## APPENDIX

We define here two measures. Let  $O \triangleq {\{\tilde{o}_j\}}_{j=1}^n$  be a set of objects, and let P and  $\dot{P}$  be two soft clusterings. Let  $\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$  be the number of clusters shared by objects  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$  in clustering P, and let  $\alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$  be similarly defined. The extended bcubed (EBC) measure [33] is based on extended bcubed precision and extended bcubed recall:

$$\mathsf{EBCP}(P, \dot{P}) \triangleq \frac{1}{n} \sum_{j_1=1}^{n} \frac{\sum_{j_2=1}^{n} \min\{\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2}), \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})\}}{\sum_{j_2=1}^{n} \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})}$$
(14a)

$$\text{EBCR}(P, \dot{P}) \triangleq \frac{1}{n} \sum_{j_1=1}^{n} \frac{\sum_{j_2=1}^{n} \min\{\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2}), \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})\}}{\sum_{j_2=1}^{n} \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})}.$$
(14b)

EBC is defined by default as

$$\operatorname{EBC}(P, \dot{P}) \triangleq 2 \cdot \frac{\operatorname{EBCP}(P, \dot{P}) \cdot \operatorname{EBCR}(P, \dot{P})}{\operatorname{EBCP}(P, \dot{P}) + \operatorname{EBCR}(P, \dot{P})}.$$
 (15)

The other measure is defined as follows. Let  $\beta_P(\tilde{o}_j)$  be the number of clusters to which object  $\tilde{o}_j$  belongs in P minus 1, and let  $\beta_{\dot{P}}(\tilde{o}_j)$  be similarly defined. The agreements and disagreements associated with a pair  $(j_1, j_2)$  are

$$a_{G}^{P,\dot{P}}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}}) = \min\left\{\alpha_{P}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}}),\alpha_{\dot{P}}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}})\right\} + \sum_{i=1}^{2}\min\left\{\beta_{P}(\tilde{o}_{j_{i}}),\beta_{\dot{P}}(\tilde{o}_{j_{i}})\right\}$$
(16)

and

$$d_{G}^{P,P}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}}) = |\alpha_{P}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}}) - \alpha_{\dot{P}}(\tilde{o}_{j_{1}},\tilde{o}_{j_{2}})| + \sum_{i=1}^{2} |\beta_{P}(\tilde{o}_{j_{i}}) - \beta_{\dot{P}}(\tilde{o}_{j_{i}})|, \qquad (17)$$

respectively. Summing up  $a_G^{P,\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$  and  $d_G^{P,\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$  over all ordered pairs  $(\tilde{o}_{j_1},\tilde{o}_{j_2})$   $(j_1 < j_2)$  results in the following overall measures of agreements  $(a_G^{P,\dot{P}})$  and disagreements  $(d_G^{P,\dot{P}})$  between P and  $\dot{P}$ :

$$a_G^{P,\dot{P}} = \sum_{j_1=1}^{n-1} \sum_{j_2=j_1+1}^n a_G^{P,\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) \text{ and } (18)$$

$$d_G^{P,\dot{P}} = \sum_{j_1=1}^{n-1} \sum_{j_2=j_1+1}^n d_G^{P,\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$$
(19)

The Campello soft index (CSI) [36] is defined by

$$\operatorname{CSI}(P, \dot{P}) \triangleq \frac{a_G^{P, \dot{P}}}{a_G^{P, \dot{P}} + d_G^{P, \dot{P}}}.$$
(20)

We hereafter assume that P,  $\dot{P}$ , and  $\hat{P}$  are the soft clustering representations of B,  $\dot{B}$ , and  $\hat{B}$ , respectively.

**Proposition 1.** There are non-equivalent biclusterings B and  $\dot{B}$  such that  $P \equiv \dot{P}$ .

*Proof:* Let *B* be a biclustering such that some of the matrix entries are not biclustered, and let  $\dot{B}$  be the biclustering *B* with a new bicluster added that has only one entry from the matrix entries not biclustered in *B*. This new bicluster is transformed into a singleton for  $\dot{P}$  by Eq. 12, whereas Eq. 13 creates an equivalent singleton for *P*. In other words, the bicluster added in *B* to produce  $\dot{B}$  is superfluous from the point of view of our transformation.

**Proposition 2.** If *B* and  $\dot{B}$  are non-equivalent nondegenerate biclusterings, then  $P \neq \dot{P}$ .

*Proof:* Let k and q be the number of biclusters in B and  $\dot{B}$ , respectively. Suppose that  $P \triangleq \{P_i\}_{i=1}^{\overline{k}} \equiv \dot{P} \triangleq \{\dot{P}_i\}_{i=1}^{\overline{q}}$ . Thus,  $\overline{k} = \overline{q}$  and there is a bijection  $\dot{P} \triangleq \{\dot{P}_i\}_{i=1}^{\overline{q}}$ . Such that  $P_{t_i} \equiv \dot{P}_{y_i}$  for all i. Without loss of generality, suppose that  $P_{t_1}, P_{t_2}, \ldots, P_{t_{\underline{k}}}$  (respectively,  $\dot{P}_{y_1}, \dot{P}_{y_2}, \ldots, \dot{P}_{y_{\underline{q}}}$ ) are the non singletons. Clearly,  $\underline{k} =$  g = k = q. The bijection  $\{(t_i, y_i)\}_{i=1}^{\underline{k}}$  implies that there is a corresponding bijection between B and  $\dot{B}$  making  $B \equiv \dot{B}$ , which contradicts the assumption that  $B \neq \dot{B}$ .

We will adopt the following notation in several proofs. Let  $C_1$  and  $C_2$  be two sets of objects from  $O = {\tilde{o}_j}_{j=1}^n$ , and let  $f(\cdot, \cdot)$  be a function on  $O \times O$ . When proving some property of the  $\mathbb{S}_{csi}$  measure,  $f(C_1, C_2) = x$  means  $f(\tilde{o}_{j_1}, \tilde{o}_{j_2}) = x$  for all  $\tilde{o}_{j_1} \in C_1$  and  $\tilde{o}_{j_2} \in C_2$  such that  $j_1 \neq j_2$ . When proving some property of the  $\mathbb{S}_{ebc}$  measure,  $f(C_1, C_2) = x$  means  $f(\tilde{o}_{j_1}, \tilde{o}_{j_2}) = x$  for all  $\tilde{o}_{j_1} \in C_1$  and  $\tilde{o}_{j_2} \in C_2$ . In both cases, for a function  $f(\cdot)$ ,  $f(C_1) = x$ means  $f(\tilde{o}_j) = x$  for all  $\tilde{o}_j \in C_1$ .

**Proposition 3.** The  $\mathbb{S}_{csi}$  measure is sensitive to the size of spurious biclusters (Def. 1).

*Proof:* Let B,  $\hat{B}$ , and  $\hat{B}$  be biclusterings, as in Def. 1, and remember that O is the set of objects. Let  $\{P_{t_i}\}_{i=1}^x$ be the set of soft clusters corresponding to the spurious biclusters  $\{B_{t_i}\}_{i=1}^x$  in B, and similarly define  $\{\hat{P}_{t_i}\}_{i=1}^x$ for  $\hat{B}$ . Define  $C_s^1 \triangleq \bigcup_{i=1}^x P_{t_i}$  and  $C_s^2 \triangleq \bigcup_{i=1}^x \hat{P}_{t_i}$ . Note that  $C_s^1 \subset C_s^2$ . We know that

$$\begin{aligned} \alpha_{\dot{P}}(C_{\rm s}^2,O) &= \beta_{\dot{P}}(C_{\rm s}^2) = 0, \\ \alpha_P(O,O-C_{\rm s}^2) &= \alpha_{\hat{P}}(O,O-C_{\rm s}^2), \\ \beta_P(O-C_{\rm s}^2) &= \beta_{\hat{P}}(O-C_{\rm s}^2), \\ \alpha_P(C_{\rm s}^2,C_{\rm s}^2) &\leq \alpha_{\hat{P}}(C_{\rm s}^2,C_{\rm s}^2), \text{ and } \\ \beta_P(C_{\rm s}^2) &\leq \beta_{\hat{P}}(C_{\rm s}^2). \end{aligned}$$

Thus,

$$a_G^{P,\dot{P}}(C_s^2, O - C_s^2) = \min\{\beta_P(O - C_s^2), \beta_{\dot{P}}(O - C_s^2)\}\$$
  
= min{ $\beta_{\dot{P}}(O - C_s^2), \beta_{\dot{P}}(O - C_s^2)$ }  
=  $a_G^{\dot{P},\dot{P}}(C_s^2, O - C_s^2),$ 

$$\begin{split} a_G^{P,\dot{P}}(C_{\rm s}^2,C_{\rm s}^2) &= 0 = a_G^{\hat{P},\dot{P}}(C_{\rm s}^2,C_{\rm s}^2), \text{ and } \\ a_G^{P,\dot{P}}(O-C_{\rm s}^2,O-C_{\rm s}^2) &= a_G^{\hat{P},\dot{P}}(O-C_{\rm s}^2,O-C_{\rm s}^2). \end{split}$$

Thus,  $a_G^{P,\dot{P}}(O,O) = a_G^{\hat{P},\dot{P}}(O,O)$ . Observe that

$$\begin{split} d_{G}^{P,\dot{P}}(C_{\rm s}^{2},O-C_{\rm s}^{2}) &= \alpha_{P}(C_{\rm s}^{2},O-C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) \\ &+ |\beta_{P}(O-C_{\rm s}^{2}) - \beta_{\dot{P}}(O-C_{\rm s}^{2})| \\ &= \alpha_{\hat{P}}(C_{\rm s}^{2},O-C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) \\ &+ |\beta_{\hat{P}}(O-C_{\rm s}^{2}) - \beta_{\dot{P}}(O-C_{\rm s}^{2})| \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},O-C_{\rm s}^{2}) + \beta_{\dot{P}}(C_{\rm s}^{2}) \\ &+ |\beta_{\hat{P}}(O-C_{\rm s}^{2}) - \beta_{\dot{P}}(O-C_{\rm s}^{2})| \\ &= d_{G}^{\hat{P},\dot{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) - \beta_{\dot{P}}(O-C_{\rm s}^{2})| \\ &= d_{G}^{\hat{P},\dot{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) + \beta_{P}(C_{\rm s}^{2}) \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) \\ &\leq \alpha_{\hat{P}}(C_{\rm s}^{2},C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) + \beta_{\hat{P}}(C_{\rm s}^{2}) \\ &= d_{G}^{\hat{P},\dot{P}}(O-C_{\rm s}^{2},O-C_{\rm s}^{2}) = d_{G}^{\hat{P},\dot{P}}(O-C_{\rm s}^{2},O-C_{\rm s}^{2}). \end{split}$$

Thus,  $d_G^{P,\dot{P}}(O,O) \le d_G^{\dot{P},\dot{P}}(O,O).$ 

Let  $P_t$  be the soft cluster corresponding to a spurious bicluster  $B_t$  that was increased, giving rise to  $\hat{B}_t$  and  $\hat{P}_t$ . Let  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$  be two objects from  $\hat{P}_t$  such that  $\tilde{o}_{j_1} \in P_t$  and  $\tilde{o}_{j_2} \notin P_t$ . Thus,  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ ,  $d_G^{P,\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) < d_G^{\dot{P},\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$  (Eq. (21)), and  $\text{CSI}(P, \dot{P}) >$  $\text{CSI}(\hat{P}, \dot{P})$ .

**Proposition 4.** The  $\mathbb{S}_{ebc}$  measure is sensitive to the size of spurious biclusters (Def. 1).

 $\square$ 

*Proof:* Let B, B, and B be biclusterings, as in Def. 1, and remember that O is the set of objects. Let  $C_s^1$  and  $C_s^2$  be the sets defined in the proof of Proposition 3. Note that

$$\alpha_{P}(C_{s}^{2}, C_{s}^{2}) \geq \alpha_{\dot{P}}(C_{s}^{2}, C_{s}^{2}),$$
  

$$\alpha_{\hat{P}}(C_{s}^{2}, C_{s}^{2}) \geq \alpha_{\dot{P}}(C_{s}^{2}, C_{s}^{2}), \text{ and }$$
  

$$\alpha_{P}(O, O - C_{s}^{2}) = \alpha_{\dot{P}}(O, O - C_{s}^{2}).$$

The nominators of Eqs. (14) are equal if one compares Pwith  $\dot{P}$  or  $\hat{P}$  with  $\dot{P}$ . Thus,  $\text{EBCR}(P, \dot{P}) = \text{EBCR}(\hat{P}, \dot{P})$ .  $\text{EBCP}(P, \dot{P}) \geq \text{EBCP}(\hat{P}, \dot{P})$  because  $\alpha_{\hat{P}}(O, O) \geq \alpha_{P}(O, O)$ .

Let  $P_t$  be the soft cluster corresponding to a spurious bicluster  $B_t$  that was increased, giving rise to  $\hat{B}_t$  and  $\hat{P}_t$ . Let  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$  be two objects from  $\hat{P}_t$  such that  $\tilde{o}_{j_1} \in P_t$  and  $\tilde{o}_{j_2} \notin P_t$ . Thus,  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ , EBCP $(P, \dot{P}) > \text{EBCP}(\hat{P}, \dot{P})$ , and EBC $(P, \dot{P}) > \text{EBC}(\hat{P}, \dot{P})$ .

**Proposition 5.** The  $S_{rnia}$  and  $S_{ce}$  measures penalize solutions that do not cover all reference biclusters (Def. 2).

*Proof:* Let *B* and *B* be as given in Def. 2. We have  $\dot{N}_{j_1,j_2} \ge N_{j_1,j_2}$  for all  $j_1$  and  $j_2$ , and there are  $j_1$  and  $j_2$  such that  $N_{j_1,j_2} > N_{j_1,j_2}$  (Eqs. (3) and (4)). Thus, |U| > |I|,

and  $\mathbb{S}_{\text{rnia}}$  follows the property given by Def. 2. We also have  $\mathbb{S}_{\text{rnia}}(B, \dot{B}) \geq \mathbb{S}_{\text{ce}}(B, \dot{B})$  by Proposition 1 in [30]. Thus,  $\mathbb{S}_{\text{ce}}$  also has the property.

**Proposition 6.** The  $\mathbb{S}_{prec}$ ,  $\mathbb{S}_{u}$ , and  $\mathbb{S}_{erec}$  measures do not always penalize solutions that do not cover all reference biclusters (Def. 2).

*Proof:* Let *B* and *B* be as given in Def. 2, where  $B \triangleq \{B_1\}$  and  $\dot{B} \triangleq \{\dot{B}_1, \dot{B}_2\}$  such that  $B_1 \equiv \dot{B}_1 \equiv \dot{B}_2$ . We would have  $\mathbb{S}_{\text{prec}}(B, \dot{B}) = \mathbb{S}_{u}(B, \dot{B}) = \mathbb{S}_{\text{erec}}(B, \dot{B}) = 1$ , violating the condition given by Def. 2.

**Proposition 7.** The  $\mathbb{S}_{csi}$  measure penalizes solutions that do not cover all reference biclusters (Def. 2).

*Proof:* Let *B* and *B* be as given in Def. 2. We have  $\alpha_P(j_1, j_2) \leq \alpha_{\dot{P}}(j_1, j_2)$  for all  $j_1 \neq j_2$ , and the inequality is attained for at least one pair  $(j_1, j_2)$ . Thus,  $d_G^{P, \dot{P}} > 0$  and  $\text{CSI}(P, \dot{P}) < 1$ .

**Proposition 8.** The  $\mathbb{S}_{ebc}$  measure penalizes solutions that do not cover all reference biclusters (Def. 2).

*Proof:* Let *B* and *B* be as given in Def. 2. We have  $\alpha_P(j_1, j_2) \leq \alpha_{\dot{P}}(j_1, j_2)$  for all  $j_1$  and  $j_2$ . The inequality is attained for at least one pair  $(j_1, j_2)$ , implying that  $\text{EBCR}(P, \dot{P}) < 1$  and  $\text{EBC}(P, \dot{P}) < 1$ .

**Proposition 9.** The  $\mathbb{S}_{rnia}$  measure penalizes solutions for non-intersecting area (Def. 3).

*Proof:* Let *B*, *B*, and *B* be three biclusterings, as in Def. 3, and let *S* be the set of matrix elements, as in Def. 3. The matrix elements in *S* are those corresponding to  $j_1$  and  $j_2$  such that  $\dot{N}_{j_1,j_2} = 0$ . We have  $N_{j_1,j_2} = \hat{N}_{j_1,j_2}$  for all  $j_1$  and  $j_2$  such that  $\dot{N}_{j_1,j_2} > 0$ . Thus,  $\min\{N_{j_1,j_2}, \dot{N}_{j_1,j_2}\} = \min\{\hat{N}_{j_1,j_2}, \dot{N}_{j_1,j_2}\}$  for all  $j_1$ and  $j_2$ . Since  $N_{j_1,j_2} \le \hat{N}_{j_1,j_2}$  for all  $j_1$  and  $j_2$ , we have  $\max\{N_{j_1,j_2}, \dot{N}_{j_1,j_2}\} \le \max\{\hat{N}_{j_1,j_2}, \dot{N}_{j_1,j_2}\}$  for all  $j_1$  and  $j_2$ . Therefore,  $S_{rnia}(B, \dot{B}) \ge S_{rnia}(\dot{B}, \dot{B})$ . Since  $N_{j_1,j_2} < \hat{N}_{j_1,j_2}$ for at least a pair  $(j_1, j_2)$  such that  $\dot{N}_{j_1,j_2} = 0$ , we have  $\max\{N_{j_1,j_2}, \dot{N}_{j_1,j_2}\} < \max\{\hat{N}_{j_1,j_2}, \dot{N}_{j_1,j_2}\}$  for such a pair and  $S_{rnia}(B, B) > S_{rnia}(\dot{B}, \dot{B})$ . □

**Proposition 10.** The  $\mathbb{S}_{ce}$  measure penalizes solutions for nonintersecting area (Def. 3).

*Proof:* Let B,  $\dot{B}$ , and  $\hat{B}$  be three biclusterings, as in Def. 3. We know from the proof of Proposition 9 that |U| increases from comparing B with  $\dot{B}$  to comparing  $\hat{B}$  with  $\dot{B}$ . On the other hand,  $d_{\max}$  (Eq. 6) does not change from comparing B with  $\dot{B}$  to comparing  $\hat{B}$  with  $\dot{B}$ . Thus,  $\mathbb{S}_{ce}(B, \dot{B}) > \mathbb{S}_{ce}(\hat{B}, \dot{B})$ .

**Proposition 11.** The  $\mathbb{S}_{wjac}$  and  $\mathbb{S}_{wdic}$  measures do not always penalize solutions for non-intersecting area (Def. 3).

*Proof:* Consider a data matrix  $A \in \mathbb{R}^{4\cdot 4}$ . Let  $B \triangleq \{B_1, B_2\}$ ,  $B_1 \triangleq (\{2, 3, 4\}, \{1, 2\})$ ,  $B_2 \triangleq (\{2, 3, 4\}, \{3\})$ ,  $\dot{B} \triangleq \{\dot{B}_1\}$ ,  $\dot{B}_1 \triangleq (\{2, 3, 4\}, \{3, 4\})$ ,  $\dot{B} \triangleq \{\dot{B}_1, \dot{B}_2\}$ ,  $\dot{B}_1 \triangleq (\{2, 3, 4\}, \{3, 4\})$ ,  $\dot{B} \triangleq \{\dot{B}_1, \dot{B}_2\}$ ,  $\dot{B}_1 \triangleq (\{2, 3, 4\}, \{1, 2\})$ , and  $\dot{B}_2 \triangleq (\{1, 2, 3, 4\}, \{3\})$ . Note that B,  $\dot{B}$ , and  $\hat{B}$  follow the biclustering definitions given in Def.

3. However,  $\mathbb{S}_{wjac}(B, \dot{B}) = 0.167 < 0.171 = \mathbb{S}_{wjac}(\hat{B}, \dot{B})$ and  $\mathbb{S}_{wdic}(B, \dot{B}) = 0.22 < 0.24 = \mathbb{S}_{wdic}(\hat{B}, \dot{B}).$ 

**Proposition 12.** Let B,  $\dot{B}$ , and  $\hat{B}$  be three biclusterings, as in Def. 3. We have  $\mathbb{S}_{csi}(B, \dot{B}) \ge \mathbb{S}_{csi}(\hat{B}, \dot{B})$ .

*Proof:* Let *S* be the set of matrix elements, as in Def. 3. Define *C* as the set of elements from *O* corresponding to the matrix elements in *S*, and let  $\overline{C} \triangleq O - C$ . We have

$$\begin{split} &\alpha_{P}(\overline{C},\overline{C}) = \alpha_{\hat{P}}(\overline{C},\overline{C}), \\ &\alpha_{P}(C,\overline{C}) \leq \alpha_{\hat{P}}(C,\overline{C}), \\ &\alpha_{P}(C,C) \leq \alpha_{\hat{P}}(C,C), \\ &\alpha_{\hat{P}}(C,\overline{C}) = \alpha_{\hat{P}}(C,C) = 0, \\ &\beta_{P}(\overline{C}) = \beta_{\hat{P}}(\overline{C}), \\ &\beta_{P}(C) \leq \beta_{\hat{P}}(C), \text{ and} \\ &\beta_{\hat{P}}(C) = 0. \end{split}$$

Thus,  $a_G^{P,\dot{P}}(\overline{C},\overline{C}) = a_G^{\hat{P},\dot{P}}(\overline{C},\overline{C})$  and  $d_G^{P,\dot{P}}(\overline{C},\overline{C}) = d_G^{\hat{P},\dot{P}}(\overline{C},\overline{C})$ . We have

$$a_{G}^{P,P}(C,\overline{C}) = \min\{\beta_{P}(\overline{C}), \beta_{\dot{P}}(\overline{C})\} = \min\{\beta_{\hat{P}}(\overline{C}), \beta_{\dot{P}}(\overline{C})\} = a_{G}^{\hat{P},\dot{P}}(C,\overline{C})$$

and

$$d_{G}^{P,P}(C,\overline{C}) = \alpha_{P}(C,\overline{C}) + \beta_{P}(C) + |\beta_{P}(\overline{C}) - \beta_{\dot{P}}(\overline{C})|$$
  
$$= \alpha_{P}(C,\overline{C}) + \beta_{P}(C) + |\beta_{\dot{P}}(\overline{C}) - \beta_{\dot{P}}(\overline{C})|$$
  
$$\leq \alpha_{\dot{P}}(C,\overline{C}) + \beta_{\dot{P}}(C) + |\beta_{\dot{P}}(\overline{C}) - \beta_{\dot{P}}(\overline{C})|$$
  
(22)

$$= d_{C}^{P,P}(C,\overline{C})$$

Note that

$$a_G^{P,\dot{P}}(C,C) = 0 = a_G^{\hat{P},\dot{P}}(C,C)$$

and

$$d_G^{P,\tilde{P}}(C,C) = \alpha_P(C,C) + 2\beta_P(C)$$
  

$$\leq \alpha_{\hat{P}}(C,C) + 2\beta_{\hat{P}}(C)$$

$$= d_G^{\hat{P},\hat{P}}(C,C).$$
(23)

 $\begin{array}{l} \text{Thus, } a_G^{P, \dot{P}} = a_G^{\dot{P}, \dot{P}}, \, d_G^{P, \dot{P}} \leq d_G^{\dot{P}, \dot{P}}, \, \text{CSI}(P, \dot{P}) \geq \text{CSI}(\dot{P}, \dot{P}), \\ \text{and } \mathbb{S}_{\text{csi}}(B, \dot{B}) \geq \mathbb{S}_{\text{csi}}(\dot{B}, \dot{B}). \end{array} \end{array}$ 

**Proposition 13.** The  $\mathbb{S}_{csi}$  measure penalizes solutions for non-intersecting area (Def. 3) in the domain of non-degenerate biclusterings.

*Proof:* Let *B*, *B*, and *B* be three biclusterings, as in Def. 3, with the additional restriction of being nondegenerates. Let *S* be the set of matrix elements, as in Def. 3. Define *C* as the set of elements from *O* corresponding to the matrix elements in *S*. If there are biclusters in  $\hat{B}$  originated from the expansion of biclusters in *B*, there is an object  $\tilde{o}_j \in C$  that belongs to more clusters in  $\hat{P}$  than in *P*, meaning that  $\beta_{\hat{P}}(\tilde{o}_j) > \beta_P(\tilde{o}_j)$ . If there are new biclusters in  $\hat{B}_i$  let  $\hat{B}_i$  be one of these. There is a pair  $\tilde{o}_{j_1}, \tilde{o}_{j_2} \in C$   $(j_1 \neq j_2)$  that belongs to more clusters in  $\hat{P}$  than in P, meaning that  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ . In the first case,  $d_G^{\hat{P}, \dot{P}} > d_G^{P, \dot{P}}$  because of Ineq. (22). In the second case,  $d_G^{\hat{P}, \dot{P}} > d_G^{P, \dot{P}}$  because of Ineq. (23). Therefore,  $\mathrm{CSI}(P, \dot{P}) > \mathrm{CSI}(\hat{P}, \dot{P})$  and  $\mathbb{S}_{\mathrm{csi}}(B, \dot{B}) > \mathbb{S}_{\mathrm{csi}}(\hat{B}, \dot{B})$ .  $\Box$ 

**Proposition 14.** Let B,  $\dot{B}$ , and  $\ddot{B}$  be three biclusterings, as in Def. 3. We have  $\mathbb{S}_{ebc}(B, \dot{B}) \ge \mathbb{S}_{ebc}(\dot{B}, \dot{B})$ .

*Proof:* Let *S* be the set of matrix elements, as in Def. 3. Define *C* as the set of elements from *O* corresponding to the matrix elements in *S*, and let  $\overline{C} \triangleq O - C$ . We have  $\alpha_P(\overline{C}, \overline{C}) = \alpha_{\hat{P}}(\overline{C}, \overline{C}), \ \alpha_{\hat{P}}(C, \overline{C}) = 0, \ \alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) = 0$  for all  $\tilde{o}_{j_1}, \tilde{o}_{j_2} \in C$  s.t.  $j_1 \neq j_2, \ \alpha_P(\tilde{o}_j, \tilde{o}_j) \ge \alpha_{\hat{P}}(\tilde{o}_j, \tilde{o}_j)$  for all  $\tilde{o}_j \in C$ , and  $\alpha_{\hat{P}}(\tilde{o}_j, \tilde{o}_j) \ge \alpha_{\hat{P}}(\tilde{o}_j, \tilde{o}_j)$  for all  $\tilde{o}_j \in C$ . Thus,  $\min\{\alpha_P(O, O), \alpha_{\hat{P}}(O, O)\} = \min\{\alpha_{\hat{P}}(O, O), \alpha_{\hat{P}}(O, O)\}$ . Since

$$\alpha_{\hat{P}}(C,\overline{C}) \ge \alpha_P(C,\overline{C}) \text{ and}$$
 (24)

$$\alpha_{\hat{P}}(C,C) \ge \alpha_P(C,C),\tag{25}$$

we have  $\text{EBC}(P, \dot{P}) \geq \text{EBC}(\hat{P}, \dot{P})$  and  $\mathbb{S}_{\text{ebc}}(B, \dot{B}) \geq \mathbb{S}_{\text{ebc}}(\hat{B}, \dot{B})$ .

**Proposition 15.** The  $\mathbb{S}_{ebc}$  measure penalizes solutions for non-intersecting area (Def. 3) in the domain of non-degenerate biclusterings.

*Proof:* Let *B*, *B*, and *B* be three biclusterings, as in Def. 3, with the additional restriction of being nondegenerate. Let S be the set of matrix elements, as in Def. 3. Define C as the set of elements from Ocorresponding to the matrix elements in  $S_{i}$  and let  $\overline{C} \triangleq O - C$ . If there are biclusters in  $\hat{B}$  originated from the expansion of biclusters in B, there is a pair  $\tilde{o}_{j_1}, \tilde{o}_{j_2} \in C$  s.t.  $j_1 \neq j_2$  or a pair  $\tilde{o}_{j_1} \in C, \tilde{o}_{j_2} \in \overline{C}$  that belongs to more clusters in  $\hat{P}$  than in P, meaning that  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ . If there are new biclusters in  $\hat{B}_i$ , let  $\hat{B}_i$  be one of these. There is a pair  $\tilde{o}_{j_1}, \tilde{o}_{j_2} \in C$ s.t.  $j_1 \neq j_2$  that belongs to more clusters in P than in *P*, meaning that  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ . In both cases, we can conclude from Ineqs. (24) and (25) that  $\operatorname{EBC}(P, \dot{P}) > \operatorname{EBC}(\dot{P}, \dot{P}) \text{ and } \mathbb{S}_{\operatorname{ebc}}(B, \dot{B}) > \mathbb{S}_{\operatorname{ebc}}(\dot{B}, \dot{B}).$  $\square$ 

**Proposition 16.** The  $\mathbb{S}_{csi}$  measure penalizes solutions for multiple biclusters coverage (Def. 4).

*Proof:* Let *B* and *B* be two biclusterings, as in Def. 4. We have  $\alpha_P(O, O) \ge \alpha_{\dot{P}}(O, O)$  and  $\beta_P(O) = \beta_{\dot{P}}(O) = 0$ . There are  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$  s.t.  $j_1 \ne j_2$  such that  $\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ , implying that  $d_G^{P, \dot{P}} > 0$ ,  $\text{CSI}(P, \dot{P}) < 1$ , and  $\mathbb{S}_{\text{csi}}(B, \dot{B}) < 1$ .

**Proposition 17.** The  $\mathbb{S}_{ebc}$  measure penalizes solutions for multiple biclusters coverage (Def. 4).

*Proof:* Let *B* and *B* be two biclusterings, as in Def. 4. Note that  $\alpha_P(O, O) \ge \alpha_{\dot{P}}(O, O)$ . There are  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$ s.t.  $j_1 \ne j_2$  such that  $\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ , implying that EBCP $(P, \dot{P}) < 1$ , EBC $(P, \dot{P}) < 1$ , and  $\mathbb{S}_{ebc}(B, \dot{B}) < 0$  1.

**Proposition 18.** The  $\mathbb{S}_{prel}$ ,  $\mathbb{S}_{prec}$ , and  $\mathbb{S}_{l\&w}$  measures penalize solutions for multiple biclusters coverage (Def. 4).

*Proof:* Let *B* and *B* be two biclusterings, as in Def. 4. Since the biclusters in *B* do not overlap, we have the proper subset relationships  $\dot{B}_i^r \subset B_1^r$  for all *i* or  $\dot{B}_i^c \subset B_1^c$  for all *i*. Thus,  $|B_1^r \cup \dot{B}_i^r| > |B_1^r \cap \dot{B}_i^r|$  for all *i* or  $|B_1^c \cup \dot{B}_i^c| > |B_1^c \cap \dot{B}_i^c|$  for all *i*. We have  $S_r(B,\dot{B}) < 1$  or  $S_c(B,\dot{B}) < 1$  (Eqs. (1) and (2)), implying that  $\mathbb{S}_{\text{prec}}(B,\dot{B}) < 1$ .  $\Box$ 

**Proposition 19.** The  $S_{stm}$ ,  $S_{wjac}$ ,  $S_{wdic}$ ,  $S_{ay}$ ,  $S_{erel}$ , and  $S_{erec}$  measures penalize solutions for multiple biclusters coverage (Def. 4).

*Proof:* Let *B* and *B* be two biclusterings, as in Def. 4. Since the biclusters in *B* do not overlap, we have the proper subset relationship  $\dot{B}_i^{\rm r} \times \dot{B}_i^{\rm c} \subset B_1^{\rm r} \times B_1^{\rm c}$  for all *i*. Thus,  $\mathbb{D}(B_1, \dot{B}_i) < 1$  and  $\mathbb{J}(B_1, \dot{B}_i) < 1$  for all *i*, implying that  $\mathbb{S}_{\rm stm}(B, \dot{B}) < 1$ ,  $\mathbb{S}_{\rm wjac}(B, \dot{B}) < 1$ ,  $\mathbb{S}_{\rm wdic}(B, \dot{B}) < 1$ ,  $\mathbb{S}_{\rm erel}(B, \dot{B}) < 1$ , and  $\mathbb{S}_{\rm erec}(B, \dot{B}) < 1$ . From  $\mathbb{S}_{\rm ay}(B, \dot{B}) < \mathbb{S}_{\rm erel}(B, \dot{B})$ , we also have  $\mathbb{S}_{\rm ay}(B, \dot{B}) < 1$ . □

**Proposition 20.** The  $S_{csi}$  measure penalizes solutions with repetitive biclusters (Def. 5).

*Proof:* Let B,  $\dot{B}$ , and  $\dot{B}$  be biclusterings, as in Def. 5. Let  $C_r$  be the set of objects from O corresponding to the matrix entries of the biclusters in B that were replicated. We have

$$\alpha_P(O, O - C_r) = \alpha_{\hat{P}}(O, O - C_r),$$
 (26)

$$\alpha_{\hat{P}}(C_{\mathrm{r}}, C_{\mathrm{r}}) > \alpha_{P}(C_{\mathrm{r}}, C_{\mathrm{r}}) \ge \alpha_{\hat{P}}(C_{\mathrm{r}}, C_{\mathrm{r}}), \qquad (27)$$

$$\beta_P(O - C_{\mathbf{r}}) = \beta_{\hat{P}}(O - C_{\mathbf{r}}), \text{ and} \beta_{\hat{P}}(C_{\mathbf{r}}) > \beta_P(C_{\mathbf{r}}) \ge \beta_{\hat{P}}(C_{\mathbf{r}}).$$

We conclude that  $a_G^{P,\dot{P}}(O,O) = a_G^{\hat{P},\dot{P}}(O,O)$  and  $a_G^{P,\dot{P}} = a_G^{\hat{P},\dot{P}}$ .

We have

$$\begin{split} d_{G}^{P,\dot{P}}(O,O-C_{\rm r}) &= |\alpha_{P}(O,O-C_{\rm r}) - \alpha_{\dot{P}}(O,O-C_{\rm r})| \\ &+ |\beta_{P}(O) - \beta_{\dot{P}}(O)| \\ &+ |\beta_{P}(O-C_{\rm r}) - \beta_{\dot{P}}(O-C_{\rm r})| \\ &= |\alpha_{\dot{P}}(O,O-C_{\rm r}) - \alpha_{\dot{P}}(O,O-C_{\rm r})| \\ &+ |\beta_{P}(O) - \beta_{\dot{P}}(O)| \\ &+ |\beta_{\dot{P}}(O-C_{\rm r}) - \beta_{\dot{P}}(O-C_{\rm r})| \\ &\leq d_{G}^{\hat{P},\dot{P}}(O,O-C_{\rm r}) \end{split}$$

and

$$\begin{aligned} d_G^{P,\dot{P}}(C_{\mathbf{r}},C_{\mathbf{r}}) &= |\alpha_P(C_{\mathbf{r}},C_{\mathbf{r}}) - \alpha_{\dot{P}}(C_{\mathbf{r}},C_{\mathbf{r}})| \\ &+ 2|\beta_P(C_{\mathbf{r}}) - \beta_{\dot{P}}(C_{\mathbf{r}})| \\ &< |\alpha_{\hat{P}}(C_{\mathbf{r}},C_{\mathbf{r}}) - \alpha_{\dot{P}}(C_{\mathbf{r}},C_{\mathbf{r}})| \\ &+ 2|\beta_{\hat{P}}(C_{\mathbf{r}}) - \beta_{\dot{P}}(C_{\mathbf{r}})| \\ &= d_G^{\hat{P},\dot{P}}(C_{\mathbf{r}},C_{\mathbf{r}}) \end{aligned}$$

Thus, 
$$d_G^{\hat{P},\hat{P}} > d_G^{\hat{P},\hat{P}}$$
,  $\operatorname{CSI}(P,\dot{P}) > \operatorname{CSI}(\hat{P},\dot{P})$ , and  $\mathbb{S}_{\operatorname{csi}}(B,\dot{B}) > \mathbb{S}_{\operatorname{csi}}(\hat{B},\dot{B})$ .

**Proposition 21.** The  $\mathbb{S}_{ebc}$  measure penalizes solutions with repetitive biclusters (Def. 5).

*Proof:* Let *B*, *B*, and *B* be biclusterings, as in Def. 5. Let  $C_r$  be the set of objects from *O* corresponding to the matrix entries of the biclusters in *B* that were replicated. We know from Eqs. (26) and (27) that the nominators of Eqs. (14) do not change from comparing *P* with  $\dot{P}$  to comparing  $\hat{P}$  with  $\dot{P}$ , and that  $\alpha_{\hat{P}}(O,O) \geq \alpha_P(O,O)$ . We have  $\tilde{o}_{j_1}$  and  $\tilde{o}_{j_2}$  (for which  $j_1 = j_2$  is allowed) such that  $\alpha_{\hat{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2}) > \alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2})$ . Therefore, EBCP $(P, \dot{P}) >$  EBCP $(\hat{P}, \dot{P})$ , EBC $(P, \dot{P}) >$  EBC $(\hat{P}, \dot{P})$ , and  $\mathbb{S}_{ebc}(B, \dot{B})$ .

**Proposition 22.** The  $\mathbb{S}_{\text{prec}}$  and  $\mathbb{S}_{\text{erec}}$  measures do not have the homogeneity property (Def. 7).

*Proof:* Consider the non-overlapping biclusterings B and  $\hat{B}$  represented by Figs. 13b and 13c and the reference solution  $\dot{B}$  represented by Fig. 13a. We have  $\mathbb{S}_{\text{prec}}(B, \dot{B}) = \mathbb{S}_{\text{prec}}(\hat{B}, \dot{B}) = 0.74$  and  $\mathbb{S}_{\text{erec}}(B, \dot{B}) = \mathbb{S}_{\text{erec}}(\hat{B}, \dot{B}) = 0.55$ .





**Proposition 23.** The  $\mathbb{S}_{csi}$  measure has the homogeneity property (Def. 7).

*Proof:* Let B,  $\hat{B}$ , and  $\hat{B}$  be three biclusterings, as in Def. 7. Let  $C_s^1$  be the x objects swapped from  $P_{i_1}$ ,  $C_n^1$  be the objects from the minor category in  $P_{i_1}$  that were not swapped, and  $C_r^1$  be the objects from the main category in  $P_{i_1}$ . Analogously, define  $C_s^2$ ,  $C_n^2$ , and  $C_r^2$ . Since B,  $\hat{B}$ , and  $\dot{B}$  are non-overlapping solutions, we have  $\beta_P(O) = \beta_{\hat{P}}(O) = \beta_{\hat{P}}(O) = 0$ . Thus, the eventual difference between  $a_G^{P,\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$  (respectively,  $d_G^{P,\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$ ) and  $a_G^{\hat{P},\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$  ( $d_G^{\hat{P},\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$ ) can only be due to the eventual difference between  $\alpha_P(\tilde{o}_{j_1},\tilde{o}_{j_2})$ and  $\alpha_{\hat{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})$  (see Eqs. (16) and (17)).

We conclude from Table 12 that  $a_G^{P,\dot{P}} = a_G^{\hat{P},\dot{P}} + |C_s^1||C_n^1| + |C_s^2||C_n^2| = a_G^{\hat{P},\dot{P}} + x(|C_n^1| + |C_n^2|)$ , where  $x = |C_s^1| = |C_s^2|$ , as in Def. 7. Table 13 shows the differences in

TABLE 12: Differences in  $a_G^{\cdot,\cdot}(\cdot, \cdot)$  by changing P to  $\hat{P}$ .

 $\begin{aligned} d_{G}^{\gamma}(\cdot,\cdot), \text{ implying that } d_{G}^{P,\dot{P}} &= d_{G}^{\hat{P},\dot{P}} - |C_{s}^{1}||C_{n}^{1}| - |C_{s}^{2}||C_{n}^{2}| - |C_{s}^{1}||C_{n}^{2}| - |C_{s}^{2}||C_{n}^{2}| - |C_{s}^{1}||C_{s}^{2}| - |C_{s}^{1}||C_{s}^{2}| + |C_{s}^{1}||C_{r}^{1}| + |C_{s}^{2}||C_{r}^{2}| = d_{G}^{\hat{P},\dot{P}} - 2x(|C_{n}^{1}| + |C_{n}^{2}|). \text{ Thus,} \end{aligned}$ 

$$\operatorname{CSI}(\hat{P}, \dot{P}) = \frac{a_G^{1,2} - x(|C_n^1| + |C_n^2|)}{a_G^{P,\dot{P}} + d_G^{P,\dot{P}} + x(|C_n^1| + |C_n^2|)}$$

and  $\mathbb{S}_{csi}(B, \dot{B}) \ge \mathbb{S}_{csi}(\hat{B}, \dot{B}).$ 

TABLE 13: Differences in  $d_G^{r,\cdot}(\cdot, \cdot)$  by changing P to  $\hat{P}$ .

$d_G^{P,\dot{P}}(C_{\rm s}^1,C_{\rm n}^1) =  1-1  <  0-1  = d_G^{\dot{P},\dot{P}}(C_{\rm s}^1,C_{\rm n}^1)$
$d_G^{P,\dot{P}}(C_{\rm s}^2,C_{\rm n}^2) =  1-1  <  0-1  = d_G^{\hat{P},\dot{P}}(C_{\rm s}^2,C_{\rm n}^2)$
$d_G^{P,\dot{P}}(C_{\rm s}^1,C_{\rm r}^1) =  1-0  >  0-0  = d_G^{\hat{P},\dot{P}}(C_{\rm s}^1,C_{\rm r}^1)$
$d_G^{P,\dot{P}}(C_{\rm s}^2,C_{\rm r}^2) =  1-0  >  0-0  = d_G^{\hat{P},\dot{P}}(C_{\rm s}^2,C_{\rm r}^2)$
$d_G^{P,\dot{P}}(C_{\rm s}^1,C_{\rm n}^2) =  0-0  <  1-0  = d_G^{\hat{P},\dot{P}}(C_{\rm s}^1,C_{\rm n}^2)$
$d_G^{P,\dot{P}}(C_{\rm n}^1,C_{\rm s}^2) =  0-0  <  1-0  = d_G^{\hat{P},\dot{P}}(C_{\rm n}^1,C_{\rm s}^2)$
$d_G^{P,\dot{P}}(C_{\rm s}^1,C_{\rm r}^2) =  0-0  <  1-0  = d_G^{\hat{P},\dot{P}}(C_{\rm s}^1,C_{\rm r}^2)$
$d_G^{P,\dot{P}}(C_{\rm r}^1,C_{\rm s}^2) =  0-0  <  1-0  = d_G^{\hat{P},\dot{P}}(C_{\rm r}^1,C_{\rm s}^2)$

If  $x = |I(B_{i_1}, \dot{B}_{mi(i_1)})| = |I(B_{i_2}, \dot{B}_{mi(i_2)})|$ , then  $|C_n^1| = |C_n^2| = 0$  and  $\mathbb{S}_{csi}(B, \dot{B}) = \mathbb{S}_{csi}(\hat{B}, \dot{B})$ . If  $\mathbb{S}_{csi}(B, \dot{B}) = \mathbb{S}_{csi}(\hat{B}, \dot{B})$ , then  $|C_n^1| + |C_n^2| = 0$  (because x > 0, Def. 7) and  $x = |I(B_{i_1}, \dot{B}_{mi(i_1)})| = |I(B_{i_2}, \dot{B}_{mi(i_2)})|$ .

**Proposition 24.** The  $\mathbb{S}_{ebc}$  measure has the homogeneity property (Def. 7).

*Proof:* Let B,  $\hat{B}$ , and  $\hat{B}$  be three biclusterings, as in Def. 7. Let  $C_s^1$  be the x objects swapped from  $P_{i_1}$ ,  $C_n^1$  be the objects from the minor category in  $P_{i_1}$  that were not swapped, and  $C_r^1$  be the objects from the main category in  $P_{i_1}$ . Analogously, define  $C_s^2$ ,  $C_n^2$ , and  $C_r^2$ . Let

$$\delta_{\mathbf{p}}^{P,\dot{P}}(\tilde{o}_{j_{1}}) \triangleq \frac{\sum_{j_{2}=1}^{n} \min\{\alpha_{P}(\tilde{o}_{j_{1}}, \tilde{o}_{j_{2}}), \alpha_{\dot{P}}(\tilde{o}_{j_{1}}, \tilde{o}_{j_{2}})\}}{\sum_{j_{2}=1}^{n} \alpha_{P}(\tilde{o}_{j_{1}}, \tilde{o}_{j_{2}})}$$

such that EBCP $(P, \dot{P}) = (1/n) \sum_{j_1=1}^n \delta_{\mathbf{p}}^{P, \dot{P}}(\tilde{o}_{j_1})$ . Note that

$$\sum_{\tilde{o}_{j_1} \notin P_{i_1} \cup P_{i_2}} \delta_{\mathbf{p}}^{P, \dot{P}}(\tilde{o}_{j_1}) = \sum_{\tilde{o}_{j_1} \notin P_{i_1} \cup P_{i_2}} \delta_{\mathbf{p}}^{\hat{P}, \dot{P}}(\tilde{o}_{j_1}).$$

TABLE 14: Differences in  $\delta_{p}^{\cdot,\cdot}(\cdot)$  by changing *P* to  $\hat{P}$ .

We conclude from Table 14 and after some algebraic manipulation that

$$\sum_{\tilde{o}_{j_1} \in P_{i_1} \cup P_{i_2}} \delta_{\mathbf{p}}^{P,\dot{P}}(\tilde{o}_{j_1}) = \frac{(|C_{\mathbf{s}}^1| + |C_{\mathbf{n}}^1|)^2}{|P_{i_1}|} + \frac{|C_{\mathbf{r}}^1|^2}{|P_{i_1}|} + \frac{(|C_{\mathbf{s}}^2| + |C_{\mathbf{n}}^2|)^2}{|P_{i_2}|} + \frac{(|C_{\mathbf{r}}^2|^2}{|P_{i_2}|}$$

and

$$\sum_{\tilde{o}_{j_1} \in P_{i_1} \cup P_{i_2}} \delta_{\mathbf{p}}^{\hat{P}, \dot{P}}(\tilde{o}_{j_1}) = \frac{|C_{\mathbf{s}}^2|^2 + |C_{\mathbf{n}}^1|^2 + |C_{\mathbf{r}}^1|^2}{|P_{i_1}|} + \frac{|C_{\mathbf{s}}^1|^2 + |C_{\mathbf{n}}^2|^2 + |C_{\mathbf{r}}^2|^2}{|P_{i_2}|}$$

From  $x = |C_{s}^{1}| = |C_{s}^{2}|$ , we have

$$\text{EBCP}(\hat{P}, \dot{P}) - \text{EBCP}(P, \dot{P}) = \frac{-2x}{n} \left( \frac{|C_{n}^{1}|}{|P_{i_{1}}|} + \frac{|C_{n}^{2}|}{|P_{i_{2}}|} \right).$$
(28)

Let

$$\delta_{\mathbf{r}}^{P,\dot{P}}(\tilde{o}_{j_1}) \triangleq \frac{\sum_{j_2=1}^n \min\{\alpha_P(\tilde{o}_{j_1},\tilde{o}_{j_2}), \alpha_{\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})\}}{\sum_{j_2=1}^n \alpha_{\dot{P}}(\tilde{o}_{j_1},\tilde{o}_{j_2})}$$

such that  $\text{EBCR}(P, \dot{P}) = (1/n) \sum_{j_1=1}^n \delta_r^{P, \dot{P}}(\tilde{o}_{j_1})$ . The only difference between  $\delta_p^{P, \dot{P}}(\tilde{o}_{j_1})$  and  $\delta_r^{P, \dot{P}}(\tilde{o}_{j_1})$  lies in the denominators. Thus,

$$\sum_{\tilde{o}_{j_1} \in P_{i_1} \cup P_{i_2}} \delta_{\mathbf{r}}^{\mathbf{P}, \dot{\mathbf{P}}}(\tilde{o}_{j_1}) = \frac{(|C_{\mathbf{s}}^1| + |C_{\mathbf{n}}^1|)^2}{|\dot{P}_{\mathrm{mi}(i_1)}|} + \frac{(|C_{\mathbf{s}}^2| + |C_{\mathbf{n}}^2|)^2}{|\dot{P}_{\mathrm{mi}(i_2)}|} \\ + \frac{|C_{\mathbf{r}}^1|^2}{|\dot{P}_{\mathrm{ma}(i_1)}|} + \frac{|C_{\mathbf{r}}^2|^2}{|\dot{P}_{\mathrm{ma}(i_2)}|}$$

and

$$\sum_{\tilde{p}_{j_1} \in P_{i_1} \cup P_{i_2}} \delta_{\mathbf{r}}^{\hat{P}, \dot{P}}(\tilde{o}_{j_1}) = \frac{|C_{\mathbf{s}}^1|^2 + |C_{\mathbf{n}}^1|^2}{|\dot{P}_{\mathrm{mi}(i_1)}|} + \frac{|C_{\mathbf{s}}^2|^2 + |C_{\mathbf{n}}^2|^2}{|\dot{P}_{\mathrm{mi}(i_2)}|} + \frac{|C_{\mathbf{r}}^1|^2}{|\dot{P}_{\mathrm{mi}(i_2)}|} + \frac{|C_{\mathbf{r}}^2|^2}{|\dot{P}_{\mathrm{ma}(i_1)}|} + \frac{|C_{\mathbf{r}}^2|^2}{|\dot{P}_{\mathrm{ma}(i_2)}|}.$$

Therefore,

$$\operatorname{EBCR}(\hat{P}, \dot{P}) - \operatorname{EBCR}(P, \dot{P}) = \frac{-2x}{n} \Big( \frac{|C_{n}^{1}|}{|\dot{P}_{\operatorname{mi}(i_{1})}|} + \frac{|C_{n}^{2}|}{|\dot{P}_{\operatorname{mi}(i_{2})}|} \Big).$$
(29)

We conclude from (28) and (29) that  $\text{EBC}(P, \dot{P}) \ge \text{EBC}(\hat{P}, \dot{P})$  and  $\mathbb{S}_{\text{ebc}}(B, \dot{B}) \ge \mathbb{S}_{\text{ebc}}(\hat{B}, \dot{B})$ . If  $x = |I(B_{i_1}, \dot{B}_{\text{mi}(i_1)})| = |I(B_{i_2}, \dot{B}_{\text{mi}(i_2)})|$ , then  $|C_n^1| = |C_n^2| = 0$  and  $\mathbb{S}_{\text{ebc}}(B, \dot{B}) = \mathbb{S}_{\text{ebc}}(\hat{B}, \dot{B})$ . If  $\mathbb{S}_{\text{ebc}}(B, \dot{B}) = \mathbb{S}_{\text{ebc}}(\hat{B}, \dot{B})$ , then  $|C_n^1| = |C_n^2| = 0$  (because x > 0, Def. 7) and  $x = |I(B_{i_1}, \dot{B}_{\text{mi}(i_1)})| = |I(B_{i_2}, \dot{B}_{\text{mi}(i_2)})|$ .

## **Proposition 25.** We have $\mathbb{S}_{ce}(B, \dot{B}) = 1$ iff $B \equiv \dot{B}$ .

Proof: Clearly,  $B \equiv \dot{B}$  implies that  $\mathbb{S}_{ce} = 1$ . Let k be the number of biclusters in B and q the number of biclusters in  $\dot{B}$ . Suppose that  $\mathbb{S}_{ce}(B, \dot{B}) = 1$ , and let  $\{(t_i, y_i)\}_{i=1}^{\min\{k,q\}}$  be the unique relation that maximizes Eq. (6). Note that  $|U| \ge \sum_{j_1, j_2} N_{j_1, j_2} = \sum_{i=1}^k |B_i^r \times B_i^c| \ge d_{\max}$  and  $|U| \ge \sum_{j_1, j_2} N_{j_1, j_2} = \sum_{i=1}^q |\dot{B}_i^r \times \dot{B}_i^c| \ge d_{\max}$ . We have from  $|U| = d_{\max}$  that  $\sum_{i=1}^k |B_i^r \times B_i^c| = d_{\max} \le \sum_{i=1}^{\min\{k,q\}} |B_{t_i}^r \times B_{t_i}^c| \le \sum_{i=1}^k |B_i^r \times B_i^c|$ , implying that  $\sum_{i=1}^k |B_i^r \times B_i^c| = \sum_{i=1}^{\min\{k,q\}} |B_{t_i}^r \times \dot{B}_i^c| = \sum_{i=1}^{\min\{k,q\}} |\dot{B}_{i}^r \times \dot{B}_{i_i}^c|$  and  $k = \min\{k,q\}$ . Similarly,  $\sum_{i=1}^q |\dot{B}_i^r \times \dot{B}_i^c| = \sum_{i=1}^{\min\{k,q\}} |\dot{B}_{y_i}^r \times \dot{B}_{y_i}^c|$  and  $q = \min\{k,q\}$ . Thus, k = q. From  $d_{\max} = \sum_{i=1}^{\min\{k,q\}} |B_{t_i}^r \times B_{t_i}^c|$  we have  $B_{t_i}^r \times B_{t_i}^c \subseteq \dot{B}_{y_i}^r \times \dot{B}_{y_i}^c$  for all i. Similarly,  $\dot{B}_{y_i}^r \times \dot{B}_{y_i}^c \subseteq B_{t_i}^r \times B_{t_i}^c$  for all i, and then  $B_{t_i}^r \times B_{t_i}^c = \dot{B}_{y_i}^r \times \dot{B}_{y_i}^c$  for all i. Thus,  $B \equiv \dot{B}$ .

## **Proposition 26.** We have $\mathbb{S}_{\text{fabi}}(B, \dot{B}) = 1$ iff $B \equiv \dot{B}$ .

*Proof:* Clearly,  $B \equiv \dot{B}$  implies that  $\mathbb{S}_{\text{fabi}} = 1$ . Suppose that  $\mathbb{S}_{\text{fabi}}(B, \dot{B}) = 1$ , and let  $\{(t_i, y_i)\}_{i=1}^{\min\{k,q\}}$  be the optimal unique relation required by  $\mathbb{S}_{\text{fabi}}$ . The denominator of Eq. (9) shows that  $\mathbb{S}_{\text{fabi}}$  attains 1 only when comparing solutions with the same number of biclusters, which makes  $\{(t_i, y_i)\}_{i=1}^{\min\{k,q\}}$  a bijection.  $\mathbb{S}_{\text{fabi}}$  attains 1 only if  $\mathbb{J}(B_{t_i}, \dot{B}_{y_i}) = 1$  for all i, and  $\mathbb{J}(B_{t_i}, \dot{B}_{y_i})$  attains 1 only if  $B_{t_i} \equiv \dot{B}_{y_i}$ . Thus,  $B \equiv \dot{B}$ .

**Proposition 27.** There are two non-equivalent biclusterings *B* and  $\dot{B}$  such that  $\mathbb{S}_{csi}(B, \dot{B}) = \mathbb{S}_{ebc}(B, \dot{B}) = 1$ .

*Proof:* Let *B* be a biclustering in which one or more matrix elements were not biclustered. Then add one bicluster in *B* that has only one of the matrix elements that were not biclustered, and let  $\dot{B}$  be the resulting solution. Applying the transformation approach given in Section 5 to *B* and  $\dot{B}$ , we have two equivalent soft clusterings *P* and  $\dot{P}$ , implying that CSI(*P*, $\dot{P}$ ) = EBC(*P*, $\dot{P}$ ) = 1 and  $\mathbb{S}_{csi}(B,\dot{B}) = \mathbb{S}_{ebc}(B,\dot{B}) = 1$ .

**Proposition 28.** There are two non-equivalent nondegenerate biclusterings B and  $\dot{B}$  for which  $\mathbb{S}_{csi}(B, \dot{B}) = \mathbb{S}_{ebc}(B, \dot{B}) = 1$ .

*Proof:* The biclusterings in Fig. 14 are given by  $B \triangleq \{B_i\}_{i=1}^4$ ,  $\dot{B} \triangleq \{\dot{B}_i\}_{i=1}^3$ ,  $B_1 \triangleq (\{1\}, \{1, 2\})$ ,  $B_2 \triangleq (\{2\}, \{1, 2\})$ ,  $B_3 \triangleq (\{3\}, \{1, 2\})$ ,  $B_4 \triangleq (\{1, 2, 3\}, \{1, 2\})$ ,

 $\dot{B}_{1} \triangleq (\{1,2\},\{1,2\}), \ \dot{B}_{2} \triangleq (\{2,3\},\{1,2\}), \text{ and } \dot{B}_{3} \triangleq (\{1,3\},\{1,2\}). \text{ We have } P = \{P_{i}\}_{i=1}^{4} \text{ and } \dot{P} = \{\dot{P}_{i}\}_{i=1}^{3}, \text{ where } P_{1} = \{\tilde{o}_{1},\tilde{o}_{4}\}, \ P_{2} = \{\tilde{o}_{2},\tilde{o}_{5}\}, \ P_{3} = \{\tilde{o}_{3},\tilde{o}_{6}\}, P_{4} = \{\tilde{o}_{j}\}_{j=1}^{6}, \dot{P}_{1} = \{\tilde{o}_{1},\tilde{o}_{2},\tilde{o}_{4},\tilde{o}_{5}\}, \ \dot{P}_{2} = \{\tilde{o}_{2},\tilde{o}_{3},\tilde{o}_{5},\tilde{o}_{6}\}, \text{ and } \dot{P}_{3} = \{\tilde{o}_{1},\tilde{o}_{3},\tilde{o}_{4},\tilde{o}_{6}\}.$ 

Note that  $\alpha_P(\tilde{o}_{j_1}, \tilde{o}_{j_2}) = \alpha_{\dot{P}}(\tilde{o}_{j_1}, \tilde{o}_{j_2})$  for all  $j_1$  and  $j_2$ , and we have  $\beta_P(\tilde{o}_j) = \beta_{\dot{P}}(\tilde{o}_j)$  for all j. Thus,  $d_G^{P, \dot{P}} = 0$ ,  $\text{CSI}(P, \dot{P}) = 1$ , and  $\mathbb{S}_{\text{csi}}(B, \dot{B}) = 1$ . Similarly,  $\mathbb{S}_{\text{ebc}}(B, \dot{B}) = 1$ .



Fig. 14: Indistinguishable biclusterings for  $\mathbb{S}_{\rm csi}$  and  $\mathbb{S}_{\rm ebc}.$ 

Since  $P \neq \dot{P}$ , the above proof contradicts Proposition 1 in [36], which states (in terms of matrices) that  $CSI(P, \dot{P}) = 1$  iff  $P \equiv \dot{P}$ .

Algorithm	Implementation	Source	Reference
bbc	С	http://www.people.fas.harvard.edu/~junliu/BBC/	[16]
bcca	Matlab	http://sn.im/26fzpck	[57]
bibit	Java	http://www.upo.es/eps/bigs/BiBit_algorithm.html	[55]
bimax	R biclust package	http://cran.r-project.org/web/packages/biclust/index.html	[8]
сс	R biclust package	http://cran.r-project.org/web/packages/biclust/index.html	[4]
las	Matlab	https://genome.unc.edu/las/	[58]
msbe	Java	http://www.cs.cityu.edu.hk/~lwang/software/msbe/help.html	[39]
pcluster	Windows binary	http://haixun.olidu.com/proj/delta.html	[54]
xmotifs	R biclust package	http://cran.r-project.org/web/packages/biclust/index.html	[56]
fabia	R fabia package	http://www.bioconductor.org/packages/2.12/bioc/html/fabia.html	[37]

TABLE 15: Biclustering	algorithms	used in	the experiment	ments.
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TABLE 16: Algorithm configuration.

Algorithm	Configuration
bbc	-k (number of biclusters to be found): k*
	<ul> <li>-n (normalization method): zero-mean, unit-variance column normalization</li> </ul>
1	• -minc (minimum number of columns): min(nc)
bcca	• -maxk (maximum number of biclusters to be found): $\kappa$ • -theta (Pearson correlation threshold): 0.90
1.11.1.	<ul> <li>- minr (minimum number of rows): min(nr)</li> </ul>
bibit	• -minc (minimum number of cols): min(nc)
	<ul> <li>-minr (minimum number of rows): min(nr)</li> </ul>
bimax	• -minc (minimum number of cols): min(nc)
	• -K (number of biclusters to be found): $k'$
66	• -alpha (scaling factor): 1.2 (as in the original paper) • -delta (maximum acceptable score): $(max(A)-min(A))^2/12 * 0.005$ (first experiment in the original paper)
ee	<ul> <li>-k (top biclusters having the smallest errors to return): k*</li> </ul>
las	• -maxk (maximum number of biclusters to be found): $k^*$
	<ul> <li>-alpha: 0.3 (original paper, page 54, central value)</li> </ul>
	• -beta: 0.25 (original paper, page 54, central value)
msbe	• -bitype: additive
	• -nrr (number of reference rows): n
	<ul> <li>-nrc (number of reference columns): p</li> </ul>
	<ul> <li>-delta (maximum number of biclusters to be found): 1</li> </ul>
pcluster	• -minr (minimum number of rows): min(nr)
	• -mile (number of code): 10 (original paper)
	<ul> <li>-Ins (number of seeds). 10 (original paper)</li> <li>-nr (number of repetitions): 1000 (original paper)</li> </ul>
xmotifs	• -ss (sample size): 5 (implementation's default value)
	<ul> <li>-alpha: 0.05 (implementation's default value)</li> </ul>
	• -n (normalization method): 0.75-0.25 quantile
fabia	<ul> <li>-C (data centering): 2</li> <li>-alpha (sparseness loadings): 0.01</li> </ul>
	<ul> <li>-spl (sparseness prior loadings): 0</li> </ul>
	• -spz (sparseness factors): 0.5
	• -k (number of biclusters to be found): k*

**Definitions.** min(nr): minimum number of rows that the reference biclusters have (similarly for min(nc)); minr: refer to the rows of biclusters (similarly for minc);  $k^*$  is the ideal number of biclusters; and min(A): minimum value of the data matrix (similarly for max(A)).