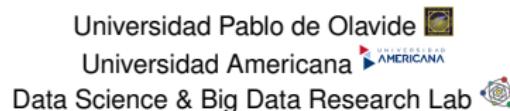


# A Fast Multivariate Symmetrical Uncertainty based Heuristic for High Dimensional Feature Selection

**Miguel García Torres**, Federico Divina, Francisco A. Gómez Vela, José L. Vázquez Noguera  
-PINV18-1129-



5-7 May 2021 - Entropy 2021: The Scientific Tool of the 21st Century

## 1 Feature selection

- Feature relevance and redundancy
- Multivariate SU based Feature Selection Heuristic

## 2 Computational results

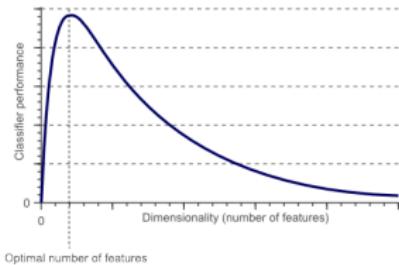
- Microarray data
- Melanoma data

## 3 Conclusions

# Introduction

## Feature selection

#	Sepal length (cm)	Sepal width (cm)	petal length (cm)	petal width (cm)	type
1	5.1	3.5	1.4	0.2	<i>Iris setosa</i>
2	4.9	3.0	1.4	0.2	<i>Iris setosa</i>
3	4.7	3.2	1.4	1.3	<i>Iris setosa</i>
...					
51	7.0	3.2	4.7	1.4	<i>Iris versicolor</i>
52	6.4	3.2	4.5	1.5	<i>Iris versicolor</i>
53	6.9	3.1	4.9	1.5	<i>Iris versicolor</i>
...					
101	6.3	5.8	7.1	2.5	<i>Iris virginica</i>
102	6.4	2.7	5.1	1.9	<i>Iris virginica</i>
103	6.9	3.0	5.9	2.1	<i>Iris virginica</i>



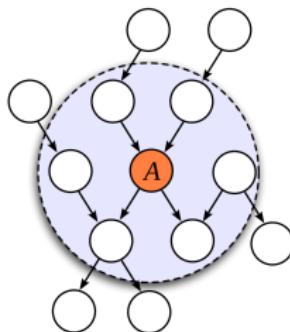
⇒ The objective of feature selection is to find the subset of features  $S \in X$  with which  $\mathcal{C}$  achieves the lowest error rate.

A feature is considered **irrelevant** if it contains no information about the class.

## Markov blanket

Given a feature  $X_i$ ,  $M_i \subset \mathcal{X}$  ( $X_i \notin M_i$ ) is said to be a Markov blanket for  $X_i$  iff

$$P(\mathcal{X} - M_i - \{X_i\}, \mathcal{Y} | X_i, M_i) = P(\mathcal{X} - M_i - \{X_i\}, \mathcal{Y} | M_i).$$



# Feature redundancy

## Entropybased measures

- Mutual Information of a given variable  $X$  with respect to variable  $Y$  ( $MI(Y;X)$ ) measures the reduction in uncertainty about the value of  $X$  given the value of  $Y$ .

$$MI(X|Y) = H(X) - H(X|Y).$$

- MI is biased in favor of r.v. with more values  $\Rightarrow$  Normalize.

$$SU(X, Y) = 2 \left[ \frac{MI(X|Y)}{H(X) + H(Y)} \right].$$

## Feature relevance

Given the threshold  $\delta$ , a feature  $X_i$  is relevant if its correlation with the class  $Y$  is  $SU(X_i, Y) > \delta$ .

## Feature redundancy: Approximate Markov blanket

Given two features  $X_i$  and  $X_j$  ( $i \neq j$ ) so that  $SU(X_j, \mathcal{Y}) \geq SU(X_i, \mathcal{Y})$ , then  $X_j$  forms an approximate Markov blanket for  $X_i$  iff  $SU(X_i, X_j) \geq SU(X_i, \mathcal{Y})$ .

# The Multivariate SU

Total Correlation (TC) is a generalization of MI:

$$C(X_{1:n}) := \sum_{i=1}^n H(X_i) - H(X_{1:n}).$$

TC is the amount of information shared among the variables in the set.

MSU is defined as follows:

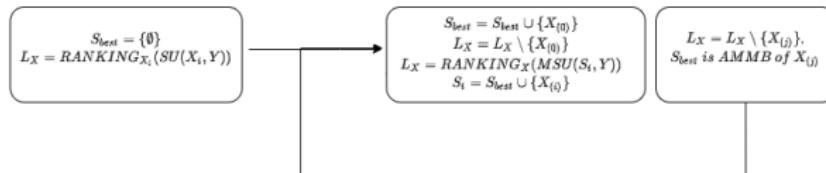
$$MSU(X_{1:n}) := \frac{n}{n-1} \left[ \frac{C(X_{1:n})}{\sum_{i=1}^n H(X_i)} \right] = \frac{n}{n-1} \left[ 1 - \frac{H(X_{1:n})}{\sum_{i=1}^n H(X_i)} \right].$$

with  $H(X_{1:n})$  the joint entropy of the random variables and  $C(X_{1:n})$  defined as

# MSU based Feature Selection (MSUFS) Heuristic

## Approximate multivariate Markov blanket

Given two features  $X_i$  and  $X_j$  ( $i \neq j$ ), let  $S_i \subset X$  so that  $X_i \in S_i$  and  $X_j \notin S_i$ . Then,  $S_i$  forms an approximate multivariate Markov blanket for  $X_j$  iff  $SU(X_i, X_j) \geq SU(X_j, Y)$  or  $MSU(S_i, X_j) \geq SU(X_j, Y)$ .



Proposed heuristic workflow

# Experiments

- ① Microarray data. Study the performance of MSUFS on small high-dimensional data.
- ② Case study: melanoma data. Inspect the relevant features on melanoma data.

In all experiments the results achieved with MSUFS were compared with those obtained by FCBF.

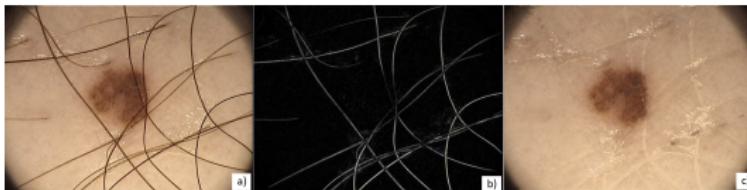
dataset	id	#inst.	#feat.	labels	#inst./label
colon	cln	62	2000	normal/tumor	22/40
lymphoma	lym	77	2647	diffuse/follicular	58/19
breast	bcd	168	2905	good/poor	111/57
prostate	prt	1545	10935	tumor/not	52/50
lung	lnc	181	12533	MPM/ADCA	31/150
breast	bcc	118	22215	positive/negative	75/43
breast/colon	bco	104	22283	breast/colon	62/42

id	naive Bayes			Logistic Regression		
	$\mathcal{C}$	FCBF	MSUFS	$\mathcal{C}$	FCBF	MSUFS
clin	54.62 (17.68)	75.77 (8.09)	72.82 (9.99)	83.97 (5.25)	79.10 (3.94)	77.44 (8.72)
lym	81.92 (4.93)	87.00 (4.74)	80.42 (10.69)	94.83 (5.53)	88.17 (13.65)	80.42 (10.69)
bco	70.20 (13.75)	71.44 (11.27)	73.74 (12.00)	75.56 (6.22)	74.96 (11.28)	72.53 (9.12)
prt	99.61 (0.27)	99.74 (0.27)	98.96 (0.84)	99.68 (0.32)	99.29 (0.42)	99.55 (0.37)
lng	97.79 (2.32)	100.00 (0.00)	95.59 (3.15)	100.00 (0.00)	98.35 (2.48)	97.79 (2.32)
bcc	88.12 (3.67)	85.62 (8.12)	88.91 (5.03)	89.00 (4.76)	83.95 (4.46)	88.04 (6.54)
bco	68.29 (7.11)	96.14 (2.16)	96.19 (3.98)	96.10 (4.16)	94.19 (4.10)	96.19 (3.98)
mean	80.08	87.96	86.66	91.31	88.29	87.42

id	#feat.	#Features	
		FCBF	MSUFS
cln	2000	13.80 (1.64)	3.80 (0.84)
lym	2647	43.00 (1.41)	4.60 (0.55)
bcg	2905	36.20 (8.35)	5.00 (0.71)
prt	10935	197.20 (46.98)	2.00 (0.00)
lng	12533	107.80 (22.04)	3.60 (0.89)
bcc	22215	135.20 (9.40)	3.00 (0.00)
bco	22283	47.40 (1.46)	3.00 (1.00)
mean	—	82.94	3.57

# Melanoma dataset

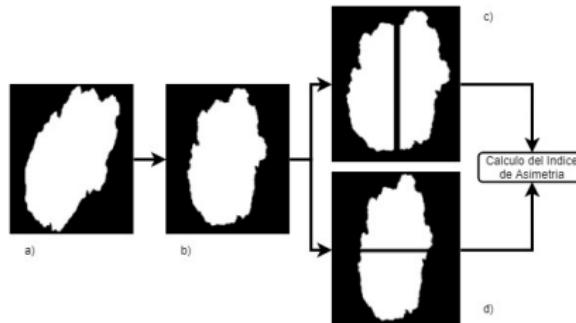
ABCD method



Criterion	Feature	Id	Description
asymmetry	index of asymmetry	as	#pixels into irregular disjoint areas
borders	segment 1-8	b1 – 8	variation of colors from center pixel to border pixels
colors	white light brown dark brown black	wh lb db bk	#pixels with this color
dermatoscopic structures	linear branches irregular pigment network structureless areas dots and globules	lr ip ne sa dg	variation of distance from center to border number of unconnected pixels micro-regions number of pixels into the area number of dots and globules

# Melanoma dataset

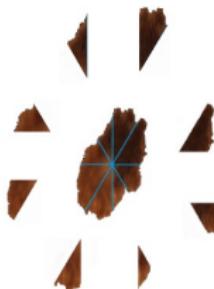
## Asymmetry



Criterion	Feature	Id	Description
asymmetry	index of asymmetry	<i>as</i>	#pixels into irregular disjoint areas
borders	segment 1-8	<i>b1 – 8</i>	variation of colors from center pixel to border pixels
colors	white light brown dark brown black	<i>wh</i> <i>lb</i> <i>db</i> <i>bk</i>	#pixels with this color
dermatoscopic structures	linear branches irregular pigment network structureless areas dots and globules	<i>lr</i> <i>ip</i> <i>ne</i> <i>sa</i> <i>dg</i>	variation of distance from center to border number of unconnected pixels micro-regions number of pixels into the area number of dots and globules

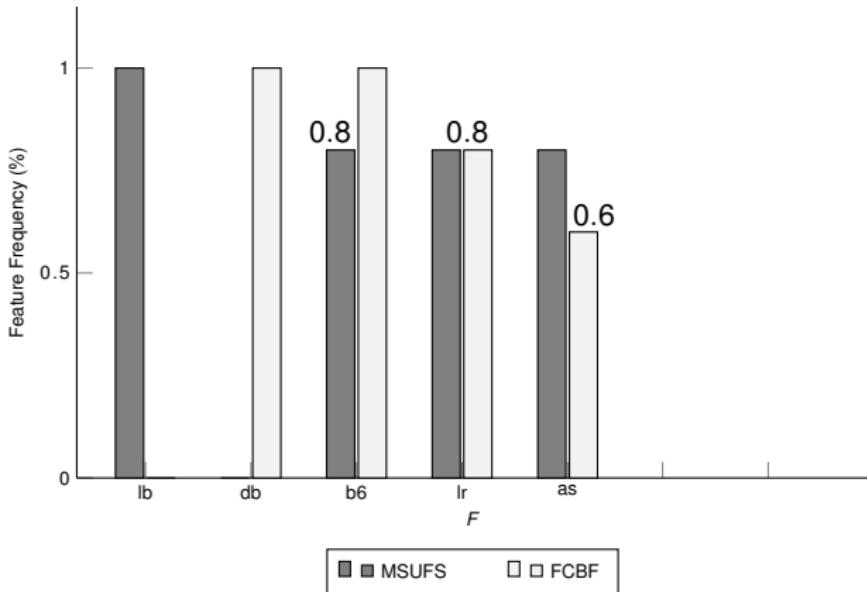
# Melanoma dataset

## Borders



Criterion	Feature	Id	Description
asymmetry	index of asymmetry	as	#pixels into irregular disjoint areas
borders	segment 1-8	b1 – 8	variation of colors from center pixel to border pixels
colors	white light brown dark brown black	wh lb db bk	#pixels with this color
dermatoscopic structures	linear branches irregular pigment network structureless areas dots and globules	lr ip ne sa dg	variation of distance from center to border number of unconnected pixels micro-regions number of pixels into the area number of dots and globules

id	#feat.	Accuracy		#Features	
		FCBF	MSUFS	FCBF	MSUFS
melanoma	18	79.86 ± 3.73	81.76 ± 6.11	3.4 ± 0.55	3.40 ± 0.55



- MSUFS can identify interaction among three or more features.
- MSUFS is a competitive strategy.
- The identification of multivariate interactions allow th discovery of a reduce subset of relevant features.