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PowerHC: non linear normalization of distances for advanced nearest neighbor classification

Manuele Bicego, Mauricio Orozco-Alzate University of Verona (Italy), Universidad Nacional de Colombia (Colombia) manuele.bicego@univr.it, morozcoa@unal.edu.co

The nearest neighbor rule

 The simplest classification technique: it assigns the testing object to the class of the most similar object of the training set (the nearest neighbor)



The nearest neighbor rule

- Many advantages:
 - Accurate: non linear classifier
 - No parameters
 - It works also for non vectorial data
 - Many theoretical results available



• Simple and interpretable



Crucial need in recent years:

eXplainable Artificial Intelligence!

Variants of Nearest Neighbor

- Several variants have been proposed in literature to improve this technique (Condensing, Editing, Adaptation, Discriminative information...)
- Among others, there are two interesting variants based on a similar idea:
 - **ANN**: the Adaptive Nearest Neighbor rule (Wang et al. 2007)
 - HC: the Hypersphere Classifier (Lopes et al. 2015)

• **Starting observation**: Some training objects are "better" than others for the NN rule

Points which are **far away from other classes** are more "trustable" that points which are not



 ANN and HC quantify this concept by defining the radius of a training point: "The distance from its nearest object of another class"

The larger the radius the more trustable (the better) the point



- ANN and HC employ a mechanism to favour in the NN rule "better" training points
- In practice, HC and ANN use the radius to correct the distances from the testing object:
 - Better points become nearer to the testing objects than other points







Better points \rightarrow nearer Worst points \rightarrow farther



Better points \rightarrow nearer Worst points \rightarrow farther

HC rule:
$$d_{HC}(\mathbf{x}^{te}, \mathbf{x}_i^{tr}) = d(\mathbf{x}^{te}, \mathbf{x}_i^{tr}) - \text{radius}(\mathbf{x}_i^{tr})$$

ANN rule: $d_{ANN}(\mathbf{x}^{te}, \mathbf{x}_i^{tr}) = \frac{d(\mathbf{x}^{te}, \mathbf{x}_i^{tr})}{\text{radius}(\mathbf{x}_i^{tr})}$

The distance from points with large radius will be reduced more than that of points with a small radius (i.e. a training point with a larger radius will be preferred)

Relation between HC and ANN

 Recently it has been shown that the relation between HC and ANN is based on logarithms

> ANN is the HC rule applied to distances which have been **non linearly scaled** with a logarithm function

[Orozco-Alzate et al., ICIAP19]

Relation between HC and ANN

Non linear scaling: an alternative to linear scaling

Linear scaling

Z-score standardization

$$x^{new} = \frac{x - \mu_j}{\sigma_j}$$

Non linear scaling $x^{new} = x^{\rho} \quad (\rho > 0)$ Power $x^{new} = \begin{cases} \frac{x^{\lambda} - 1}{\lambda} & \text{if } \lambda \neq 0\\ \log(x) & \text{otherwise} \end{cases}$ Box-Cox Logistic $x^{new} = \frac{1}{1 + e^{-x}}$ $x^{new} = \log(x)$ Logarithm

Relation between HC and ANN

- It has been shown that non linear scaling of feature spaces can be useful for classification
- Further, it has been shown that non linear scaling of distances can be useful for some distance-based classifiers

Carli et al ICCV2009W Carli et al ICPR2010 Bicego et al Neurocomputing 2016 Duin et al S+SSPR2014 Orozco-Alzate et al S+SSPR2016

The PowerHC rule

- ANN rule is the HC rule applied to distances scaled with logarithm
- What about investigating **other non linear scalings**?
 - Logistic transformation
 - Power transformation

The PowerHC rule

- ANN rule is the HC rule applied to distances scaled with logarithm
- What about investigating other non linear scalings?
 - Logistic transformation
 - Power transformation

Best variant for non linear scaling of feature spaces

Almost never used for distances



The Power-HC rule!

The powerHC rule

 The rule performs a non linear scaling of the distances using the power transform before applying the HC rule

powerHC rule: $d_{\rho HC}(\mathbf{x}^{te}, \mathbf{x}_i^{tr}) = d(\mathbf{x}^{te}, \mathbf{x}_i^{tr})^{\rho} - \operatorname{radius}(\mathbf{x}_i^{tr})^{\rho}$

In other words: distances are normalized via the **power transform**

All details in the paper!



Experimental evaluation

 We tested PowerHC using 24 standard UCI-ML datasets (of different dimensionality, cardinality and number of classes)

Moreover we tested PowerHC on a real world challenging problem (classification of **seismicvolcanic signals**)

We used DTW/Euclidean distances between spectrograms



Experimental evaluation

- We compared PowerHC with ANN and HC
 - PowerHC: the power p varies between 0.2 and 10 (step 0.2)
 - We report both accuracies for the best $\rho\,$ and accuracies for automatically estimated $\rho\,$
- We used both NN and K-NN
- We evaluate statistical significance of differences with a statistical test

TABLE II

ACCURACIES, AS PERCENTAGES, ALONG WITH STANDARD ERRORS FOR 50 REPETITIONS AND T-TESTS AT 5% OF SIGNIFICANCE FOR THE COMPARED METHODS WHEN USING NN FOR DECISION. ARROWS POINT TO THE BEST METHOD WHEN DIFFERENCES ARE SIGNIFICANT.

> Mathad	Accuracies					t-tests		7			
Method	A	B	C	D	110	B vs D	C vs D	1			
vataset	NN 68 72 ± 0.20	NN-ANN 71.22±0.20	NN-HC 71.58±0.20	NN-Power	THC (1)	Daiaat 2	Deiest 2	-			
german-credit	68.72 ± 0.29 69.70 ± 0.33	71.32 ± 0.29 72.43±0.32	71.38 ± 0.29 72.70 ± 0.32	72.59 ± 0.28 (μ	= 6.2)	Reject Z	Reject 7				
tic-tac-too	7052 ± 0.26	72.45±0.52	83.04±0.24	73.34±0.32 (μ 84.36±0.23 (μ	-5.8	Reject Z	Reject 7				
tic-tac-toe	51.02 ± 0.26	80.80±0.25	83.04±0.24	84.30±0.25 (μ) = 3.8)	Reject/	Reject	1			
yeast	57.88±0.48										
hoart	76 55 + 0.49						т	ABLE III			
haborman	66 32 +0 54	ACCURACIE	S AS DEDCEN	TAGES ALON	WITH ST		EPPOPS FO	P 50 PEPETITIC	NS AND T-TESTS AT 5% O	E SIGNIEICAI	NCE FOR TH
udba	05.06±0.18	Accorden	METHODS WH	EN USING KN	IN FOR DE	CIEION	A DROWS DO	INT TO THE DE	AS AND PIESIS AT 5 % C	ENCES ADE	SIGNIFICANS
ecoli	81 79+0.42		METHODS wh	EN USING A N	IN FOR DE	cision.	ARROWS PU	INT TO THE BE	ST METHOD WHEN DIFFER	LENCES ARE 3	SIGNIFICAN
volcano DTW	72.55+0.27							Accuraciae		t_te	aete
glass	68.50 ± 0.64			Mathod	-		D	Accuracies	D	1-10	1
sonar	83.44+0.52		D. L. L	Method						B vs D	C vs D
iris	93.33+0.41		Dataset		KNN	N P	NN-ANN	K NN-HC	KNN-PowerHC		
liver	61.45 ± 0.52		★ german	-credit	73.82±0	0.28 7	2.75 ± 0.28	73.22±0.28	$74.22 \pm 0.28 \ (\rho = 8.8)$	Reject /	Reject /
vehicles	69.11 ± 0.32		★ tic-ta	c-toe	83.37±0	0.24 8	2.66 ± 0.24	83.04±0.24	$84.36 \pm 0.23 \ (\rho = 5.8)$	Reject >	Reject >
malavsia	70.64 ± 0.53		\star arrhyt	hmia	63.00±	0.47 6	1.57 ± 0.47	64.98±0.47	$68.89 \pm 0.45 \ (\rho = 1.8)$	Reject >	Reject /
ionosphere	85.21±0.38		\star haberm	an	75.03±	0.49 7	4.64±0.50	74.76±0.50	$75.26 \pm 0.49 \ (\rho = 2.0)$	Reject >	Reject >
wpbc	65.59 ± 0.68		★ liver		63.74±0	0.52 6	2.48 ± 0.52	64.15±0.52	$65.08 \pm 0.51 \ (\rho = 2.8)$	Reject >	Reject >
wine	95.00±0.33		★ volcan	DTW_	73.62±0	0.27 7	8.78±0.25	80.95±0.24	$82.19 \pm 0.23 \ (\rho = 2.2)$	Reject /	Reject >
											ept
			▲ sonar ▲ malaysi	.â	83.44±0 70.64±0	0.52 8 0.53 6 0.25 6	4.82±0.50 9.05±0.54	84.49±0.50 68.72±0.54	84.85 \pm 0.50 (ρ = 0.2) 69.08 \pm 0.54 (ρ = 0.2) 04.42 \pm 0.27 (ρ = 0.2)	Accept Accept	ept Reject / Reject /
			▲ sonar ▲ malaysi ▲ iris	a	83.44± 70.64± 95.25±	0.52 8 0.53 6 0.35 9	4.82±0.50 9.05±0.54 4.40±0.38	84.49±0.50 68.72±0.54 93.89±0.39	84.85 \pm 0.50 (ρ = 0.2) 69.08 \pm 0.54 (ρ = 0.2) 94.43 \pm 0.37 (ρ = 0.2)	Accept Accept Accept	Reject A Reject A Reject A
			▲ sonar ▲ malaysi ▲ iris	a	83.44±0 70.64±0 95.25±0 96.14±0	0.52 8 0.53 6 0.35 9 0.16 9	4.82±0.50 9.05±0.54 4.40±0.38	84.49±0.50 68.72±0.54 93.89±0.39 96.39±0.16	84.85 \pm 0.50 (ρ = 0.2) 69.08 \pm 0.54 (ρ = 0.2) 94.43 \pm 0.37 (ρ = 0.2) 96.44 \pm 0.16 (ρ = 1.6)	Accept Accept Accept Accept	Reject A Reject Reject A Reject A Accept
			▲ sonar ▲ malaysi ▲ iris ▲ wdbc	a	83.44±0 70.64±0 95.25±0 96.14±0	0.52 8 0.53 6 0.35 9 0.16 9	4.82±0.50 9.05±0.54 4.40±0.38 6 30±0.16	84.49±0.50 68.72±0.54 93.89±0.39 96.39±0.16 76.31±0.61	84.85 \pm 0.50 (ρ = 0.2) 69.08 \pm 0.54 (ρ = 0.2) 94.43 \pm 0.37 (ρ = 0.2) 96.44 \pm 0.16 (ρ = 1.6) 76.41 \pm 0.61 (ρ = 8.2)	Accept Accept Accept Accept Accept	Reject × Reject × Reject × Accept Accept
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NNPowerHC-Be	est NNPowerH	C-Auto	▲ sonar ▲ malaysi ▲ iris	.a KNNPowerH	83.44±0 70.64±0 95.25±0 06.14±0	0.52 8 0.53 6 0.35 9 0.16 0	4.82±0.50 9.05±0.54 4.40±0.38 6.30±0.16	$\begin{array}{r} 84.49 {\pm} 0.50 \\ 68.72 {\pm} 0.54 \\ 93.89 {\pm} 0.39 \\ 96.39 {\pm} 0.16 \\ 76.31 {\pm} 0.61 \\ 55.28 {\pm} 0.29 \\ 75.73 {\pm} 0.26 \end{array}$	$\begin{array}{l} 84.85 \pm 0.50 \ (\rho = 0.2) \\ 69.08 \pm 0.54 \ (\rho = 0.2) \\ 94.43 \pm 0.37 \ (\rho = 0.2) \\ 96.44 \pm 0.16 \ (\rho = 1.6) \\ 76.41 \pm 0.61 \ (\rho = 8.2) \\ 55.35 \pm 0.29 \ (\rho = 0.8) \\ 75.79 \pm 0.26 \ (\rho = 3.0) \end{array}$	Accept Accept Accept Accept Accept Accept Accept	Reject A Reject Reject A Reject A Accept Accept Accept Accept
NNPowerHC-Be	est NNPowerH	C-Auto	▲ sonar ▲ malaysi ▲ iris	.a KNNPowerH	83.44±0 70.64±0 95.25±0 96.14±0 C-Best	0.52 8 0.53 6 0.35 9 0.16 0	4.82±0.50 9.05±0.54 4.40±0.38 6.30±0.16 C-Auto	$\begin{array}{c} 84.49 {\pm} 0.50 \\ 68.72 {\pm} 0.54 \\ 93.89 {\pm} 0.39 \\ \hline 96.39 {\pm} 0.16 \\ 76.31 {\pm} 0.61 \\ 55.28 {\pm} 0.29 \\ 75.73 {\pm} 0.26 \\ 96.00 {\pm} 0.29 \end{array}$	$\begin{array}{l} 84.85 \pm 0.50 \ (\rho = 0.2) \\ 69.08 \pm 0.54 \ (\rho = 0.2) \\ 94.43 \pm 0.37 \ (\rho = 0.2) \\ 96.44 \pm 0.16 \ (\rho = 1.6) \\ 76.41 \pm 0.61 \ (\rho = 8.2) \\ 55.35 \pm 0.29 \ (\rho = 0.8) \\ 75.79 \pm 0.26 \ (\rho = 3.0) \\ 96.05 \pm 0.29 \ (\rho = 0.6) \end{array}$	Accept Accept Accept Accept Accept Accept Accept Accept	ept Reject ≯ Reject ≯ Reject ≯ Accept Accept Accept Accept Accept
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Fig. 2. Comparison of Optimal (Best) vs Automatic Approach for tuning ρ in: (left) NN-PowerHC and (right) KNN-PowerHC

Main findings

- Results with NN:
 - For a large group of datasets (16 over 26) PowerHC is better than ANN, HC (with a stastical significance)
 - In most of the other cases (9 over 26) there is not a statistically significant improvement
 - In 1 case PowerHC is outperformed by ANN

Main findings

- Similar results obtained with K-NN
- Automatic tuning of the parameter is satisfactory
- The best value for the parameter is always larger than 1 (concave transformation)
 - Different from what has been found for feature space!

Conclusions

- We proposed a novel variant of the Nearest Neighbor rule
 - Distances are non linearly scaled with the power tranformation before applying the HC rule
- Experiments show that non linear scaling are indeed useful
- To be investigated further: why concave transformation?

