} \ln \frac{2|\mathcal{F}|}{\delta}}$$

assumes the learner minimizes training error. This may be difficult.

Consistency vs. Error Minimization

Class	Find f, $e(S,f) = 0$	Find $\arg\min_{f \in \mathcal{F}} e(S,f)$
k-DT, k-leave DT	NP-hard	NP-hard
any $\mathcal{C}$ where $\lvert\mathcal{C}\rvert$ poly	easy	easy
.. such as k-conjunctions	easy	easy
general conjunctions	easy	NP-hard

Minimizing $e(S,f)$ for general conjunctions can be reduced to the NP-hard vertex-cover graph problem.