



Study of Instance Selection Methods

Seminar at Aston University

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Universidad de Burgos



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3. Motivation and goals
4. Instance selection for regression by discretization
5. Fusion of instance selection methods in regression tasks
6. Instance selection for regression: adapting DROP
7. Instance selection of linear complexity for big data
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1. First of all



Researchers in Universidad de Burgos

Research group: 'ADMIRABLE' (Advanced Data Mining Research And (Business intelligence | Bioinformatics | Big Data) LEarning – <http://admirable-ubu.es/>)

- Álgvar Arnaiz González
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 - PhD on Computer Science (University of The West of Scotland)
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 - PhD on Computer Science (Universidad de Valladolid)
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 - PhD candidate on Computer Science (Universidad de Burgos)

Where is Burgos?¹



¹Copyright by NordNordWest - own work, using United States National Imagery and Mapping Agency data, CC BY-SA 3.0

Why is Burgos famous for? (i)²



²Copyright by Camino del Cid - Own work, CC BY-SA 3.0

Why is Burgos famous for? (ii)³



³Copyright by Sueños de aire azul - Own work

Why is Burgos famous for? (iii)⁴



But it also has got this!



⁴Copyright by Universidad de Burgos - Own work

2. Introduction

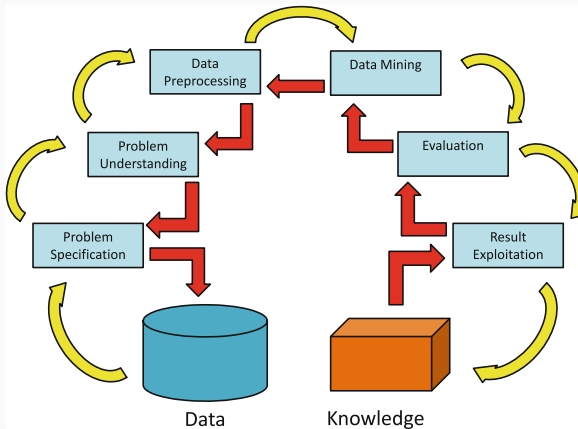


Figure 1: KDD process. Picture reproduced from⁵.

⁵Salvador García, Julián Luengo, and Francisco Herrera. *Data preprocessing in data mining*. Springer, 2015.

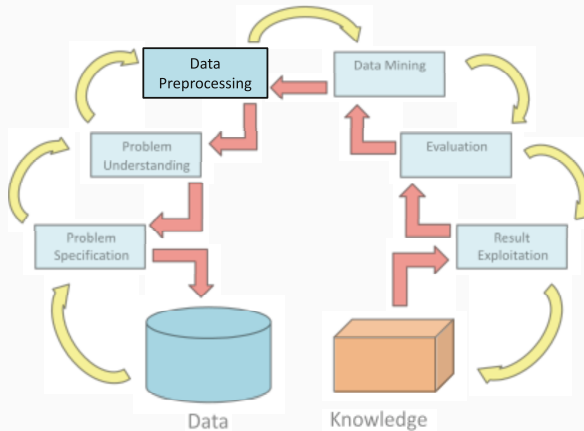


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Data preparation: set of techniques that initialize the data properly to serve as an input for a certain DM algorithm.

- Data cleaning.
- Data transformation.
- Data integration.
- Data normalization.
- Missing data imputation.
- Noise identification.

Data reduction: set of techniques that obtain a reduced representation of the original data.

- Discretization.
- Feature selection.
- Instance selection.



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- Feature selection.
- **Instance selection.**



- Its aim: the selection of a subset of instances.
- One restriction: keeping, or even improving, the prediction capabilities of the whole data set.

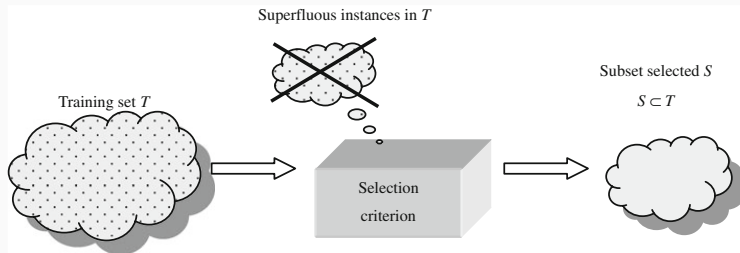


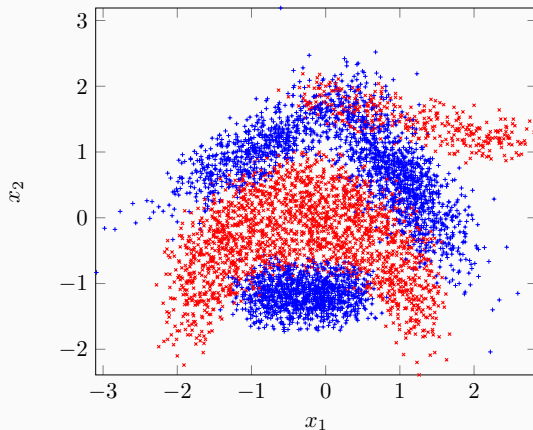
Figure 2: Instance selection process. Picture reproduced from⁶.

⁶J. Arturo Olvera-López et al. "A review of instance selection methods". In: *Artificial Intelligence Review* 34.2 (2010), pp. 133–143. ISSN: 1573-7462.

An example (i)



Banana⁷ data set (original): 5 300 instances.

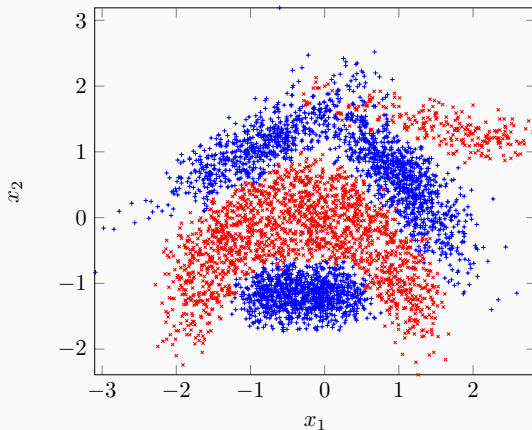


⁷Fraunhofer Institute for Intelligent Analysis and Information Systems. *Benchmark Repository*. URL: <http://www.iais.fraunhofer.de/>.

An example (ii)



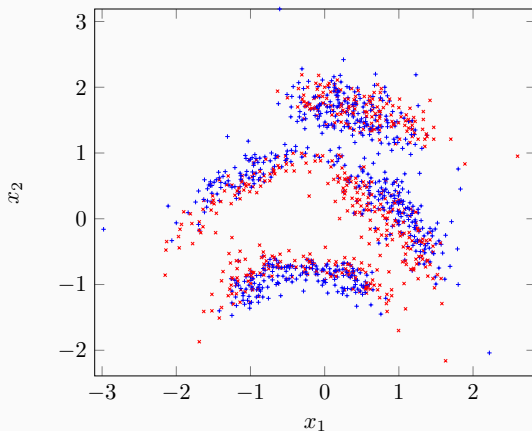
After ENN or *Wilson Editing*⁸: 4 696 inst.



⁸Dennis L. Wilson. "Asymptotic Properties of Nearest Neighbor Rules Using Edited Data". In: *Systems, Man and Cybernetics, IEEE Transactions on SMC-2.3* (1972), pp. 408–421. ISSN: 0018-9472.



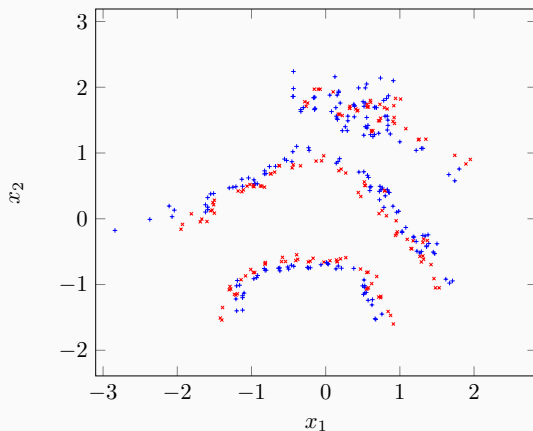
After *Condensed Nearest Neighbour*⁹ (CNN): 1 199 inst.



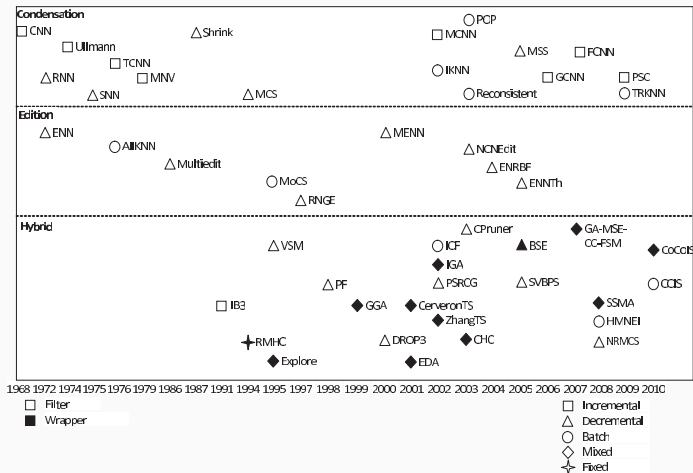
⁹P. Hart. "The condensed nearest neighbor rule (Corresp.)" In: *Information Theory, IEEE Transactions on* 14.3 (1968), pp. 515–516. ISSN: 0018-9448.



After *Decr. Red. Optimization Procedure 3* (DROP3)¹⁰: 350 inst.

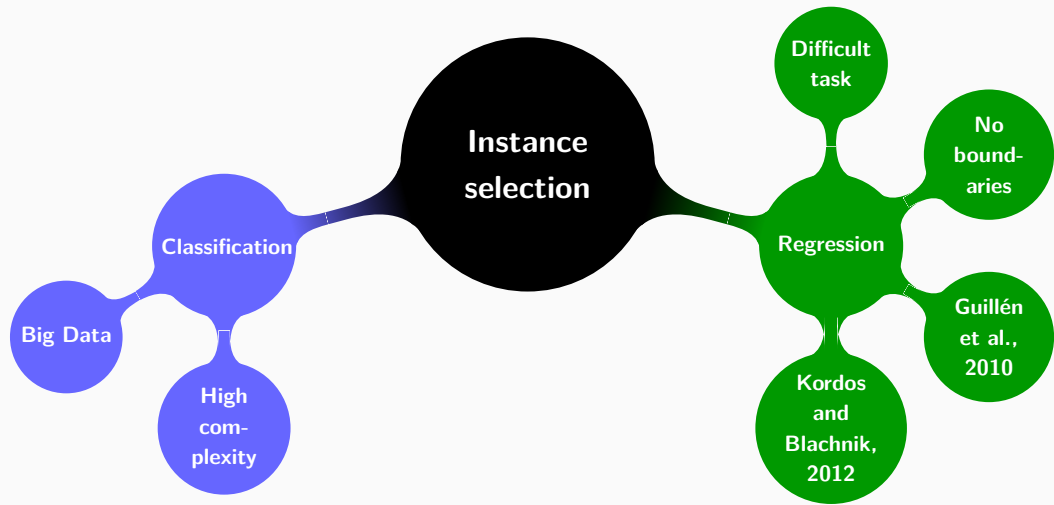


¹⁰D.Randall Wilson and Tony R. Martinez. "Reduction Techniques for Instance-Based Learning Algorithms". English. In: *Machine Learning* 38.3 (2000), pp. 257–286. ISSN: 0885-6125.



¹¹S. Garcia et al. "Prototype Selection for Nearest Neighbor Classification: Taxonomy and Empirical Study". In: *Pattern Analysis and Machine Intelligence, IEEE Transactions on* 34.3 (2012), pp. 417–435. ISSN: 0162-8828.

3. Motivation and goals





- Instance selection for classification has been broadly researched.



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- However, instance selection for regression has not, due to its difficulties.



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-



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- However, instance selection for regression has not, due to its difficulties.
- There are not well-defined boundaries between classes.
- Two journal papers faced this issue:^{12, 13}.

¹²Álvar Arnaiz-González et al. "Instance selection for regression by discretization". In: *Expert Systems with Applications* 54 (2016), pp. 340 –350. ISSN: 0957-4174.

¹³Álvar Arnaiz-González et al. "Instance selection for regression: Adapting DROP". . In: *Neurocomputing* 201 (2016), pp. 66 –81. ISSN: 0925-2312.



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¹⁴Nicolás García-Pedrajas and Aida de Haro-García. “Boosting instance selection algorithms”. In: *Knowledge-Based Systems* 67 (2014), pp. 342 –360. ISSN: 0950-7051.



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- However, *ensembles* of instance selection for regression had not been tested before.

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¹⁵Álvar Arnaiz-González et al. “Fusion of instance selection methods in regression tasks”. In: *Information Fusion* 30 (2016), pp. 69 –79. ISSN: 1566-2535.



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- Some scale up approaches based on divide-and-conquer have emerged.

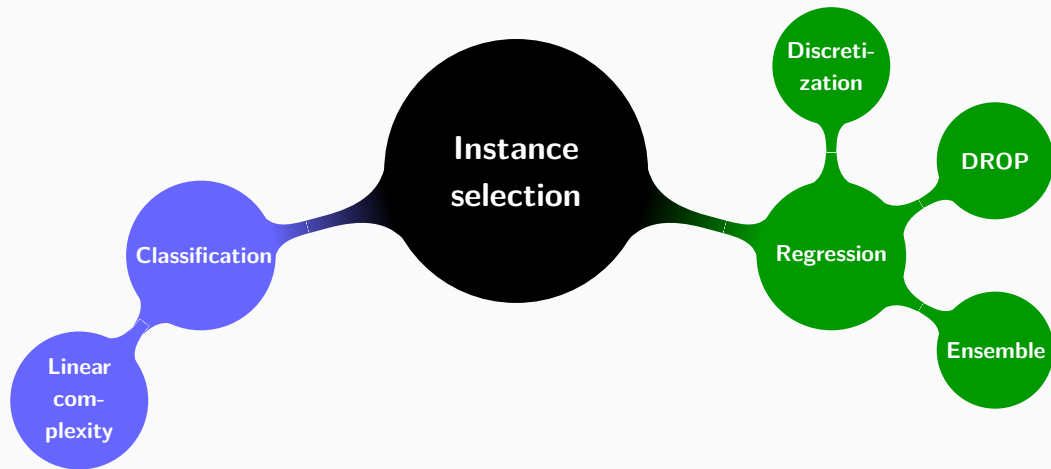


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- We propose a method that, without being based on divide and conquer, is capable of achieving a linear complexity.



- The computational complexity of instance selection methods is commonly very high.
- This makes its use almost impossible for huge data sets
- Some scale up approaches based on divide-and-conquer have emerged.
- We propose a method that, without being based on divide and conquer, is capable of achieving a linear complexity.
- The key to the method is in the use it makes of *locality sensitive hashing* (LSH)¹⁶.

¹⁶Álvar Arnaiz-González et al. "Instance selection of linear complexity for big data". In: *Knowledge-Based Systems* 107 (2016), pp. 83 –95. ISSN: 0950-7051.



4. Instance selection for regression by discretization



The idea

Discretize the numeric class and apply a well-known IS method for classification



Algorithm 1: Proposed meta-model based on discretization of the output variable

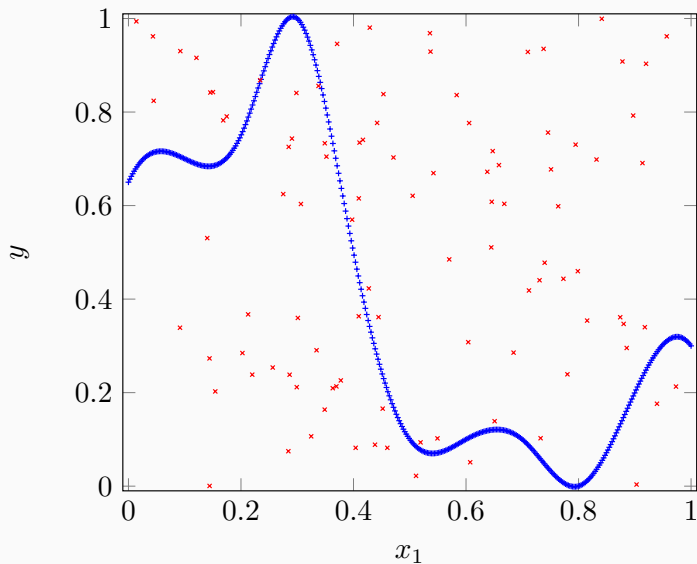
Input: Training set $\{\mathbf{X}, Y\} = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$, Discretization algorithm and all the parameters that it needs

Output: Instance set $S \subseteq \{\mathbf{X}, Y\}$

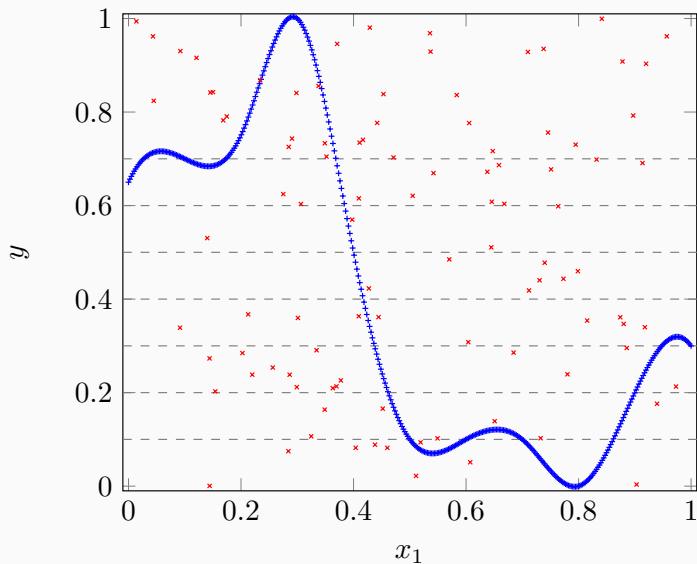
- 1 $Y_D =$ Discretization of the numerical target Y
- 2 Apply classification-based instance selection algorithm over $\{\mathbf{X}, Y_D\}$ to obtain subset S
- 3 Restore the numerical value of the output variable in S

return S

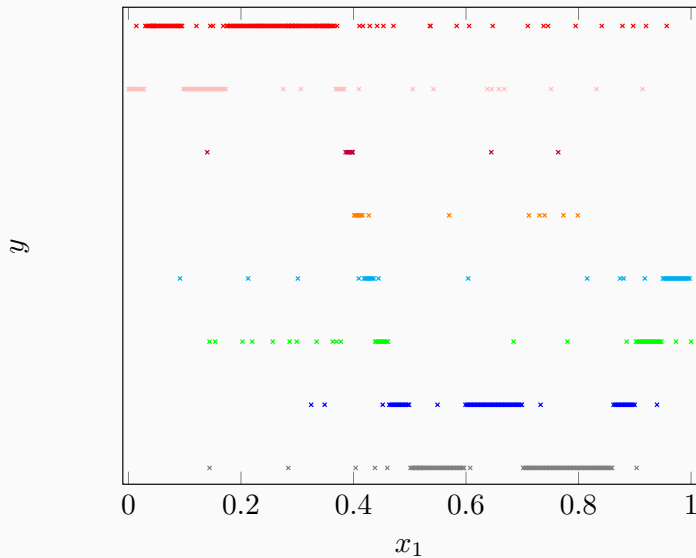
How does it work? An example (i)



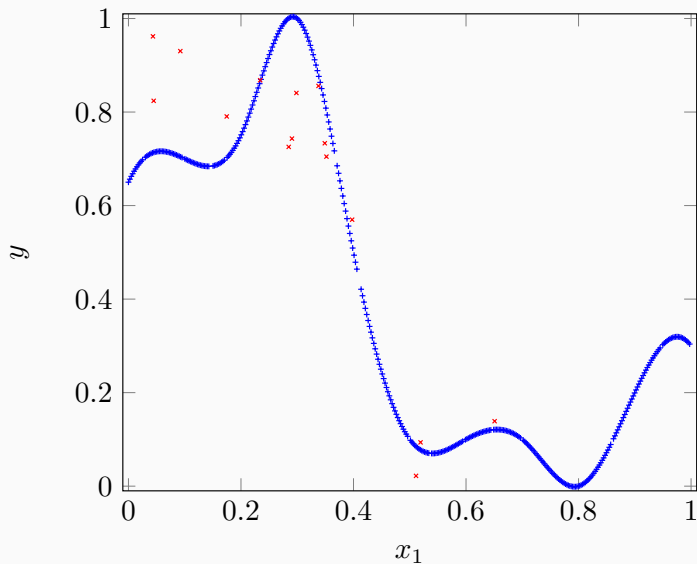
How does it work? An example (ii)



How does it work? An example (iii)



How does it work? An example (iv)



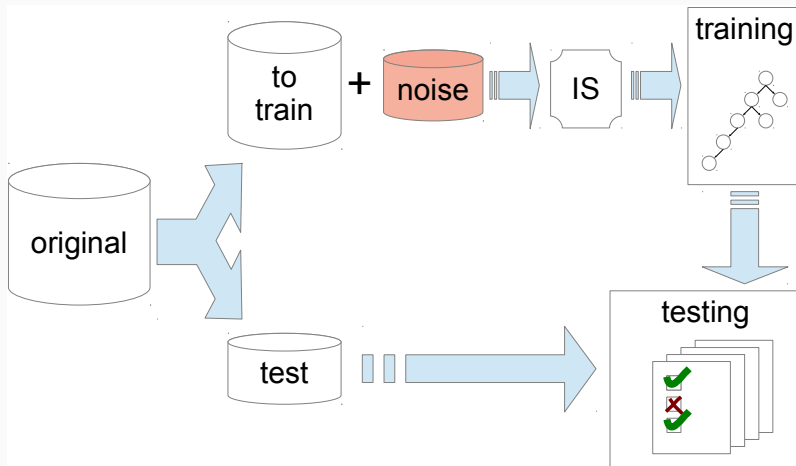


Figure 3: Configuration of the experiments.



Data set	# Instances	# Attributes	RMSE		
			kNN	RBF	REPTree
machineCPU	209	6	73.3861	54.9182	74.1478
baseball	337	16	681.9675	694.5271	784.2473
dee	365	6	0.4136	0.4024	0.4886
autoMPG8	392	7	2.9245	2.6252	3.2893
autoMPG6	392	5	2.7766	2.9610	3.2841
ele-1	495	2	647.7872	637.9696	709.1737
stock	950	9	0.7816	1.0196	1.1843
laser	993	4	10.2126	7.4007	14.0605
concrete	1030	8	9.3890	7.2785	7.4055
treasury	1049	15	0.2423	0.2265	0.3214
mortgage	1049	15	0.1917	0.1063	0.2562
ele-2	1056	4	271.1403	123.7133	185.0631
friedman	1200	5	1.7855	1.5425	2.7496
wizmir	1461	9	1.7195	1.1542	1.7374
wankara	1609	9	1.9401	1.2973	2.0441
plastic	1650	2	1.6412	1.5113	1.7518
quake	2178	3	0.1954	0.1887	0.1887
ANACALT	4052	7	0.1188	0.1889	0.0709
abalone	4177	8	2.2223	2.0983	2.3359
delta-ail	7129	5	0.0002	0.0002	0.0002
compactiv	8192	21	3.0811	3.5825	3.2458
puma32h	8192	32	0.0273	0.0232	0.0089
delta-elv	9517	6	0.0015	0.0014	0.0015
aileron	13750	40	0.0002	0.0002	0.0002
pole	14998	26	8.2376	16.7730	7.1492
elevators	16599	18	0.0036	0.0022	0.0036
california	20640	8	61915.5979	62456.4909	58826.3442
house	22784	16	38444.1767	38512.3930	38854.6220
mv	40768	10	1.8591	0.6156	0.3047



Three regressors were used: k NN, REPTree and RBF.

The proposed meta-model was compared against:

- Mutual information (MI)¹⁷: $k = 6$ and $\alpha = 0.05$.
- ENN based on threshold (RegENN)¹⁸: $k = 9$ and $\alpha = 5$.

Noise levels: 10%, 20%, 30%, and 40%, adding or subtracting a random value to the target attribute.

¹⁷A. Guillen et al. “New method for instance or prototype selection using mutual information in time series prediction”. In: *Neurocomputing* 73.10-12 (2010). Subspace Learning / Selected papers from the European Symposium on Time Series Prediction, pp. 2030 –2038. ISSN: 0925-2312.

¹⁸Mirosław Kordos and Marcin Blachnik. “Instance selection with neural networks for regression problems”. In: *Proceedings of the 22nd international conference on Artificial Neural Networks and Machine Learning - Volume Part II*. ICANN'12. Lausanne, Switzerland: Springer-Verlag, 2012, pp. 263–270. ISBN: 978-3-642-33265-4.



Confusion matrix:

Predicted	Actual	
	Noise	No noise
Noise	TP	FP
No noise	FN	TN

Using it we calculated F_1 score:

$$F_1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} \quad (1)$$

And G mean:

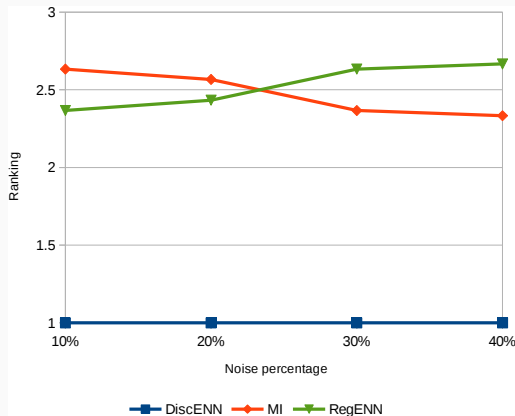
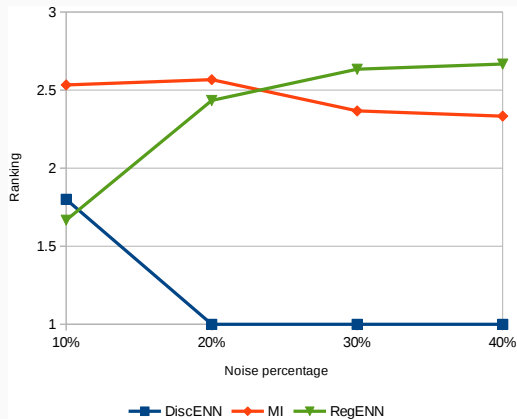
$$G \text{ mean} = \sqrt{\text{specifity} \cdot \text{recall}} \quad (2)$$

where $\text{specifity} = TN/(TN + FP)$, $\text{precision} = TP/(TP + FP)$ and $\text{recall} = TP/(TP + FN)$.

Results: F_1 and G mean



Average ranks over F_1 score (left) and G mean (right).



Results: average ranks over RMSE



kNN				
IS Algorithm	% noise			
	10	20	30	40
DiscENN	2.172	1.465	1.172	1.207
MI	2.534	2.638 ✖	2.207 ✖	2.086 ✖
RegENN	1.776	2.224 ✖	3.965 ✖	3.965 ✖
NoFilter	3.517 ✖	3.672 ✖	2.655 ✖	2.741 ✖

RBF				
IS Algorithm	% noise			
	10	20	30	40
DiscENN	2.327	1.672	1.431	1.465
MI	2.483	2.603 ✖	2.707 ✖	2.758 ✖
RegENN	1.983	2.121	2.327 ✖	2.379 ✖
NoFilter	3.207 ✖	3.603 ✖	3.534 ✖	3.396 ✖

REPTree				
IS Algorithm	% noise			
	10	20	30	40
DiscENN	2.172	1.638	1.431	1.396
MI	2.621	2.862 ✖	2.810 ✖	2.931 ✖
RegENN	2.000	2.034	2.172 ✖	2.293 ✖
NoFilter	3.207 ✖	3.465 ✖	3.586 ✖	3.379 ✖



Average ranks and Hochberg procedure over compression.

IS Algorithm	% noise			
	10	20	30	40
DiscENN	1.000	1.000	1.000	1.000
MI	2.414 ✖	2.414 ✖	2.345 ✖	2.345 ✖
RegENN	2.586 ✖	2.586 ✖	2.655 ✖	2.655 ✖



- Simple idea: easy to implement.
- Meta-model: it can be used with any IS algorithm for classification.
- Competitive results as noise filter.

5. Fusion of instance selection methods in regression tasks



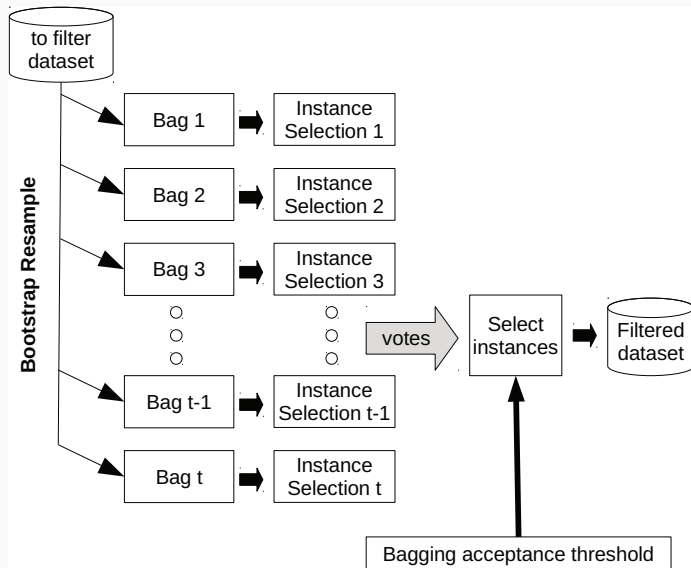
Ensembles have been successfully applied to several problems.

The ensembles' hypothesis claims that the combination of classifiers or regressors performs better than the base methods alone.

The idea

Create ensembles of instance selection methods and test them against the instance selection methods alone.

Schematic view of the IS bagging process





Algorithm 2: ISBagging - Instance Selection Bagging

Input:

- Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$
- Instance selection algorithm ISAlg
- Number of bags t
- Percent of instances in the bootstrapped training subsets p
- Threshold z

Output: Instance set $P \subseteq T$

```
1 for  $i = 1 \dots t$  do
2    $S_t = \text{Bootstrap}(T, p)$ 
3    $P_t = \text{ISAlg}(S_t)$ 
4    $v = \text{CollectVotes}(P_t, v)$ 
end
5  $P = \text{SelectInstancesByVotes}(T, v, z)$ 
return  $P$ 
```



Regressor: k NN.

Instance selection algorithms tested:

- Threshold-based¹⁹ ENN and CNN: T-ENN and T-CNN.
- Discretization-based²⁰ ENN and CNN: D-ENN and D-CNN.

Each algorithm was tested alone and into ensemble: 8 combinations.

¹⁹Mirosław Kordos and Marcin Blachnik. “Instance selection with neural networks for regression problems”. In: *Proceedings of the 22nd international conference on Artificial Neural Networks and Machine Learning - Volume Part II*. ICANN'12. Lausanne, Switzerland: Springer-Verlag, 2012, pp. 263–270. ISBN: 978-3-642-33265-4.

²⁰Álvar Arnaiz-González et al. “Instance selection for regression by discretization”. In: *Expert Systems with Applications* 54 (2016), pp. 340–350. ISSN: 0957-4174.



Dataset	Instances	Attributes			
		Total	real	integer	nominal
diabetes	43	2	2	0	0
machineCPU	209	6	0	6	0
baseball	337	16	2	14	0
dee	365	6	6	0	0
autoMPG8	392	7	2	5	0
autoMPG6	392	5	2	3	0
ele-1	495	2	1	1	0
forestFires	517	12	7	5	0
stock	950	9	9	0	0
laser	993	4	4	0	0
concrete	1 030	8	7	1	0
treasury	1 049	15	15	0	0
mortgage	1 049	15	15	0	0
ele-2	1 056	4	4	0	0
friedman	1 200	5	5	0	0
wizmir	1 461	9	9	0	0
wankara	1 609	9	9	0	0
plastic	1 650	2	2	0	0
quake	2 178	3	2	1	0
ANACALT	4 052	7	7	0	0
abalone	4 177	8	7	1	0
compactiv	8 192	21	21	0	0
tic	9 822	85	0	85	0
aileron	13 750	40	36	4	0
pole	14 998	26	26	0	0
elevators	16 599	18	14	4	0
california	20 640	8	3	5	0
house	22 784	16	10	6	0



Instance selection is a multi-objective problem.

For joining into a single measure:

$$BF_{\gamma} = \gamma \cdot Accuracy + (1 - \gamma) \cdot Compression \quad (3)$$

For accuracy: *correlation coefficient* was used.

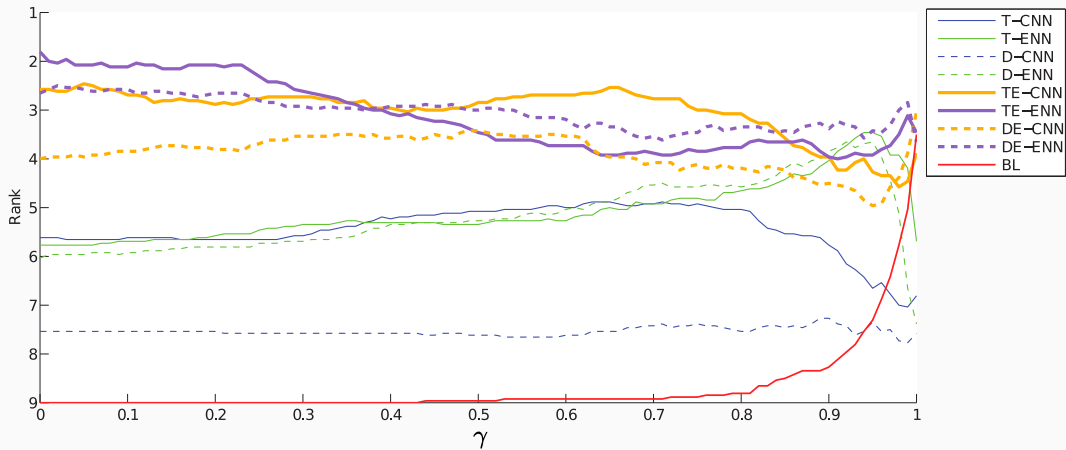
For compression:

$$C = 1 - \frac{|\text{instances after selection}|}{|\text{instances before selection}|} \quad (4)$$

Results: Benefit Function



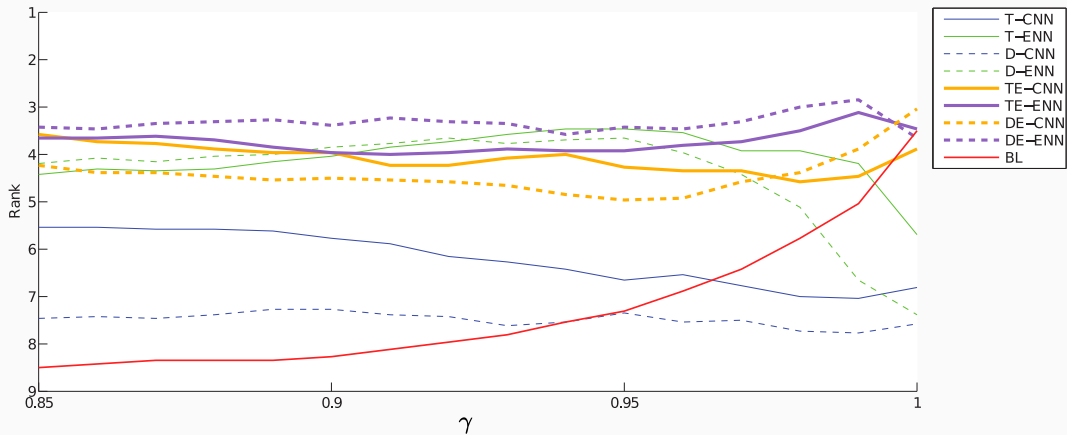
Average ranks over the benefit function.



Results: Benefit Function (zoom)



Zoom: $\gamma \in [0.85 - 1]$





Average ranks and Hochberg procedure over correlation coefficient.

IS algorithm	Ranking	ρ Hoch.
DE-CNN	3.04	
TE-ENN	3.46	0.577
Baseline	3.50	0.577
DE-ENN	3.65	0.577
TE-CNN	3.88	0.577
T-ENN	5.69	2.38E-3
T-CNN	6.80	4.17E-6
D-ENN	7.38	7.37E-8
D-CNN	7.57	1.84E-8



Average ranks and Hochberg procedure over compression.

IS algorithm	Ranking	p Hoch.
TE-ENN	1.81	
TE-CNN	2.58	0.257
DE-ENN	2.65	0.257
DE-CNN	4.00	3.75E-3
T-CNN	5.62	8.34E-8
T-ENN	5.77	2.75E-8
D-ENN	6.04	2.84E-9
D-CNN	7.54	2.31E-16



The table shows:

- wins/losses (w/l): according to benefit function.
- Wilcoxon test: ✓ indicates that the ensemble method is significantly better than the base method.

Algorithms	γ						
	0.0	0.25	0.50	0.70	0.80	0.90	1.00
TE-ENN vs. T-ENN	26 / 0 ✓	22 / 4 ✓	18 / 8 ✓	17 / 9 ✓	16 / 10 =	13 / 13 =	22 / 4 ✓
TE-CNN vs. T-CNN	25 / 1 ✓	26 / 0 ✓	25 / 1 ✓	25 / 1 ✓	23 / 3 ✓	21 / 5 ✓	25 / 1 ✓
DE-ENN vs. D-ENN	26 / 0 ✓	22 / 4 ✓	22 / 4 ✓	15 / 11 ✓	15 / 11 ✓	16 / 10 =	24 / 2 ✓
DE-CNN vs. D-CNN	26 / 0 ✓	26 / 0 ✓	25 / 1 ✓	25 / 1 ✓	24 / 2 ✓	24 / 2 ✓	25 / 1 ✓



- Ensembles give better results than the base methods alone.
- Versatility: the threshold (z) guides the performance of the IS.
 - More accuracy.
 - More reduction.
- Easy to parallelize: each IS execution is independent to others.

6. Instance selection for regression: adapting DROP



Decremental Reduction Optimization Procedure²¹ is a family of IS algorithms. It consists of 5 algorithms: DROP1, DROP2, DROP3, DROP4, and DROP5. DROP3 is one of the best IS methods for classification²².

The idea

Adapt the family of DROP algorithms to regression

²¹D.Randall Wilson and Tony R. Martinez. “Reduction Techniques for Instance-Based Learning Algorithms”. English. In: *Machine Learning* 38.3 (2000), pp. 257–286. ISSN: 0885-6125.

²²Salvador García, Julián Luengo, and Francisco Herrera. “Tutorial on practical tips of the most influential data preprocessing algorithms in data mining”. In: *Knowledge-Based Systems* 98 (2016), pp. 1 –29. ISSN: 0950-7051.



Algorithm 3: Decremental Reduction Optimization Procedure 1

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

Result: Instance set $S \subseteq T$

```
1 Let  $S = T$ 
2 foreach instance  $\mathbf{x} \in S$  do
3   Find  $\mathbf{x}.N_{1\dots k+1}$ , the  $k+1$  nearest neighbours of  $\mathbf{x}$  in  $S$ 
4   Add  $\mathbf{x}$  to each of its neighbours' lists of associates
5 end
6 foreach instance  $\mathbf{x} \in S$  do
7   Let  $\text{with} = \#$  of associates of  $\mathbf{x}$  classified correctly with  $\mathbf{x}$  as a neighbour
8   Let  $\text{without} = \#$  of associates of  $\mathbf{x}$  classified correctly without  $\mathbf{x}$  as a neighbour
9   if  $\text{without} \geq \text{with}$  then
10    Remove  $\mathbf{x}$  from  $S$ 
11    foreach associate  $\mathbf{a}$  of  $\mathbf{x}$  do
12      Remove  $\mathbf{x}$  from  $\mathbf{a}$ 's list of nearest neighbours
13      Find a new nearest neighbour for  $\mathbf{a}$ 
14      Add  $\mathbf{a}$  to its new neighbour's list of associates
15    end
16    foreach neighbour  $\mathbf{n}$  of  $\mathbf{x}$  do Remove  $\mathbf{x}$  from  $\mathbf{n}$ 's list of associates
17  end
18 end
19 return  $S$ 
```



Algorithm 3: Decremental Reduction Optimization Procedure 1

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

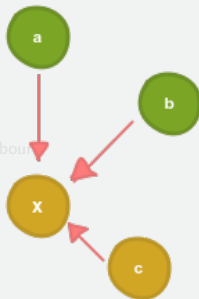
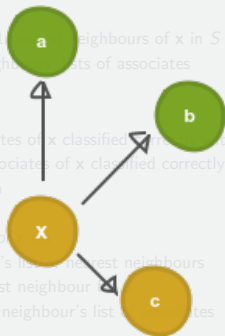
Result: Instance set $S \subseteq T$

```

1 Let  $S = T$ 
2 foreach instance  $\mathbf{x} \in S$  do
3   Find  $\mathbf{x}.N_{1\dots k+1}$ , the  $k+1$  nearest neighbours of  $\mathbf{x}$  in  $S$ 
4   Add  $\mathbf{x}$  to each of its neighbours' lists of associates
end
5 foreach instance  $\mathbf{x} \in S$  do
6   Let  $\text{with} = \#$  of associates of  $\mathbf{x}$  classified correctly with  $\mathbf{x}$  as a neighbour
7   Let  $\text{without} = \#$  of associates of  $\mathbf{x}$  classified correctly without  $\mathbf{x}$  as a neighbour
8   if  $\text{without} \geq \text{with}$  then
9     Remove  $\mathbf{x}$  from  $S$ 
10    foreach associate  $a$  of  $\mathbf{x}$  do
11      Remove  $\mathbf{x}$  from  $a$ 's list of nearest neighbours
12      Find a new nearest neighbour
13      Add  $a$  to its new neighbour's list of associates
14    end
15    foreach neighbour  $n$  of  $\mathbf{x}$  do Remove  $\mathbf{x}$  from  $n$ 's list of associates
16  end
end
return  $S$ 
    
```

Nearest neighbours of \mathbf{x}

\mathbf{x} is an associate of a , b and c





Algorithm 3: Decremental Reduction Optimization Procedure 1

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$

Result: Instance set $S \subseteq T$

```
1 Let  $S = T$ 
2 foreach instance  $\mathbf{x} \in S$  do
3   Find  $\mathbf{x}.N_{1\dots k+1}$ , the  $k+1$  nearest neighbours of  $\mathbf{x}$  in  $S$ 
4   Add  $\mathbf{x}$  to each of its neighbours' lists of associates
5 end
6 foreach instance  $\mathbf{x} \in S$  do
7   Let  $\text{with} = \#$  of associates of  $\mathbf{x}$  classified correctly with  $\mathbf{x}$  as a neighbour
8   Let  $\text{without} = \#$  of associates of  $\mathbf{x}$  classified correctly without  $\mathbf{x}$  as a neighbour
9   if  $\text{without} \geq \text{with}$  then
10     Remove  $\mathbf{x}$  from  $S$ 
11     foreach associate  $\mathbf{a}$  of  $\mathbf{x}$  do
12       Remove  $\mathbf{x}$  from  $\mathbf{a}$ 's list of nearest neighbours
13       Find a new nearest neighbour for  $\mathbf{a}$ 
14       Add  $\mathbf{a}$  to its new neighbour's list of associates
15     end
16     foreach neighbour  $\mathbf{n}$  of  $\mathbf{x}$  do Remove  $\mathbf{x}$  from  $\mathbf{n}$ 's list of associates
17   end
18 end
19 return  $S$ 
```



The key is how the counters `with` and `without` are computed.

Two ideas:

- DROP using error accumulation.
- DROP using thresholding.



Algorithm 4: Computation of eWith and eWithout

```
...
5 foreach instance  $\mathbf{x} \in S$  do
6   Let eWith = 0
7   Let eWithout = 0
8   foreach associate  $\mathbf{a}$  of  $\mathbf{x}$  do
9     Add  $|Y(\mathbf{a}) - \text{Model}(\mathbf{a}.N, \mathbf{a})|$  to eWith
10    Add  $|Y(\mathbf{a}) - \text{Model}(\mathbf{a}.N \setminus \mathbf{x}, \mathbf{a})|$  to eWithout
11  end
12  if  $e\text{Without} \leq e\text{With}$  then
13    Remove  $\mathbf{x}$  from  $S$ 
14    ...
15  end
end
```



Algorithm 5: Computation of with and without

```
...
5 foreach instance  $\mathbf{x} \in S$  do
6   Let with = 0
7   Let without = 0
8   foreach  $\mathbf{a}$  associate of  $\mathbf{x}$  do
9      $\theta_D = \alpha_D \cdot \text{std}(Y(\mathbf{a}.N))$ 
10    if  $|Y(\mathbf{a}) - \text{Model}(\mathbf{a}.N, \mathbf{a})| \leq \theta_D$  then
11      Add 1 to with
12    end
13    if  $|Y(\mathbf{a}) - \text{Model}(\mathbf{a}.N \setminus \mathbf{x}, \mathbf{a})| \leq \theta_D$  then
14      Add 1 to without
15    end
16  end
17  if without  $\geq$  with then
18    Remove  $\mathbf{x}$  from  $S$ 
19  end
20  ...
21 end
```



Regressors: k NN, MLP, and REPTree.

DROP algorithms tested:

- Using error accumulation (DROP_x-RE): DROP2-RE and DROP3-RE.
- Using thresholding (DROP_x-RT): DROP2-RT and DROP3-RT.

The Model used inside DROP: k NN ($k = 9$).

DROP was compared against RegCNN and the regressor trained over the whole data set.

Experiments were made without and with noise: 10%, 20% and 30%.



	Dataset	# attributes	# instances	Correlation coefficient		
				kNN	MLP	REPTree
1	MachineCPU	6	209	0.9335	0.9433	0.8127
2	Baseball	16	337	0.8291	0.7350	0.7775
3	DEE	6	365	0.9013	0.9061	0.8631
4	AutoMPG8	7	392	0.9276	0.9330	0.9133
5	AutoMPG6	5	392	0.9345	0.9277	0.9081
6	Ele-1	2	495	0.8321	0.8402	0.7969
7	Stock	9	950	0.9927	0.9864	0.9832
8	Laser	4	993	0.9725	0.9873	0.9527
9	Concrete	8	1030	0.8296	0.9103	0.8978
10	Treasury	15	1049	0.9974	0.9981	0.9955
11	Mortgage	15	1049	0.9981	0.9995	0.9965
12	Ele-2	4	1056	0.9904	0.9969	0.9950
13	Friedman	5	1200	0.9425	0.9135	0.8495
14	Wizmir	9	1461	0.9930	0.9967	0.9926
15	Wankara	9	1609	0.9924	0.9964	0.9912
16	Plastic	2	1650	0.8773	0.9024	0.8606
17	Quake	3	2178	0.1074	0.0808	0.0699
18	ANACALT	7	4052	0.9755	0.9890	0.9898
19	Abalone	8	4177	0.7253	0.7516	0.6918
20	Delta-ail	5	7129	0.8267	0.8314	0.8035
21	Compactiv	21	8192	0.9860	0.9903	0.9839
22	Puma32h	32	8192	0.4286	0.3200	0.9562
23	Delta-elv	6	9517	0.7768	0.7913	0.7760
24	Ailerons	40	13750	0.8966	0.8947	0.8728
25	Pole	26	14998	0.9807	0.9491	0.9851
26	Elevators	18	16599	0.8487	0.9499	0.8448
27	California	8	20640	0.8438	0.8468	0.8612
28	House	16	22784	0.6863	0.6736	0.6827
29	Mv	10	40768	0.9853	0.9999	0.9995



Instance selection is a multi-objective problem.

For joining into a single measure:

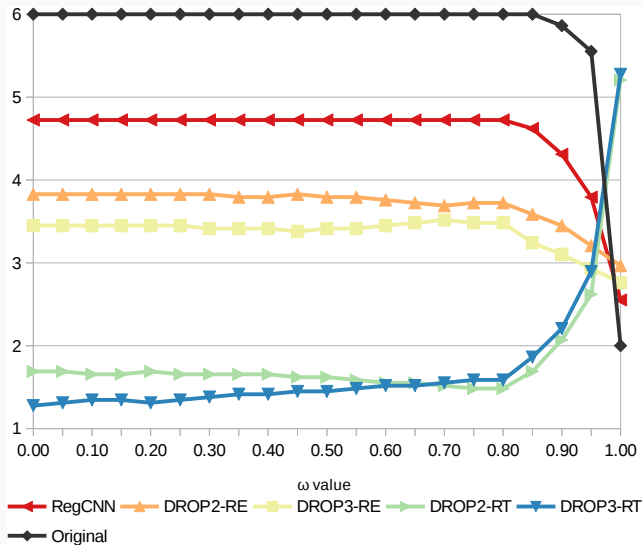
$$l_{\omega} = \omega \cdot \epsilon + (1 - \omega) \cdot m \quad (5)$$

For ϵ (error): $1 - \text{correlation coefficient}$ was used.

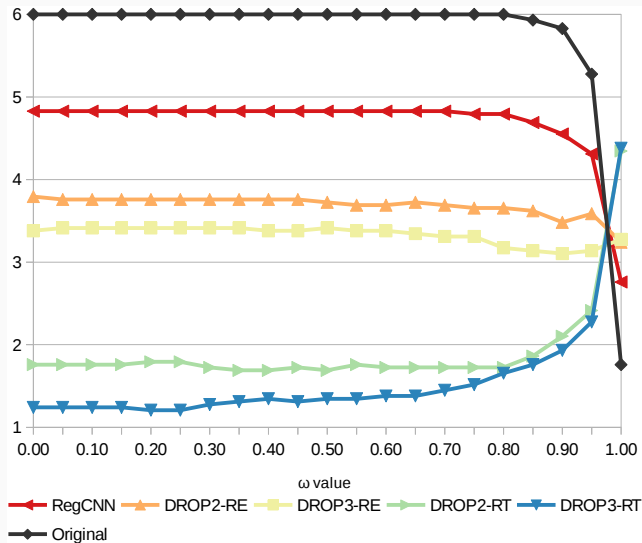
For m (retention ratio):

$$m = \frac{|\text{instances after selection}|}{|\text{instances before selection}|} \quad (6)$$

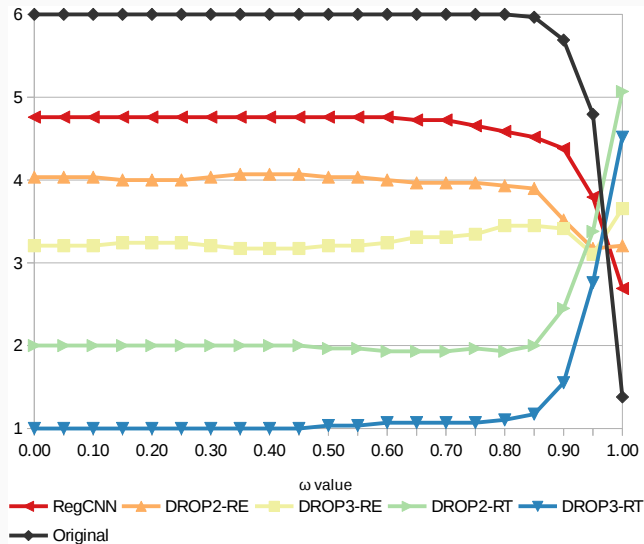
Results: k NN (no noise)



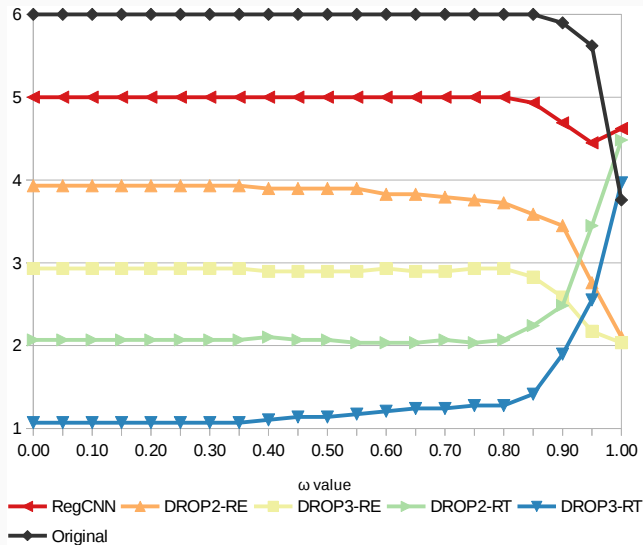
Results: MLP (no noise)



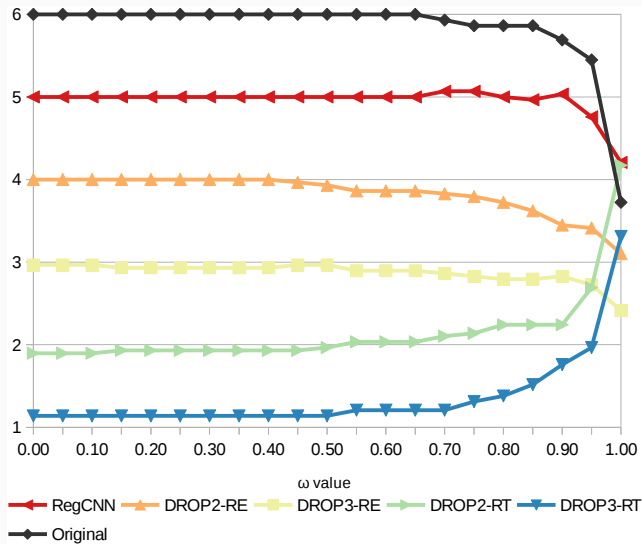
Results: REPTree (no noise)



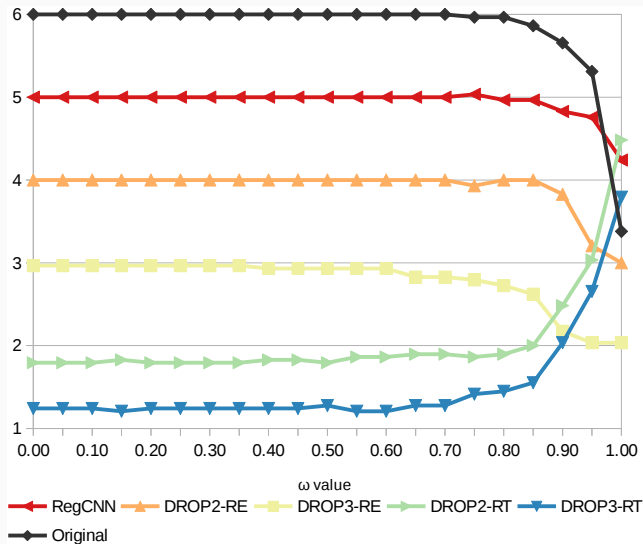
Results: k NN (10% noise)



Results: MLP (10% noise)



Results: REPTree (10% noise)





Average compression and Hochberg procedure.

IS algorithms	Avg. rank	Avg. compression
DROP3-RT	1.2931	0.532
DROP2-RT	1.7069	0.529
DROP2-RE	3.4483	0.366 ✖
DROP3-RE	3.8276	0.369 ✖
RegCNN	4.7241	0.213 ✖



More accuracy

DROP_x-RE: DROP using error accumulation

More compression

DROP_x-RT: DROP using thresholding

DROP3-Rx outperforms significantly DROP2-Rx: noise filter gives an advantage.

RegCNN is highly affected by noise: as the original CNN is.

7. Instance selection of linear complexity for big data



Instance selection methods suffer from high computational complexity.

Hashing functions perform in linear time.

The idea

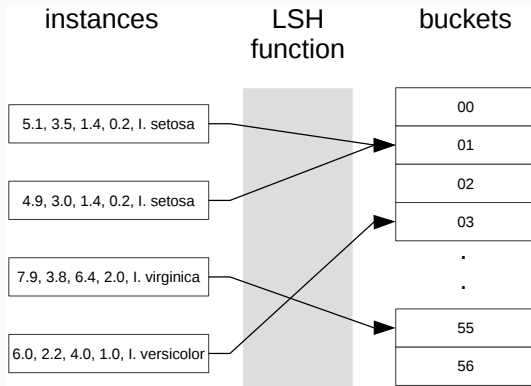
Use LSH functions for designing fast instance selection methods

LSH: how does it work?



Common hashing functions try to avoid collisions: assigning different buckets to similar elements.

LSH functions does not: they assign the same bucket to elements that are close in the input space.

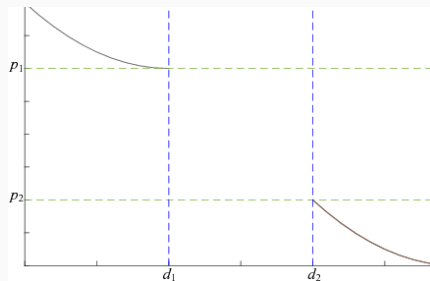




Given a set of objects S and a distance measure D , a family of hash functions $\mathcal{H} = \{h : S \rightarrow U\}$ is said to be (d_1, d_2, p_1, p_2) -sensitive, if all functions of h in the family \mathcal{H} follow:

- For all x, y in S , if $D(x, y) \leq d_1$, then the probability that $h(x) = h(y)$ is at least p_1 .
- For all x, y in S , if $D(x, y) > d_2$, then the probability that $h(x) = h(y)$ is at most p_2 .

It is possible to make the distances d_1 and d_2 can be as close as possible, but the cost will be that p_1 and p_2 are also closer. However, it is possible to combine families of hash functions that separate the probabilities p_1 and p_2 without modifying the distances d_1 and d_2 .





The hash functions in the base family were obtained using the following equation²³.

$$h_{\vec{a},b}(\vec{x}) = \left\lfloor \frac{\vec{a} \cdot \vec{x} + b}{w} \right\rfloor \quad (7)$$

- \vec{a} is a random vector (Gaussian distribution with mean 0 and standard deviation 1)
- b is a random real value from the interval $[0, w]$
- w is the width of each bucket in the hash table

This equation gives a $(w/2, 2w, 1/2, 1/3)$ -sensitive family.

²³Mayur Datar et al. “Locality-sensitive Hashing Scheme Based on P-stable Distributions”. In: *Proceedings of the Twentieth Annual Symposium on Computational Geometry*. SCG '04. Brooklyn, New York, USA: ACM, 2004, pp. 253–262. ISBN: 1-58113-885-7.



Given a (d_1, d_2, p_1, p_2) -sensitive family of hash functions \mathcal{H} , it is possible to obtain a new family \mathcal{H}' using the following operations (only if the independence of functions in \mathcal{H} can be guaranteed)²⁴:

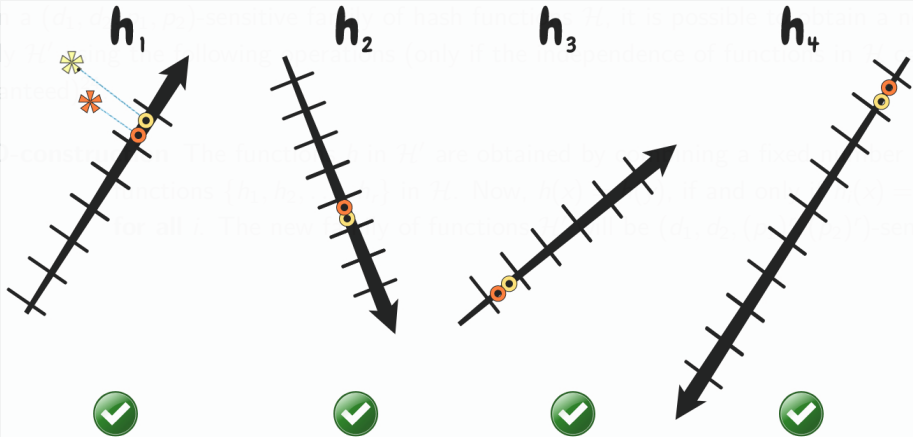
AND-construction The functions h in \mathcal{H}' are obtained by combining a fixed number r of functions $\{h_1, h_2, \dots, h_r\}$ in \mathcal{H} . Now, $h(x) = h(y)$, if and only if $h_i(x) = h_i(y)$ **for all** i . The new family of functions \mathcal{H}' will be $(d_1, d_2, (p_1)^r, (p_2)^r)$ -sensitive.

²⁴The AND-construction decreases the probabilities and the OR-construction increases them.



Given a (d_1, d_2) -sensitive family \mathcal{H} of hash functions, it is possible to obtain a new family \mathcal{H}' of (d_1, d_2) -sensitive functions (only if the independence of functions in \mathcal{H} can be guaranteed).

AND-construction The functions h in \mathcal{H}' are obtained by taking a fixed number r of functions $\{h_1, h_2, \dots, h_r\}$ in \mathcal{H} . Now, $h(x) = 1$ if and only if $h_i(x) = 1$ for all i . The new family of functions is (d_1, d_2) -sensitive.

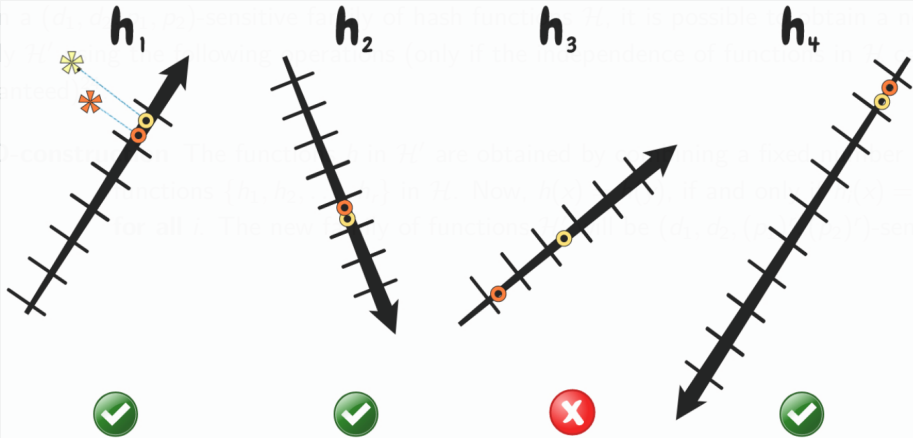


²⁴The AND-construction decreases the probabilities and the OR-construction increases them.



Given a (d_1, d_2) -sensitive family of hash functions \mathcal{H} , it is possible to obtain a new family \mathcal{H}' using the following operations (only if the independence of functions in \mathcal{H} can be guaranteed):

AND-construction: The functions h in \mathcal{H}' are obtained by taking a fixed number r of functions $\{h_1, h_2, \dots, h_r\}$ in \mathcal{H} . Now, $h(x) = h(y)$ if and only if $h_i(x) = h_i(y)$ for all i . The new family of functions will be (d_1, d_2) -sensitive.



²⁴The AND-construction decreases the probabilities and the OR-construction increases them.

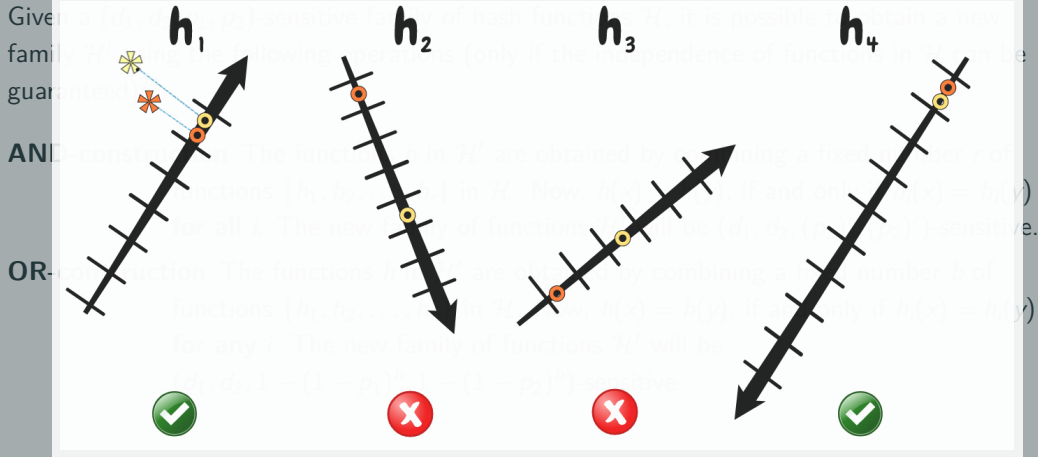


Given a (d_1, d_2, p_1, p_2) -sensitive family of hash functions \mathcal{H} , it is possible to obtain a new family \mathcal{H}' using the following operations (only if the independence of functions in \mathcal{H} can be guaranteed)²⁴:

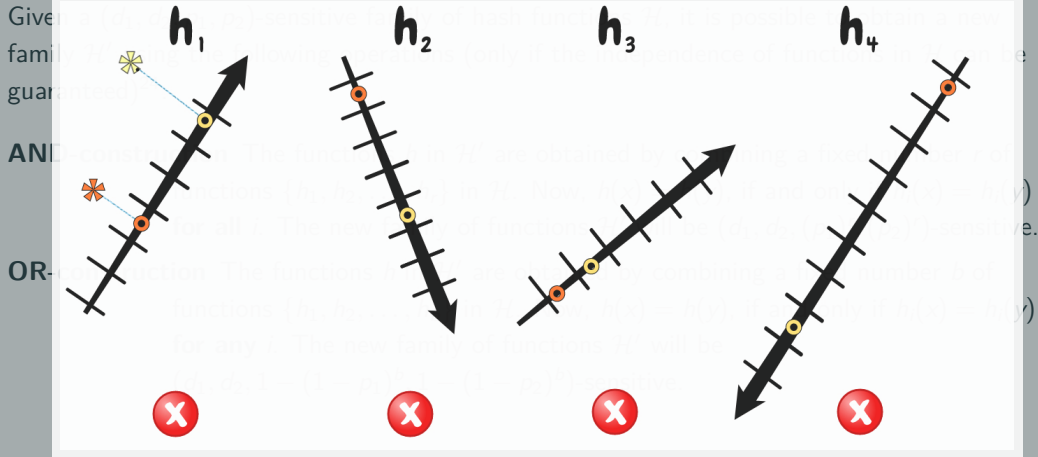
AND-construction The functions h in \mathcal{H}' are obtained by combining a fixed number r of functions $\{h_1, h_2, \dots, h_r\}$ in \mathcal{H} . Now, $h(x) = h(y)$, if and only if $h_i(x) = h_i(y)$ **for all** i . The new family of functions \mathcal{H}' will be $(d_1, d_2, (p_1)^r, (p_2)^r)$ -sensitive.

OR-construction The functions h in \mathcal{H}' are obtained by combining a fixed number b of functions $\{h_1, h_2, \dots, h_b\}$ in \mathcal{H} . Now, $h(x) = h(y)$, if and only if $h_i(x) = h_i(y)$ **for any** i . The new family of functions \mathcal{H}' will be $(d_1, d_2, 1 - (1 - p_1)^b, 1 - (1 - p_2)^b)$ -sensitive.

²⁴The AND-construction decreases the probabilities and the OR-construction increases them.



²⁴The AND-construction decreases the probabilities and the OR-construction increases them.



²⁴The AND-construction decreases the probabilities and the OR-construction increases them.



Algorithm 6: LSH-IS-S: Instance selection algorithm by hashing in one pass.

Input: A training set $X = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, set \mathcal{G} of hash function families

Output: The set of selected instances $S \subseteq X$

```
1  $S = \emptyset$ 
2 foreach instance  $\mathbf{x} \in X$  do
3   foreach function family  $g \in \mathcal{G}$  do
4      $u \leftarrow$  bucket assigned to  $\mathbf{x}$  by family  $g$ 
5     if there is no other instance of the same class of  $\mathbf{x}$  in  $u$  then
6       Add  $\mathbf{x}$  to  $S$ 
7       Add  $\mathbf{x}$  to  $u$ 
     end
   end
end
return  $S$ 
```



Algorithm 7: LSH-IS-F: Instance selection algorithm by hashing with two passes.

Input: A training set $X = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, set \mathcal{G} of hash function families

Output: The set of selected instances $S \subseteq X$

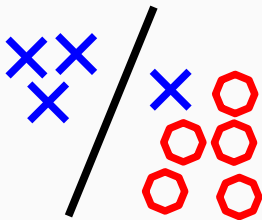
```
1  $S = \emptyset$ 
2 foreach instance  $\mathbf{x} \in X$  do
3   foreach function family  $g \in \mathcal{G}$  do
4      $u \leftarrow$  bucket assigned to  $\mathbf{x}$  by family  $g$ 
5     Add  $\mathbf{x}$  to  $u$ 
6   end
7 end
8 foreach function family  $g \in \mathcal{G}$  do
9   foreach bucket  $u$  of  $g$  do
10    foreach class  $y$  with some instance in  $u$  do
11       $I_y \leftarrow$  all instances of class  $y$  in  $u$ 
12      if  $|I_y| > 1$  then
13        Add to  $S$  one random instance of  $I_y$ 
14      end
15    end
16  end
17 end
18 return  $S$ 
```

How do they work? An example

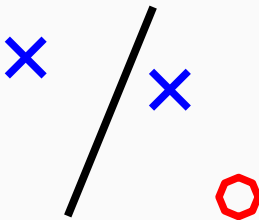


Two buckets are identified by LSH and the line shows the boundary:

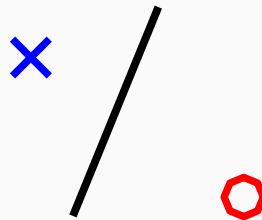
- (a) Initial instances.
- (b) Instances selected by LSH-IS-S.
- (c) Instances selected by LSH-IS-F.



(a)



(b)



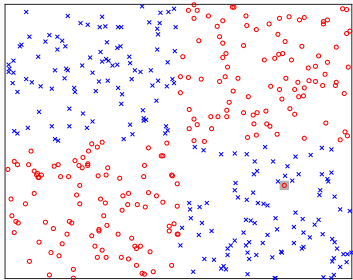
(c)

How do they work? XOR example

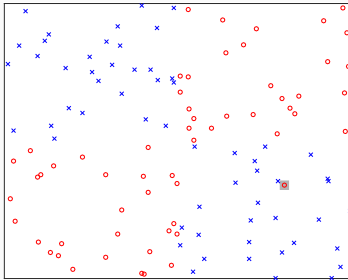


Example with XOR data set:

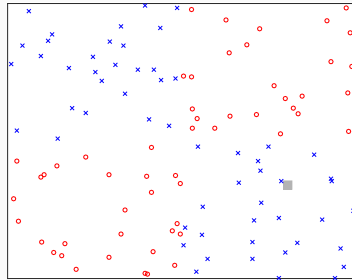
- (a) Original data set, an outlier is highlighted in gray.
- (b) LSH-IS-S maintains the outlier.
- (c) LSH-IS-F removes the outlier.



(a)



(b)



(c)



Data sets		# attributes		# instances	# classes	Accuracy	
		Continuous	Nominal			1NN	J48
1	German	7	13	1000	2	72.90	71.80
2	Flare	0	11	1066	6	73.26	73.55
3	Contraceptive	9	0	1473	3	42.97	53.22
4	Yeast	8	0	1484	10	52.22	56.74
5	Wine-quality-red	11	0	1599	11	64.85	62.04
6	Car	0	6	1728	4	93.52	92.36
7	Titanic	3	0	2201	2	79.06	79.06
8	Segment	19	0	2310	7	97.23	96.62
9	Splice	0	60	3190	3	74.86	94.17
10	Chess	0	35	3196	2	72.12	81.85
11	Abalone	7	1	4174	29	19.84	20.72
12	Spam	0	57	4597	2	91.04	92.97
13	Wine-quality-white	11	0	4898	11	65.40	58.23
14	Banana	2	0	5300	2	87.21	89.04
15	Phoneme	5	0	5404	2	90.19	86.42
16	Page-blocks	10	0	5472	5	95.91	97.09
17	Texture	40	0	5500	11	99.04	93.13
18	Optdigits	63	0	5620	10	98.61	90.69
19	Mushroom	0	22	5644	2	100.00	100.00
20	Satimage	37	0	6435	7	90.18	86.28
21	Marketing	13	0	6876	10	28.74	31.06
22	Thyroid	21	0	7200	3	92.35	99.71
23	Ring	20	0	7400	2	75.11	90.95
24	Twonorm	20	0	7400	2	94.81	85.12
25	Coil 2000	85	0	9822	2	90.62	93.95
26	Penbased	16	0	10992	10	99.39	96.53
27	Nursery	0	8	12960	5	98.13	97.13
28	Magic	10	0	19020	2	80.95	85.01
29	Letter	16	0	20000	27	96.04	87.98
30	KR vs. K	0	6	28058	18	73.05	56.58



Classifiers used: 1NN and J48.

The proposed methods were compared against:

- CNN, MSS²⁵, HMN-EI²⁶, and LSBo.
- ICF²⁷ and DROP3: $k = 3$.
- PSC²⁸: *num clusters* = 6r.

²⁵Ricardo Barandela, Francesc J. Ferri, and José Salvador Sánchez. “Decision boundary preserving prototype selection for nearest neighbor classification”. In: *IJPRAI* 19.6 (2005), pp. 787–806.

²⁶Elena Marchiori. “Hit Miss Networks with Applications to Instance Selection”. In: *J. Mach. Learn. Res.* 9 (June 2008), pp. 997–1017. ISSN: 1532-4435.

²⁷Henry Brighton and Chris Mellish. “Advances in Instance Selection for Instance-Based Learning Algorithms”. English. In: *Data Mining and Knowledge Discovery* 6.2 (2002), pp. 153–172. ISSN: 1384-5810.

²⁸J.Arturo Olvera-López, J.Ariel Carrasco-Ochoa, and J.Francisco Martínez-Trinidad. “A new fast prototype selection method based on clustering”. In: *Pattern Analysis and Applications* 13.2 (2009), pp. 131–141. ISSN: 1433-755X.



Average ranks over accuracy: 1NN classifier (left) and J48 (right).

Algorithm	Ranking	p Hoch.
HMN-EI	2.92	
LSBo	3.85	0.1869
LSH-IS-F	4.45	0.0602
MSS	4.58	0.0553
LSH-IS-S	4.98	0.0139
DROP3	5.03	0.0138
CNN	5.17	0.0088
ICF	5.75	0.0004
PSC	8.27	0.0000

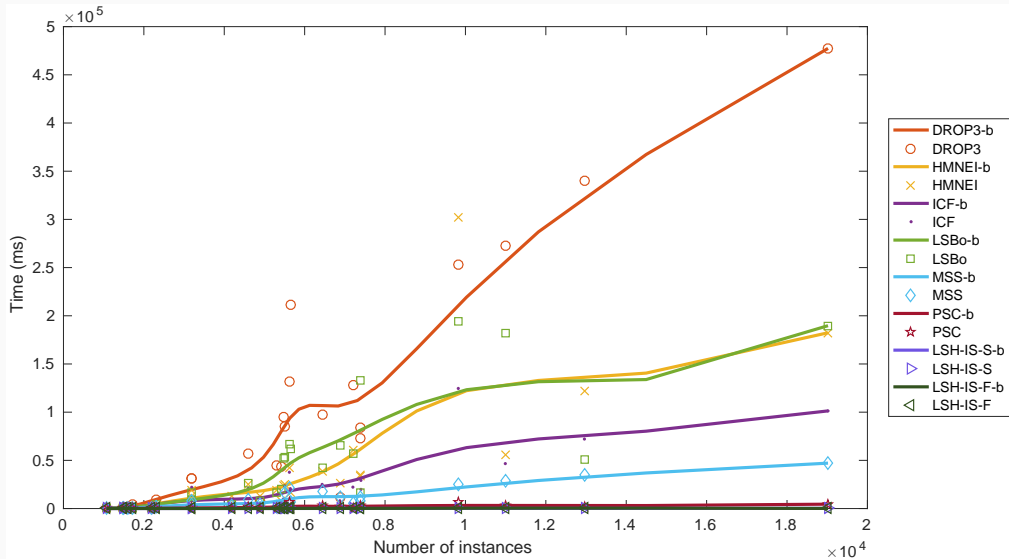
Algorithm	Ranking	p Hoch.
LSH-IS-F	3.63	
LSH-IS-S	3.88	0.7237
HMN-EI	4.10	0.7237
LSBo	4.57	0.5606
MSS	5.03	0.1909
CNN	5.28	0.0981
ICF	5.67	0.0242
DROP3	5.90	0.0094
PSC	6.93	0.0000



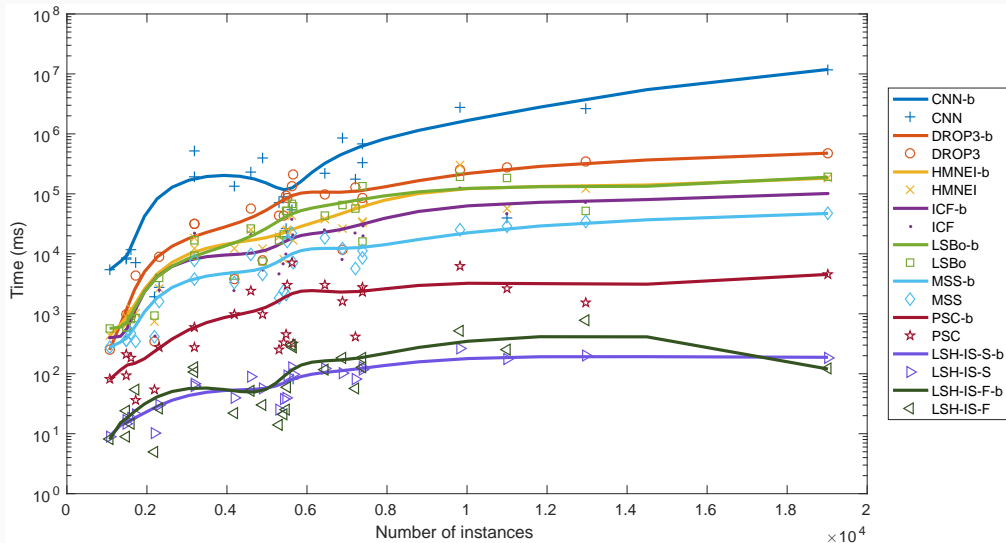
Average ranks and Hochberg procedure over storage reduction, and average reduction rate.

Algorithm	Ranking	p Hoch.	Reduction rate
DROP3	1.67		0.896
ICF	3.10	0.0427	0.813
LSBo	3.70	0.0081	0.737
PSC	4.70	0.0001	0.762
CNN	5.43	0.0000	0.658
MSS	6.00	0.0000	0.665
HMN-EI	6.10	0.0000	0.577
LSH-IS-F	6.62	0.0000	0.455
LSH-IS-S	7.68	0.0000	0.405

Results: filtering time



Results: filtering time (Log. scale)





Data sets		# attributes		# instances	# classes	Accuracy
		Continuous	Nominal			
31	Census	7	30	299 285	2	92.70
32	KDDCup99	33	7	494 021	23	99.95
33	CovType	54	0	581 012	7	94.48
34	KDDCup991M	33	7	1 000 000	23	99.98
35	Poker	5	5	1 025 010	10	50.61



Classifier used: 1NN.

The proposed methods were compared against: Democratic Instance Selection²⁹:

- RNN.
- ICF and DROP3: $k = 3$.

²⁹César García-Osorio, Aida de Haro-García, and Nicolás García-Pedrajas. “Democratic instance selection: A linear complexity instance selection algorithm based on classifier ensemble concepts”. In: *Artificial Intelligence* 174.5-6 (2010), pp. 410–441. ISSN: 0004-3702.



Average ranks: accuracy (left) and compression (right).

Algorithm	Ranking
LSH-IS-F	2.0
DIS.RNN	2.2
LSH-IS-S	2.6
DIS.DROP3	3.6
DIS.ICF	4.6

Algorithm	Ranking
DIS.RNN	1.8
DIS.DROP3	2.4
LSH-IS-F	3.2
DIS.ICF	3.4
LSH-IS-S	4.2



- Linear complexity: $\mathcal{O}(n)$
- One of the methods does not need that the data fits in memory (*on-the-fly*).
- Competitive results as instance selection for medium and huge data sets.

8. Conclusions



The lack of instance selection methods for regression sparked my initial interest in this task.

We designed and tested three ideas of instance selection for regression:



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- Discretization: to transform the continuous output variable into discrete counterparts \implies good performance on noise identification.



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- Combination of several instance selection methods for regression was evaluated: it upholds the 'ensemble' hypothesis.



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We designed and tested three ideas of instance selection for regression:

- Discretization: to transform the continuous output variable into discrete counterparts \implies good performance on noise identification.
- Combination of several instance selection methods for regression was evaluated: it upholds the 'ensemble' hypothesis.
- Adaptation of DROP to regression: it mimics the benefits of DROP for classification.



High computational complexity of instance selection methods for classification.

We faced the problem from two points of view:



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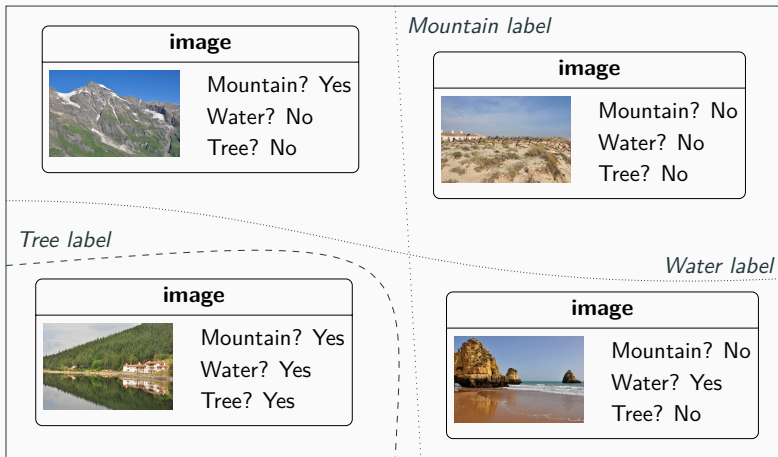
- Locality-Sensitive Hashing: linear complexity in relation to the number of instances.
- Democratic Instance Selection: we designed and implemented a parallel version of DIS method by following the MapReduce model³⁰.

³⁰Álvar Arnaiz-González et al. “MR-DIS: Democratic Instance Selection for Big Data by MapReduce”. In: *Progress in Artificial Intelligence* 6.3 (2017), pp. 211–219. ISSN: 2192-6360.

9. Current research



There is a relatively new topic where the usefulness of instance selection is starting to become apparent.





The work on this topic has already borne fruit, as a result, the following couple of papers have recently been published:

- Local sets for multi-label instance selection³¹.
- Study of data transformation techniques for adapting single-label prototype selection algorithms to multi-label learning³².

³¹Álvar Arnaiz-González et al. “Local sets for multi-label instance selection”. In: *Applied Soft Computing* (in press) (2018). ISSN: 1568-4946.

³²Álvar Arnaiz-González et al. “Study of data transformation techniques for adapting single-label prototype selection algorithms to multi-label learning”. In: *Expert Systems with Applications* (in press) (2018). ISSN: 0957-4174.



A topic closely related to multi-label is multi-target regression.

Each instance in multi-target data sets has a group of numeric output values, not a set of labels.

There are many real-world problems to which multi-target regression can be applied: environmental sciences, bio-informatics, medicine...

There are not any instance selection algorithm for multi-target regression in the literature.

Thanks!



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dblp: `dblp.uni-trier.de/pers/hd/a/Arnaiz=Gonz=acute=lez:=Acute=lvar`



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Appendix

10. Discretization

Discretization algorithm (i)

An unsupervised filter incorporated in Weka was used for discretization.

The equal-width option was selected, so all bins in which the target attribute was split had the same size.

The number of bins is selected from one to ten by the Weka filter using leave-one-out cross-validation to select the best way of separating the numerical output variable, i.e. the one that maximizes the entropy.

Discretization algorithm (ii)

Algorithm 8: Equal-width binning using leave-one-out estimated entropy.

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$

Maximum number of bins b

Output: Discretized set $D = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$

```
1 bestEntropy  $\leftarrow$  MAX_VALUE
2 for  $i = 1 \dots b$  do
3   entropy = LOUEstimatedEntropy( $T, i$ )
4   if entropy < bestEntropy then
5     bestEntropy  $\leftarrow$  entropy
6     bestNumBins  $\leftarrow$   $i$ 
7   end
8 end
9 cutPoints = CalcCutPoints( $T, i$ )
10  $D =$  DiscretizeClass( $T, \text{cutPoints}$ )
11 return  $D$ 
```

RegENN

Algorithm 9: RegENN: Edited Nearest Neighbour for regression using a threshold

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, parameter α to control how the threshold is calculated from the standard deviation

Output: Instance set $P \subseteq T$

```
1 for  $i = 1 \dots n$  do
2    $\bar{Y}(\mathbf{x}_i) = \text{Model}(T \setminus \mathbf{x}_i, \mathbf{x}_i)$ 
3    $S = \text{kNN}(T, \mathbf{x}_i)$ 
4    $\theta = \alpha \cdot \text{std}(Y(X_S))$ 
5   if  $|Y(\mathbf{x}_i) - \bar{Y}(\mathbf{x}_i)| > \theta$  then
6      $T \leftarrow T \setminus \mathbf{x}_i$ 
  end
end
7  $P \leftarrow T$ 
return  $P$ 
```

Class noise

The noise configurations were tested at 10, 20, 30 and 40% adding or subtracting a random value to the target attribute.

Mutual Information IS

Algorithm 10: Algorithm based on mutual information

Input: Training set $\{X, Y\} = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$, the number k of neighbours

Output: Edited set $S \subseteq \{X, Y\}$

```
1  $S = \emptyset$ 
2 for  $i = 1 \dots n$  do
3   | Calculate  $NN[\mathbf{x}_i, j]$ , the  $k$  nearest neighbours ( $j = 1 \dots k$ ) in the input space
   end
4 for  $i = 1 \dots n$  do
5   | Calculate the value of mutual information  $I(X, Y)_i$  when  $\mathbf{x}_i$  is eliminated from  $X$ 
   end
6 Normalize  $I(X, Y)_i$  in  $[0, 1]$ 
7 for  $i = 1 \dots n$  do
8   |  $Cdiff = 0$ 
9   for  $j = 1 \dots k$  do
10    |  $diff = I(X, Y)_i - I(X, Y)_{NN[\mathbf{x}_i, j]}$ 
11    | if  $diff > \alpha$  then  $Cdiff = Cdiff + 1$ 
   end
12  | if  $Cdiff < k$  then add  $(\mathbf{x}_i, y_i)$  to  $S$ 
  end
return  $S$ 
```

11. Fusion

T-CNN

Algorithm 11: T-CNN: Condensed Nearest Neighbour for regression using a threshold

Input: Training set $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, parameter α to control how the threshold is calculated from the standard deviation

Output: Instance set $P \subseteq T$

```
1  $P = \emptyset$ 
2  $P \leftarrow P \cup \mathbf{x}_1$ 
3 for  $i = 2 \dots n$  do
4    $\bar{Y}(\mathbf{x}_i) = \text{Model}(P, \mathbf{x}_i)$ 
5    $S = \text{kNN}(T, \mathbf{x}_i)$ 
6    $\theta = \alpha \cdot \text{std}(Y(X_S))$ 
7   if  $|Y(\mathbf{x}_i) - \bar{Y}(\mathbf{x}_i)| > \theta$  then
8      $P \leftarrow P \cup \mathbf{x}_i$ 
9      $T \leftarrow T \setminus \mathbf{x}_i$ 
  end
end
return  $P$ 
```

Experimental setup

Bagging parameters:

- The bagging ensemble was set to 30 members.
- Each subset was created by randomly drawing instances without replacement.
- The number of instances in the subset was 80% of the original.

Other parameters:

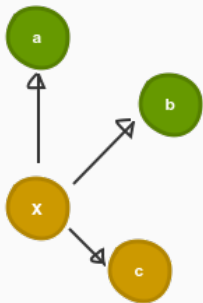
- Number of k -nearest neighbours used by k NN: from 1 to 13 in steps of 2.
- Number of k -nearest neighbours used by instance selection algorithms: from 1 to 13 in steps of 2.
- Threshold controlled by α : from 0.1 to 1 in steps of 0.1.
- Maximum number of bins D : from 5 to 15 in steps of 1.
- Percentage of votes to select an instance z : from 0.1 to 0.9 in steps of 0.1.

12. DROP for regression

Nearest neighbours and associate concepts

The nearest neighbours of x are a , b , and c instances.

$$\text{NN}(x) = \{a, b, c\}$$

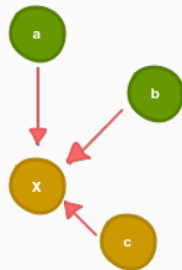


Therefore, a , b , and c have x as associate.

$$x \in \text{associate}(a)$$

$$x \in \text{associate}(b)$$

$$x \in \text{associate}(c)$$



Differences between DROP algorithms: (i)

The differences between the variants of DROP methods are as follows:

- DROP1 eliminates an instance \mathbf{p} of S , if its associates in S are correctly classified without \mathbf{p} , that is, if the elimination of \mathbf{p} does not affect the classification results.
- The DROP2 removes an instance³³; \mathbf{p} of S if the associates that \mathbf{p} has in the original set, T , are correctly classified without \mathbf{p} . Before starting the selection, it sorts the instances in descending order from their distance to their *nearest enemy*. In this way, instances are processed in an order that is the reverse of its distance to the class boundary, the furthest instance is processed first, then the second furthest, and so on.

³³The DROP2, DROP3, DROP4 and DROP5 algorithms verify the effect that causes the removal of an instance on the original sample.

Differences between DROP algorithms: (ii)

The differences between the variants of DROP methods are as follows:

- The DROP3 algorithm, applies a noise filter before starting. The filtering state removes all instances that are not correctly classified by their k nearest neighbours.
- DROP4 is identical to DROP3 but applies a slightly different noise filter, involving the removal of an instance only if it is misclassified by its k nearest neighbours and its removal does not mean that another instance is badly classified. This avoids the removal of too many instances in the filtering stage.
- The DROP5 algorithm is similar to DROP2, but it begins to analyse the instances that are found close to its nearest enemy (those on the class boundary).

Experimental setup: regressors

The regressors used were:

- nearest neighbours (with $k = 8$).
- multilayer perceptron (trained with backpropagation with the following parameters: learning rate = 0.3, momentum = 0.2, number of hidden neurons = $\frac{\#attr+1}{2}$).
- REPTrees (with Weka default parameters).

Class noise

In the experiments that were carried out, the noise was introduced by exchanging the output values of two randomly selected instances.

This way, the distribution of the sample, both for the input variables and for the output variables was not modified.

Experimental setup: DROP_x-R_x

Value of α_E which has achieved lower errors for the different regressors and noise levels.

Noise	IS algorithm	k NN	MLP	REPTree
0 %	DROP3-RE	5	5	3
	DROP2-RT	4	2	1
	DROP3-RT	4	5	2
10 %	DROP3-RE	3	2	2
	DROP2-RT	3	5	2
	DROP3-RT	3	2	3
20 %	DROP3-RE	2	2	2
	DROP2-RT	3	1	3
	DROP3-RT	4	2	1
30 %	DROP3-RE	2	1	1
	DROP2-RT	1	3	5
	DROP3-RT	4	1	1

Experimental setup: RegCNN

It is influenced by two parameters α and k .

With the aim to use reasonable values for these parameters, we first launched several experiments with different values: 0.25, 0.5, 0.75 and 1 for α ; and 3, 5, 7 and 9 for k .

The best results, for all regressors, were achieved using $\alpha = 0.25$.

The optimal values for k depended on the regressor, as the table shows:

Noise	k NN	MLP	REPTree
0 %	9	9	9
10 %	3	7	3
20 %	9	7	9
30 %	7	7	7

13. LSH-IS

Complexity

Summary of state-of-the-art IS methods (taxonomy from³⁴; computational complexity from³⁵ and authors' papers).

Strategy	Direction	Algorithm	Complexity	Year
Condensation	Incremental	CNN	$\mathcal{O}(n^3)$	1968
	Incremental	PSC	$\mathcal{O}(n \log n)$	2010
	Decremental	RNN	$\mathcal{O}(n^3)$	1972
	Decremental	MSS	$\mathcal{O}(n^2)$	2002
Hybrid	Decremental	DROP1-5	$\mathcal{O}(n^3)$	2000
	Batch	ICF	$\mathcal{O}(n^2)$	2002
	Batch	HMN-EI	$\mathcal{O}(n^2)$	2008
	Batch	LSBo	$\mathcal{O}(n^2)$	2015

³⁴S. Garcia et al. "Prototype Selection for Nearest Neighbor Classification: Taxonomy and Empirical Study". In: *Pattern Analysis and Machine Intelligence, IEEE Transactions on* 34.3 (2012), pp. 417–435. ISSN: 0162-8828.

³⁵Norbert Jankowski and Marek Grochowski. "Comparison of Instances Seletion Algorithms I. Algorithms Survey". English. In: *Artificial Intelligence and Soft Computing - ICAISC 2004*. Ed. by Leszek Rutkowski et al. Vol. 3070. Lecture Notes in Computer Science. Springer Berlin Heidelberg, 2004, pp. 598–603. ISBN: 978-3-540-22123-4.

LSH functions (i)

The reason for $w/2$ and $1/2$ is: if the distance d between two points is exactly $w/2$ (half the width of the buckets) the smallest probability for the two points falling in the same segment would happen for $\theta = 0$, and in this case the probability would be 0.5, since d is exactly $w/2$. For angles greater than 0, this probability will be even higher; in fact, it will be 1 for $\theta = 90$. And for shorter distances than $w/2$, the probability will equally increase. So the lower boundary for this probability is $1/2$.

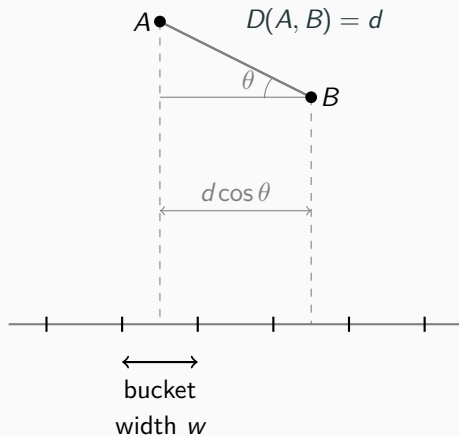


Figure 4: Two points (A, B) at distance $d \gg w$ have a small chance of being hashed to the same bucket.

LSH functions (ii)

The reason for $2w$ and $1/3$ is: if the distance d is exactly $2w$ (twice the width of the bucket), the only chance for both points to fall in the same bucket is that their distances, once projected in the segment, are lower than w , what means that $\cos \theta$ must be lower than 0.5, since the projected distance is $d \cos \theta$ and d is exactly $2w$. For θ in the interval 0 to 60 , $\cos \theta$ is greater than 0.5, so the only chance of $\cos \theta$ being lower than 0.5 is that θ is in the interval $[60, 90]$, and the chance of that happening is at most $1/3$. For distances greater than $2w$, the probabilities are even lower. So the upper boundary of this probability is $1/3$.

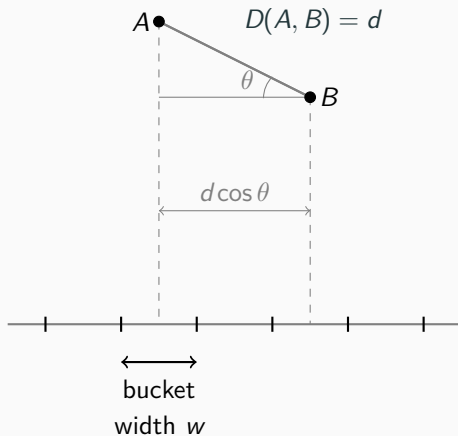


Figure 5: Two points (A, B) at distance $d \gg w$ have a small chance of being hashed to the same bucket.

LSH configuration: AND/OR constructions

- LSH-IS-S: the best configuration is one that uses OR-constructions of 6 functions obtained using an AND-construction on 10 functions of the base family.
- LSH-IS-F: the best results were obtained using OR-constructions of 5 functions obtained by combining by AND-construction 10 functions of the base family.

