

Visualization of attractiveness and performance measures

in knowledge discovery and machine learning

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Wizualizacja miar atrakcyjno ci i skuteczno ci w odkrywaniu wiedzy i uczeniu maszynowym

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Presentation plan

- Work context and motivations
- Visualization of measures
 - Motivations
 - 4D domain
 - Visualization technique
- Application of the visualization technique to measures
- Visual-based detection of properties
 - Property of monotonicity M
 - Property of weak L
 - Property of hypothesis symmetry
- Summary
- Quiz 🙂

Work context



Work context – measuring single rule attractiveness

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Height	Hair	Lyes	Nationality						Ц	_ U
tall	blond	blue	Swede		¬Ε	¬Η			11	
medium	dark	hazel	German		¬Ε	Н		E	1	0
medium	blond	blue	Swede		¬Ε	¬Η		_ F	2	3
tall	blond	blue	German		¬Ε	Н		_		0
short	red	blue	German		E	Н		a = sup b = sup)(Е,Н))(_— Е,Н) 0
medium	dark	hazel	Swede		¬Ε	¬Η		c = sup	(Е, —Н	ý o
								a = sup n=a+b	>(¬E,− +c+d	H) U

 The contingency table is a form used to calculate the value of attractiveness measures (e.g. confirmation measures)

Confirmation measures

An interestingness measure c(H,E) has the property of confirmation (i.e. is a confirmation measure) if is satisfies the following condition:

 $c(H,E) \begin{cases} > 0 \text{ if } P(H|E) > P(H) \\ = 0 \text{ if } P(H|E) = P(H) \end{cases} c(H,E) \begin{cases} > 0 \text{ if } \frac{a}{a+c} > \frac{a+b}{n} \\ = 0 \text{ if } \frac{a}{a+c} = \frac{a+b}{n} \\ < 0 \text{ if } P(H|E) < P(H) \end{cases}$

- Measures of confirmation quantify the strength of confirmation that premise E gives to conclusion H
- "H is verified more often, when E is verified, rather than when E is not verified"

There are many alternative, non-equivalent measures of confirmation

$$D(H,E) = P(H | E) - P(H) = \frac{a}{a+c} - \frac{a+b}{n}$$
(Carnap 1950/1962)

$$M(H,E) = P(E | H) - P(E) = \frac{a}{a+b} - \frac{a+c}{n}$$
(Mortimer 1988)

$$S(H,E) = P(H | E) - P(H | \neg E) = \frac{a}{a+c} - \frac{b}{b+d}$$
(Christensen 1999)

$$N(H,E) = P(E | H) - P(E | \neg H) = \frac{a}{a+b} - \frac{c}{c+d}$$
(Nozick 1981)

$$C(H,E) = 4[P(E \land H) - P(E)P(H)] = 4\left[\frac{a}{n} - \frac{(a+c)(a+b)}{n^2}\right]$$
(Carnap 1950/1962)

$$F(H,E) = \frac{P(E | H) - P(E | \neg H)}{P(E | H) + P(E | \neg H)} = \frac{ad - bc}{ad + bc + 2ac}$$
(Kemeny, Oppenheim 1952)

$$FS(H,E) = \frac{1}{2}(F(H,E) + S(H,E))$$
(Glass 2013)

The values of all of the above measures range from -1 to +1 otherwise they are undefined, e.g. when a+c=0 measure D(H,E) is NaN.

Work context – measuring classifier performance



a b

С

d

FN

FP

ΤN

 A classifier predicts the desired class label (out of two):

Nationality = Swede

 The confusion matrix (a special case of the contingency table) is a form used to calculate the value of classifier performance measures (e.g. accuracy, sensitivity)

Selected classifier performance measures

There are many alternative, non-equivalent classifier performance measures

$$accuracy = \frac{TP + TN}{TP + FN + FP + TN} = \frac{a+d}{a+b+c+d}$$

$$sensitivity = \frac{TP}{TP + FN} = \frac{a}{a+b} \qquad (recall)$$

$$specificity = \frac{TN}{FP + TN} = \frac{d}{c+d}$$

$$precision = \frac{TP}{TP + FP} = \frac{a}{a+c}$$

$$G - mean = \sqrt{sensitivity \times specificity}$$

$$F - measure = \frac{2TP}{2TP + FN + FP} = \frac{2a}{2a+b+c}$$

$$Jaccard = \frac{TP}{TP + FN + FP} = \frac{a}{a+b+c}$$

- The values of all of the above measures range from 0 to +1,
- otherwise they are undefined, e.g. when a+c=0 precision is NaN.

Visualization of measures

• Example:

- problem: in data sets with imbalanced classes (P(Cl₁) << P(Cl₂)) the classification accuracy (CA) may be a misleading measure since in general (for real life classifiers) CA ≥ P(Cl₁) and CA ≥ P(Cl₂), so high values of CA are implied by high values of P(Cl₂)
- solution: measures that take the class-imbalance into account (G-mean, F₁, Jaccard, ...) are often applied (also several at once)
 - a small issue in the solution: do those measures differ (significantly)?
 - if yes, then where (in the domain) and how much do they differ?
 - if no, then why use several of them?
 - a suggested remedy to the small issue in the solution: treat the measures as functions of four arguments and examine the behaviour of these functions
 - which may, but need not to, clarify the issue...

- What is our most common working knowledge on the measures (as functions of their arguments)?
 - the formula of the form f(a,b,c,d) (when defined analytically /most cases/)
 - the domain, the value set
 - existence of particular values
 - minima/maxima
 - undefined
 - selected properties (continuity, monotonicity, periodicity, ...)

Exemplary questions:

• ...

- what are the domains of G-mean, F_1 and CA?
- what are the value sets of G-mean, F₁ and CA?
- what are the maxima/minima of G-mean, F_1 and CA?
 - where (in the domain) are the extrema situated?
- what are the undefined values of G-mean, F₁ and CA?
 - where (in the domain) are those values situated?
- does one (of G-mean, F₁ and CA) significantly exceed the others?
 - where (in the domain) are the regions of this phenomenon situated?
- what are the growth rates of G-mean, F₁ and CA?
 - where (in the domain) are the regions of high/low growth rate situated?

- The most popular way to get a good working knowledge of how a function behaves throughout its domain:
 - charting its value set against its domain
 - easy for 1D functions
 - many, not all
 - harder for nD functions
 - although still possible when n is small
- This way we gain an insight into all areas of the domain that the visualized measure can possibly occupy, and which could be omitted and thus remain undiscovered while working on real-life data

- The visualization technique that we propose aims at describing (by the means of visualization) the measures as functions, and thus helps
 - users of the measures use those measures that meet better their needs
 - designers of the measures design such measures that possess better properties

4D domain

- Given n > 0 (the total number of observations), the domain space is generated as the set of all possible contingency tables satisfying
 a + b + c + d = n
- The set is thus exhaustive and non-redundant (i.e. it contains exactly one copy of each contingency table satisfying the above condition)

Height	Hair	Eyes	Nationality		
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tall	blond	blue	German		
short	red	blue	German		
medium	dark	hazel	Swede		

	Н	¬ H			
Е	а	С			
- E	b	d			

а	b	С	d
0	0	0	6
Ò	0	1	5
0	0	2	4
0	0	3	3
0	0	4	2
0	0	5	1
0	0	6	0
0	0	5	1
0	1	0	5
0	1	1	4
0	1	2	3
6	0	0	0

- Thus, our data set comprises t rows and 4 columns: a, b, c and d; t=(n+1)(n+2)(n+3)/6
- In general, four independent columns correspond to four degrees of freedom, visualization of such data in the form of a scatter-plot would formally require four dimensions
- Owing to the condition a + b + c + d = n however, the number of degrees of freedom is reduced to three, so it is possible to visualize such data in three dimensions (3D) using tetrahedron-based barycentric coordinates
- The tetrahedron is a 3D structure, so its every point may be assigned 3 values (3D coordinates).
- Simultaneously, its every point may be assigned 4 values (barycentric coordinates)



 The proposed 3D view of the tetrahedron, has its four vertices
 A, B, C and D coinciding with points of the following
 [x, y, z] coordinates:

> A: [1,1,1] B: [-1,1,-1] C: [-1,-1,1] D: [1,-1,-1]



 the vertex A corresponds to the (single) contingency table satisfying a=n and b=c=d=0



 the edge AB corresponds to the (multiple) contingency tables satisfying a+b=n and c=d=0



 the face ABC corresponds to the (multiple) contingency tables satisfying a+b+c=n and d=0

- Given n > 0 (the total number of observations), the domain space is generated as the set of all possible contingency tables satisfying
 a + b + c + d = n
- The set contains only samples of the 4D domain, however it is a uniform (regular) sampling, thus the best possible





• Example of poor sampling



• Example of acceptable sampling



Example of uniform (regular) sampling

Visualization technique – colour map

- Because the individual points of the tetrahedron may be displayed in colour, it is possible to visualize a function f(a,b,c,d) of the four arguments (e.g. any measure)
- It is assumed that the value set of this function is a real interval [r,s], with r < s, so that its values may be rendered using a pre-defined colour map

Visualization technique – colour map

may be rendered as colours

or special characters (e.g., "*")

not occurring in the map

 For all the analysed confirmation measures the standard colour map ranges from -1 to +1 (actually used: jet(16))



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Visualization technique – exemplary external visualizations



Visualization technique – exemplary external visualizations



 The standard view accompanied by the rotated view, designed to depict the DAB face of the tetrahedron (not visible in the standard view)

Visualization technique – exemplary internal visualizations



Visualization technique – summary of the capabilities

- The capabilities of the visualization techniques include:
 - regular views of any measure
 - specialized views of a region of interest
 - specialized views of any number of measures
 - differences between two measures
 - variances/means of a number of measures

Application of the visualization technique to confirmation measures

Visualization technique – summary of the capabilities

- The capabilities of the visualization techniques include:
 - regular views of any measure
 - specialized views of a region of interest
 - specialized views of any number of measures
 - differences between two measures
 - variances/means of a number of measures

Regular views of confirmation measures

- The regular views of the measures may be used to practically compare their general configurations of values and gradient profiles
- Such visual analyses allow to tentatively conclude about the ordinal equivalence of the visualized measures, an especially important issue in evaluating rules with multiple measures
- In general, this kind of equivalence analysis may require an insight into the interior of the tetrahedron

Regular views of confirmation measures: S(H,E)



Regular views of confirmation measures: F(H,E)





Regular views of confirmation measures

- In all faces measure S(H,E) manifests 'radial' gradients, while measure F(H,E) is characterized by constant values (no gradient) in two faces (ABD and BCD) and a 'radial' gradient in the other two
- In the case of S(H,E) and F(H,E) the different gradient profiles in the external areas of the corresponding tetrahedrons constitute conclusive counterexamples to the ordinal equivalence of those measures
Visualization techniques – summary of the capabilities

- The capabilities of the visualization techniques include:
 - regular views of any measure
 - specialized views of a region of interest
 - specialized views of any number of measures
 - differences between two meaures
 - variances/means of a number of measures

Specialized views of regions of interest

The specialized views of regions of interest are useful since they allow to instantly detect and localize interesting characteristics of the measures (extreme values, zeros, etc.), which would otherwise have to be laboriously derived from the analytic definitions of the measures

Specialized views of regions of interest: c(H,E)=0



- Regions with neutral values of confirmation measures
- The grey colour map is used only to provide the necessary perspective; the colours do not translate to values of the measure (which are constant in this case)

Specialized views of regions of interest: C(H,E)=0.5



- Regions for which |C(H,E)|=0.5; notice their full symmetry
- The grey colour map is used only to provide the necessary perspective; the colours do not translate to values of the measure (which are constant in this case)

Specialized views of regions of interest: N(H,E)=min/max/NaN



 Regions of extreme (-1 and +1) and non-numeric values (NaN) of measure N(H,E)



Visualization techniques – summary of the capabilities

- The capabilities of the visualization techniques include:
 - regular views of any measure
 - specialized views of a region of interest
 - specialized views of any number of measures
 - differences between two measures
 - variances/means of a number of measures

Specialized views – differences /variance among measures

- Visualization of differences between measures or variances among groups of measures allows to identify those arguments (i.e. values of a, b, c and d) for which two given measures differ only insignificantly (similarity of the measures) or differ considerably (dissimilarity of the measures)
- Thus, it guides practitioners towards measures that suit them most



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The exterior view of S(H,E) - N(H,E)





The inner view of S(H,E) - N(H,E)





The inner view of S(H,E) - N(H,E)



Visualization techniques – summary of the capabilities

- The capabilities of the visualization techniques include:
 - regular views of any measure
 - specialized views of a region of interest
 - specialized views of any number of measures
 - differences between two measures
 - variances/means of a number of measures

Specialized views - variance among likelihoodist measures



The variance among measures: M(H,E), N(H,E), A(H,E), c₂(H,E)



Specialized views - variance among likelihoodist measures



The inner view of the variance among: M(H,E), N(H,E), A(H,E), c₂(H,E)



Specialized views - variance among likelihoodist measures



■ The inner view of the variance among: M(H,E), N(H,E), A(H,E), c₂(H,E)





Properties of confirmation measures

The choice of a confirmation measure for a certain application is a difficult problem

- •the number of proposed measures is overwhelming
- there is no evidence which measure is the best
- the users' expectations vary

properties of confirmation measures, which reflect users' expectations towards the behaviour of measures in particular situations

 property of monotonicity M (Greco, Pawlak & Słowi ski 2004)
 Ex₁ property and its generalization to weak Ex₁
 property of logicality L and its generalization to weak L
(Fitelson 2006; Crupi, Tentori & Gonzalez 2007
Greco, Słowi ski & Szcz ch 2012)
•

need to analyze measures with respect to their properties

Motivation: Detect properties of measures and compare measures easily through their visualizations

Property of monotonicity M		Н	¬ H
	E	а	С
	¬ E	b	d

Desirable property of c(H,E) = f(a,b,c,d) : monotonicity (M)*

f should be non-decreasing with respect to a and d and non-increasing with respect to b and c

- Interpretation of (M): $(E \rightarrow H \equiv if x is a raven, then x is black)$
 - a) the more black ravens we observe, the more credible becomes $E \rightarrow H$
 - b) the more black non-ravens we observe, the less credible becomes $E \rightarrow H$
 - c) the more non-black ravens we observe, the less credible becomes $E \rightarrow H$
 - d) the more non-black non-ravens we observe, the more credible becomes $E \rightarrow H$

*S.Greco, Z.Pawlak, R.Słowi ski: Can Bayesian confirmation measures be useful for rough set decision rules? Engineering Applications of Artificial Intelligence, 17 (2004) no.4, 345-361

Property of monotonicity M		Н	¬ H
	E	а	С
	¬ E	b	d

Desirable property of c(H,E) = f(a,b,c,d) : monotonicity (M)

f should be non-decreasing with respect to a and d and non-increasing with respect to b and c

- Visual-based detection:
 - the "non-decreasing with a and d" condition should be reflected in the visualization as colours changing towards dark brown (increase of confirmation) around vertices A and D and
 - the "non-increasing with b and c" condition should be reflected in the visualization as colours changing towards dark blue (increase of disconfirmation) around vertices B and C
 - a thorough analysis with respect to property M requires an insight into the tetrahedron as potential counterexamples to this property may be located inside the shape

Does measure M(H,E) possess the property of monotonicity?



Clearly, measure M(H,E) does not satisfy property M, as in the visualization the colour changes from dark brown at vertex D to pale green at vertex A, violating the demands the of the non-decrease with a.

Does measure S(H,E) possess the property of monotonicity?



There are no observable counterexamples to property M in the external visualizations of measure S(H,E) which, together with additional analysis of the shape's inside, determines the possession of the property M by S(H,E).



Desirable property of c(H,E): weak L*

c(H,E) is maximal when E entails H and \neg E entails \neg H

c(H,E) is minimal when E entails \neg H and \neg E entails H.

Interpretation of maximality/minimality:

a measure obtains its maximum if c=b=0 and its minimum if a=d=0.

 ^{*} S.Greco, R.Słowi ski, I. Szcz ch: Properties of rule interestingness measures and alternative approaches to normalization of measures, Information Sciences 216, (2012) 1–16



Desirable property of c(H,E): weak L

c(H,E) is maximal if b=c=0 and c(H,E) is minimal if a=d=0.

- Visual-based detection:
 - the dark brown (dark blue) colour must be found on the whole AD (BC) edge of the tetrahedron

Let us observe that the AD (BC) edge contains all points for which b=c=0 (a=d=0), i.e., the points most distant from the vertices Band C (A and D)

 however, we do not demand that the dark brown (dark blue) points lie only on AD (BC) edge, and thus we do not need any insight into the tetrahedron as potential counterexamples to weak L cannot be located inside the shape

Does measure D(H,E) possess the weak L property?



Clearly, measure D(H,E) does not satisfy weak L property, since there are points on the egde AD (BC) that are not dark brown (dark blue).

Does measure F(H,E) possess the weak L property?



Visual-based detection of weak L property reveals that measure F(H,E) does satisfy this property. It is due to the fact that the points with maximal (minimal) values of F(H,E) cover the whole AD (BC) edge. No additional analysis of the inside of the shape is required.

Property of hypothesis symmetry HS

Desirable property of c(H,E): hypothesis symmetry (HS)*

 $C(H,E) = -C(\neg H,E)$

• Interpretation of (HS): $(E \rightarrow H = if x is a square, then x is rectangle)$

the strength with which

the premise (x is a square) confirms the conclusion (x is rectangle)

is the same as the strength with which

the premise disconfirms the negated conclsuion (x is not a rectangle).

- *R. Carnap: Logical Foundations of Probability, second ed. University of Chicago Press, Chicago (1962)
- E. Eells, B. Fitelson: Symmetries and asymmetries in evidential support. Philosophical Studies, 107 (2) (2002), 129-142

Pro	(Н	¬ H	esis symi		(¬H)	$\neg(\neg H) = H$	
	E	а	С			E	a'=c	c'=a
	¬ E	b	d	E→H	E→¬H	¬ E	b' = d	d'=b

Desirable property of c(H,E): hypothesis symmetry (HS)

 $C(H,E) = -C(\neg H,E)$

- Visual-based detection:
 - c(H,E)=f(a,b,c,d) = −c(¬H,E)= −f(a', b', c', d') = −f(c,d,a,b), reflecting the exchange of columns in the contingency tables (a=c', b=d', c=a' d=b')
 - two views must have the same gradient profile (i.e., the left view must be just like the right one, provided the colour map is reversed)
 - if the "recoloured" views are not the same, then the visualized measure does not possess the hypothesis symmetry
 - a thorough analysis with respect to HS requires an insight into the tetrahedron as potential counterexamples to this property may be located inside the shape

Does measure M(H,E) possess property HS?



Clearly, measure M(H,E) does not satisfy property HS since e.g., the BCD face has a gradient profile that is characterized by straight lines, while the DAB face has a profile that is characterized by curved lines.

Does measure FS(H,E) possess property HS?



There are no observable counterexamples to property HS in the external visualizations of measure FS(H,E) which, together with additional analysis of the shape's inside, determines the possession of the property by FS(H,E).

Summary

- Our proposition starts with constructing an exhaustive and nonredundant set of contingency tables, which are commonly used to calculate the values of measures
- Using such a dataset, a 3-dimensional tetrahedron is built
- The position of points in the shape translates to corresponding contingency tables and the colour of the points represents values of the visualized measure



- The visual analyses are especially useful since they allow to instantly detect and localize interesting characteristics of the measures (extreme values, zeros, etc.), which would otherwise have to be laboriously derived from the analytic definitions of the measures
- Our visualization helps to determine e.g. if the visualized measures are identical or similar in particular domain regions, or if they are ordinally equivalent



- The proposed visualization allows us to promptly detect distinct properties of the measures and compare them, increasing the general comprehension of the measures and helping the users choose one for their particular application
- Such visual-based approach is advantageous, especially when time constraints impede conducting in-depth, theoretical analyses of large numbers of such measures (e.g., generated automatically)
- Clearly, the analyses can be generalized to a wider range of measures or properties



The Quiz 😊



What does f(a,b,c,d) = a/n look like?





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f(a,b,c,d) = a/n



f(a,b,c,d) = b/n



⁺¹ NaN

72
f(a,b,c,d) = c/n



f(a,b,c,d) = d/n



What does f(a,b,c,d) = (a+b)/n look like?





75

f(a,b,c,d) = (a+b)/n



f(a,b,c,d) = (a+c)/n



f(a,b,c,d) = (a+d)/n



$f(a,b,c,d) = (a+d)/n \equiv classification accuracy$



What does f(a,b,c,d) = (b+c+d)/n look like?





f(a,b,c,d) = (b+c+d)/n



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f(a,b,c,d) = a/n



What does f(a,b,c,d) = a/(a+b+c) look like?



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f(a,b,c,d) = a/(a+b+c)





f(a,b,c,d) = a/(a+b+c) = Jaccard coefficient





What does f(a,b,c,d) = a/(a+b) look like?





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f(a,b,c,d) = a/(a+b)



f(a,b,c,d) = a/(a+b) = sensitivity, recall, true positive rate



f(a,b,c,d) = d/(c+d)



f(a,b,c,d) = d/(c+d) = specificity, true negative rate



f(a,b,c,d) = a/(a+c)



$f(a,b,c,d) = a/(a+c) \equiv precision$



The case of imbalanced data

$f(a,b,c,d) = (a+d)/n \equiv classification accuracy$ Why not useful for imbalanced data?



Let us assume that we are interested in class represented by vertex A (i.e. a in the contingency table)

- Aggregations of precision and recall:
 - arithmetic means
 - geometric means
 - harmonic means
- Aggregations of specificity and recall:
 - arithmetic means
 - geometric means
 - harmonic means

The case of imbalanced data



f(a,b,c,d) = amean(precision,recall) == (2a² + ab + ac)/(a² + ab + ac + bc)





$f(a,b,c,d) = gmean(precision,recall) = a/((a+b)(a+c))^{0.5}$





f(a,b,c,d) = hmean(precision,recall) == 2a/(2a+b+c)





f(a,b,c,d) = another-aggregation(precision,recall) == a/(a+b+c)









Thank you!