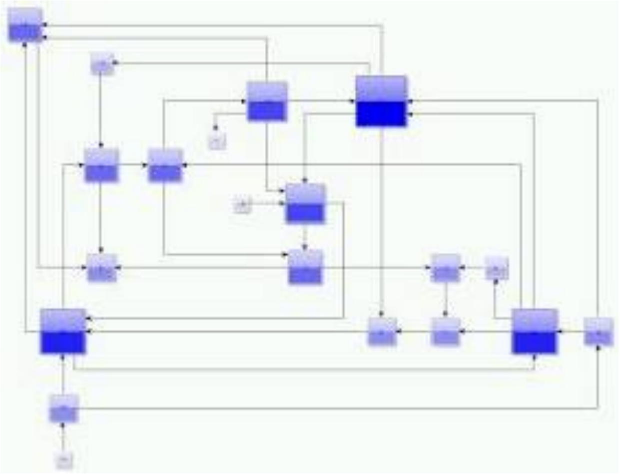
IMPROVER

systemsbiologyverification

Scoring Metrics



Prediction Format (Subject Belief Matrix)

	Class 1	…	Class *j*	…	Class q
Subject 1	s_{11}		s_{1j}		s_{1q}
Subject 2	s_{21}		s_{2j}		s_{2q}
…					
Subject *i*	s_{i1}		s_{ij}		s_{iq}
…					
Subject *N*	s_{N1}		s_{Nj}		s_{Nq}

Where s_{ij}, a number between 0 and 1, is the belief that subject *i* is in class *j* (or has phenotype *j*)

We required that for each subject the class assignments sum up to 1

$$\sum_{j=1}^{q} s_{ij} = 1$$

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True Assignments (Gold Standard Matrix)

	Class 1	…	Class *j*	…	Class q
Subject 1	t_{11}		t_{1j}		t_{1q}
Subject 2	t_{21}		t_{2j}		t_{2q}
…					
Subject *i*	t_{i1}		t_{ij}		t_{iq}
…					
Subject *N*	t_{N1}		t_{Nj}		t_{Nq}

Where $$t_{ij} = \begin{cases} 1 & \text{if subject } i \text{ is in class } j \\ 0 & \text{if subject } i \text{ is not in class } j \end{cases}$$

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Properties and definitions of the Subject Belief and GS matrices

$$T = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sum_{j=1}^{q} t_{ij} = 1$$ and

$$\sum_{i=1}^{N} t_{ij} = N_j$$

Where N_j is the number of subjects in class *j*

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Properties and definitions of the Subject Belief and GS matrices

$$T = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \qquad S = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \\ s_{41} & s_{42} & s_{43} \\ s_{51} & s_{52} & s_{53} \\ s_{61} & s_{62} & s_{63} \\ s_{71} & s_{72} & s_{73} \\ s_{81} & s_{82} & s_{83} \\ s_{91} & s_{92} & s_{93} \\ s_{10\,1} & s_{10\,2} & s_{10\,3} \\ s_{11\,1} & s_{11\,2} & s_{11\,3} \\ s_{12\,1} & s_{12\,2} & s_{12\,3} \end{pmatrix}$$

$$\sum_{\substack{i\ /\ \text{subject } i \\ \text{is in class } k}} s_{ij} \equiv v_{kj}$$

Can be interpreted as the number of subjects in class *k* believed to be in class *j*

$$\frac{1}{N_k} \sum_{\substack{i\ /\ \text{subject } i \\ \text{is in class } k}} s_{ij} \equiv b_{kj}$$

Can be interpreted the average belief that a subject in class *k* is in class *j*

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Belief Confusion Matrix

The matrix

$$b_{kj} = \frac{1}{N_k} \sum_{\substack{i \,/\, \text{subject } i \\ \text{is in class } k}} s_{ij}$$

can be interpreted as a confusion matrix. However, proper confusion matrices require a class assignment which is this case is not required.

The perfect prediction, *T* would correspond to a Belief Confusion matrix equal to the identity:

$$b_{kj}^{GldStd} = \delta_{kj}$$

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BCM: **Belief Confusion Metric**

BCM is defined as the difference between the Belief Confusion Matrix and the Perfect Confusion Matrix

$$\varepsilon_2 = \sum_{i=1}^{N} \sum_{j=1}^{q} | b_{ij} - \delta_{ij} |$$

$$= \sum_{k=1}^{q} \left\{ (1 - b_{kk}) + \sum_{j \neq k} b_{kj} \right\}$$

$$= \sum_{q=1}^{q} \{ (1 - b_{kk}) + (1 - b_{kk}) \}$$

$$= 2 \left[(1 - \frac{\nu_{11}}{N_1}) + (1 - \frac{\nu_{22}}{N_2}) + \ldots + (1 - \frac{\nu_{qq}}{N_q}) \right]$$

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Scoring Metrics AUPR

Use each column of the Subject Belief Matrix as the basis for ranking for PR curves

$$S = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \\ s_{41} & s_{42} & s_{43} \\ s_{51} & s_{52} & s_{53} \\ s_{61} & s_{62} & s_{63} \\ s_{71} & s_{72} & s_{73} \\ s_{81} & s_{82} & s_{83} \\ s_{91} & s_{92} & s_{93} \\ s_{10\,1} & s_{10\,2} & s_{10\,3} \\ s_{11\,1} & s_{11\,2} & s_{11\,3} \\ s_{12\,1} & s_{12\,2} & s_{12\,3} \end{pmatrix}$$

Order each column independently and compute AUPR

For each column *j*, compute AUPR(*j*)

Obtain the final metrics by averaging all the AUPRs (one per column)

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CCEM: Correct Class Enrichment Metric

Estimate the enrichment of the correctly assigned classes.

Compute the score as

$$CCEM = \sum_{\substack{i \text{ / subject i} \\ \text{was correctly} \\ \text{classified}}} s_{i\,a(i)} - \sum_{\substack{i \text{ / subject i} \\ \text{was incorrectly} \\ \text{classified}}} s_{i\,a(i)}$$

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Normalization to metrics

For ease of comparison we modified

- BCM_{nor} = 1 – *BCM*/q, where q is number of classes.
- $CCEM_{nor}$ = (*CCEM*/N + 1)/2, where N is number of subjects.

With these modifications all metrics range from [0,1], 1 being the perfect score.

BCM and CCEM used in the tables are the normalized ones.