

Sorting through the Safety Data Haystack: Using Machine Learning to Identify Individual Case Safety Reports (ICSRs) in Social-Digital Media

Drug Safety

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Electronic Supplementary Material 3 Machine Learning and Pharmacovigilance statistical methods

Team 2x2 Summary Comparison Table
 (AKA “Confusion Matrix”, “Classification Matrix”, etc.)*,**

	Reference System (RS) Results			
Test System (TS) Results		Pos	Neg	Totals
	Pos	A: tp	B: fp	G: Total TS Pos
	Neg	C: fn	D: tn	H: Total TS Neg
Totals	E: Total RS Pos	F: Total RS Neg	I: Total Events	

* Cell values can be raw counts or percentage of total counts;

** Note that tp, tn, etc may or may not reflect “true” positive or negative classifications depending on whether the reference standard is considered a “gold” standard or “ground truth”. When the RS is a true “Gold” standard it is customary to use tp, tn, etc. When the RS is a “non-Gold” standard or a non-reference standard, it is customary to use the cell letters for calculations instead.

Cell Definitions:

- A** = true positive (tp)
- B** = false positive (fp)
- C** = false negative (fn)
- D** = true negative (tn)
- E** = **A** + **C** (or tp + fn)
- F** = **B** + **D** (or fp + tn)
- G** = **A** + **B** (or tp + fp)
- H** = **C** + **D** (or fn + tn)

I = Total Events = **A** + **B** + **C** + **D** (or $tp + fp + fn + tn$)

Team Classification Performance Formulas

Classification Formulas	Comment(s)
Sensitivity (S_n) = $\frac{tp}{tp+fn}$	Equivalent to Positive Percent Agreement and Recall (Rc)
Specificity (S_p) = $\frac{tn}{tn+fp}$	Equivalent to Negative Percent Agreement
Accuracy (Acc) = $\frac{tp+tn}{tp+fp+tn+fn}$	Equivalent to Overall Percent Agreement and Prob(Observed Agreement)
Error Rate (Err) = $\frac{fp+fn}{tp+fp+tn+fn}$	Equivalent to Overall % Negative Agreement and Prob(Negative Agreement)
Positive Predictive Value (PPV) = $\frac{tp}{tp+fp}$	Equivalent to Precision (Pc)
Negative Predictive Value (NPV) = $\frac{tn}{tn+fn}$	
$e(\pi) = \left\{ \frac{(2tp+fn+fp)/2}{tp+fp+tn+fn} \right\}^2 + \left\{ \frac{(2tn+fp+fn)/2}{tp+fp+tn+fn} \right\}^2$	Expected chance agreement for Gwet AC1
Gwet ACI (k_g) = $\frac{Acc-e(\pi)}{1-e(\pi)}$	Chance adjusted Inter-Rater Gwet "Kappa" agreement between the TS and RS
F-Measure (F_m) = $\frac{2*Pc*Rc}{Pc+Rc}$	The harmonic mean between recall (Rc) and precision (Pc) values