Maximum Margin Separations in Finite Closure Systems

Florian Seiffarth Tamás Horváth Stefan Wrobel













Separating hyper-plane

classical machine learning problem (Rosenblatt, 1958)



Separating hyper-plane (arbitrary)

classical machine learning problem (Rosenblatt, 1958), not unique, over-fitting



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Maximum margin separation (unique)

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- support vector machines (Vapnik, 1992), unique



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Adaptions:

 \rightarrow

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 \mathbb{R}^d

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$$\rightarrow$$
 E (*finite* ground set)

Adaptions:

\mathbb{R}^{d}	\rightarrow	E (finite ground set)
convexity	\rightarrow	

Adaptions:

 \mathbb{R}^d

- \rightarrow E (finite ground set)
- convexity \rightarrow closure operator

Adaptions:

 $\begin{array}{ccc} \mathbb{R}^d & \to & E \mbox{ (finite ground set)} \\ \mbox{convexity} & \to & \mbox{closure operator} \\ \mbox{convex hull} & \to & \end{array}$

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closure operator *c* over *E*:

• $A \subseteq c(A)$

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$$A \subseteq B \Rightarrow c(A) \subseteq c(B)$$

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$$c(c(A)) = c(A)$$

Definition: closure system (E, C): • $\emptyset, E \in C$ • $A, B \in C \Rightarrow A \cap B \in C$

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- separation margin \rightarrow

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- Which properties should be preserved?
- Goal: Efficient algorithm!

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Maximum Margins in Finite Closure Systems

Florian Seiffarth, Tamás Horváth, Stefan Wrobel Maximum Margin Separations in Finite Closure Systems

Function $I: 2^E \to E$ such that

$$X \subseteq Y \Rightarrow I(X, e) \ge I(Y, e)$$

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Some Practical Motivations:

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Trees

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Graphs (e.g. molecule, social graph, ...)

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 requires semantically meaningful definition of closure system/operator and linkage function

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Maximum-Margin Property:

a + b is maximal and a = b \Leftrightarrow min(a, b) is maximal



Finite Closure Systems:



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Given $A, B \subseteq E$, the *margin* for H and H^c is defined by

$$\mu_{H,H^c}(A,B) := \min\{I(c(A),H^c), I(c(B),H)\}$$
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Given a monotone linkage closure system (E, C, I) and two sets $A, B \subseteq E$, find a half-space H which **maximizes** the margin, i.e.

$$\mathcal{H} = \operatorname*{argmax}_{\mathcal{H}_1, \mathcal{H}_1^c \in \mathcal{C}_c} \mu_{\mathcal{H}_1, \mathcal{H}_1^c}(\mathcal{A}, \mathcal{B})$$

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Solutions:

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1 restrict to Kakutani closure systems (e.g. trees, distributive lattices)

Kakutani closure system:

All disjoint closed sets are half-space separable.

Solutions:

- restrict to Kakutani closure systems (e.g. trees, distributive lattices)
- 2 relax the problem to maximal disjoint closed sets

Kakutani closure system:

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Result: Very efficient algorithm.

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requires only the ground set the closure operator and the linkage function



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Theorem: The algorithm solves the Maximum Margin Closed Set Separation problem by calling the closure operator at most 2|E| - 2 times and the linkage function at most 2|E| times. **Theorem:** The algorithm solves the Maximum Margin Closed Set Separation problem by calling the closure operator at most 2|E| - 2 times and the linkage function at most 2|E| times.

Corollary: The algorithm solves the Maximum Margin Half-Space Separation Problem if the closure system is Kakutani.

Experiments (Finite Point Sets)







(Vapnik, 1992)

Greedy Algorithm

(ECML/PKDD 2019)



Maximum Margin Algorithm (this work)

Experiments (Finite Point Sets)



svm: (Vapnik, 1992), greedy: (ECML/PDKK 2019), max margin: (this work)





Maximum Half-Space separation on trees

Maximum closed set separation on small graphs

• Maximum margin concept **differs** from that in \mathbb{R}^d

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- Maximum Margin Closed Set Separation is efficient solvable
 - outperforms simple greedy algorithm (ECML/PKDD, 2019)

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- reduce complexity of the algorithm for known closure systems (e.g. trees, lattices,...)
- allow approximate/fuzzy solutions

Further Details

Come to the Question and Answer Session or contact me:



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