Component intensities to relate difference by category with difference overall

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ABSTRACT

This article gives methods to analyze the difference between two datasets that describe a mutual set of categories. The methods can analyze classification error between mapped and reference categories, or change between two time points. Previous work showed how to compute difference size as the sum of three components: Quantity, Exchange and Shift. These components exist for difference by category and for difference overall. These components can be challenging to compare when the categories' differences vary by size. To address this challenge, this article introduces equations to compute a component's intensity, which is the size of the component divided by the size of the difference. Component intensities facilitate comparison of each category with other categories and with difference overall. The case study illustrates how to use component intensities to characterize temporal change using remotely sensed data. Results show how an intensive Exchange component can signal possible confusion of two categories with each other. The literature shows that authors could benefit from interpretation of component intensities. Readers can perform the calculations for free by using the *diffeR* package in R or the *PontiusMatrix* spreadsheet available at www.clarku.edu/~rpontius.

1. Introduction

A contingency table shows the association between categories in the table's rows and categories in the table's columns (Agresti, 2002). If the sequence of categories in the rows is the same as in the columns, then the table is square while diagonal entries show agreement and off-diagonal entries show difference. The square table has a specific name depending on the application. Confusion matrix is the name for error assessment in remote sensing, where the rows are the mapped categories and the columns are the reference categories (Foody, 2002). In a confusion matrix, a category's row difference is the category's commission error and a category's column difference is the category's omission error. Transition matrix is the name for temporal change analysis, where the rows are the initial categories and the columns are the subsequent categories. In a transition matrix, a category's row difference is the category's gross loss and a category's column difference is the category's gross gain. Pontius and Santacruz (2014) showed how to separate difference into three components: Quantity, Exchange and Shift. A category's Quantity component is the absolute value of the category's column difference minus the category's row difference. An Exchange component exists between two categories when the differences between them do not modify the size of either category, such as when category i transitions to category j for some observations while category j transitions to category i for an equal number of other observations. The Shift

component is the difference that is neither Quantity nor Exchange. Quantity, Exchange and Shift components exist by category and summed over all categories. Comber et al. (2017) expressed concern that policy makers might not immediately understand the three components. This article's purpose is to offer novel methods to deepen understanding and interpretation of the components of difference.

Examination of each component's size is helpful, but comparison among categories can be challenging because categories typically vary in size of difference. Therefore, this article establishes methods to compare categories that vary in size of difference. This article defines component intensity as the size of the component divided by the size of the difference, so that component intensities are on a single scale from 0% to 100%, which facilitates comparison.

This article is the next step in a sequence of articles that analyze a square contingency table. Terminology has evolved in the literature. Pontius et al. (2004) showed how to separate total difference in terms of two components, which they called Net and Swap. Pontius and Millones (2011) used the term Quantity difference to refer to Net and the term Allocation difference to refer to Swap. Allocation difference is the sum of Exchange and Shift. Aldwaik and Pontius (2012, 2013) established Intensity Analysis to analyze transition matrices. Intensity Analysis considers the intensity of each category's gross loss and gross gain relative to temporal change overall (Pontius et al., 2013). Intensity Analysis has not yet considered the components of Quantity,

Table 1
Square contingency table for the example where ten is the number of observations of difference overall.

	$j = 1$	$j = 2$	$j = 3$	Row Total	Row Difference
$i = 1$	C_{11}	1	2	$C_{11} + 3$	3
$i = 2$	4	C_{22}	0	$C_{22} + 4$	4
$i = 3$	1	2	C_{33}	$C_{11} + 3$	3
Column Total	$C_{11} + 5$	$C_{22} + 3$	$C_{33} + 2$	$C_{11} + C_{22} + C_{33} + 10$	
Column Difference	5	3	2		10

Exchange and Shift (Akinyemi et al., 2017; Huang et al., 2018). This article applies the concepts of Intensity Analysis to those three components.

2. Materials and methods

Table 1 gives an example of a square contingency table to illustrate the concepts. The number of categories is three, which is the minimum number to show all three components. Table 1 gives the size of each off-diagonal entry, meaning where $i \neq j$. The entries for which $i = j$ do not influence the results because diagonal entries are not differences. Table 2 gives the mathematical notation for the equations, following the rules of Pontius et al. (2017).

Eqs. (1)–(4) give the difference size for category j and its components. Eq. (1) computes the difference for each category j as the sum of the category's column difference and row difference. The first subscript of C denotes the row and the second subscript of C denotes the column. Eqs. (1) and (3) subtract C_{jj} to eliminate the diagonal entry from the calculations. Eq. (2) computes the Quantity component's size for category j as the absolute value of the category's column total minus its row total. Eq. (3) computes the Exchange between categories i and j as two times the minimum of C_{ij} and C_{ji} because Exchange occurs in pairs, where each observation in C_{ij} is paired with an observation in C_{ji}. In Table 1, Exchange between categories 1 and 2 is two, Exchange between categories 1 and 3 is two, and Exchange between categories 2 and 3 is zero. Eq. (3) gives the Exchange component's size for category j by summing the Exchanges between category j and all other categories. Eq. (4) computes the Shift component as the difference for category j minus Quantity and Exchange for category j. Shift for category j is positive when $C_{ij} < C_{ji}$ and $C_{kj} > C_{jk}$ for any categories $i \neq k$.

$$d_j = \left[\sum_{i=1}^{J} (C_{ij} + C_{ji}) \right] - 2C_{jj} \tag{1}$$

Table 2
Mathematical notation.

Symbol	Meaning
C_{ij}	number of observations in row i and column j of contingency table
C_{ji}	number of observations in row j and column i of contingency table
d_j	Difference size of category j
D	Difference size overall
e_j	Exchange size of category j
e'_j	Exchange intensity of category j
E	Exchange size overall
E'	Exchange intensity overall
i	index of a category
j	index of a category
J	number of categories
q_j	Quantity size of category j
q'_j	Quantity intensity of category j
Q	Quantity size overall
Q'	Quantity intensity overall
s_j	Shift size of category j
s'_j	Shift intensity of category j
S	Shift size overall
S'	Shift intensity overall

$$q_j = \left| \sum_{i=1}^{J} (C_{ij} - C_{ji}) \right| \tag{2}$$

$$e_j = 2\{[\sum_{i=1}^{J} \text{MINIMUM}(C_{ij}, C_{ji})] - C_{jj}\} \tag{3}$$

$$s_j = d_j - q_j - e_j \tag{4}$$

Fig. 1a shows the sizes of components for each category in Table 1. The column difference is greater than the row difference for category 1, thus category 1 has a positive sign in its Quantity component. The column difference is less than the row difference for categories 2 and 3, thus categories 2 and 3 have negative signs in their Quantity components. In general, the sign associated with each q_j is the sign of the summation that is within the absolute value symbols in Eq. 2.

Eq. (5) computes the difference size overall, while Eqs. (6)–(8) compute the component sizes overall by summing over all categories. Division by two is necessary to neutralize the summation's double counting. Double counting exists because any difference involves two categories: the row category and the column category. Eqs. (6)–(8) imply that each component overall derives from the categories in proportion to the sum of the categories' corresponding component. The second equals sign in Eq. (8) reflects the fact that the difference overall is the sum of its three components.

$$D = \sum_{j=1}^{J} d_j/2 \tag{5}$$

$$Q = \sum_{j=1}^{J} q_j/2 \tag{6}$$

$$E = \sum_{j=1}^{J} e_j/2 \tag{7}$$

$$S = \sum_{j=1}^{J} s_j/2 = D - Q - E \tag{8}$$

Eqs. (9)–(11) compute the intensity of each component by category. Each intensity is the size of the category's component divided by the size of the category's difference, expressed as a percentage.

$$q'_j = 100\% \ q_j/d_j \tag{9}$$

$$e'_j = 100\% \ e_j/d_j \tag{10}$$

$$s'_j = 100\% \ s_j/d_j \tag{11}$$

Eqs. (12)–(14) compute the intensity of each component overall, where each intensity is the size of the component overall divided by the size of the difference overall, expressed as a percentage. The second equals sign in Eqs. (12)–(14) shows how each component overall is a weighted average of the components for each category, where the weight is the ratio in the round parentheses. Eq. (5) implies that the weights sum to one.

$$Q' = 100\% \ Q/D = 100\% \ \sum_{j=1}^{J} [q'_j(d_j/2D)] \tag{12}$$

$$E' = 100\% \ E/D = 100\% \ \sum_{j=1}^{J} [e'_j(d_j/2D)] \tag{13}$$

$$S' = 100\% \ S/D = 100\% \ \sum_{j=1}^{J} [s'_j(d_j/2D)] \tag{14}$$

All intensities in Eqs (9)–(14) are on a scale from 0% to 100%. The sum of q'_j, e'_j, and s'_j is 100% for each category j; similarly, the sum of Q', E' and S' is 100%, regardless of the sizes of the categories and their differences. This mutual scale facilitates comparison among categories and comparison of each category's component to the corresponding component overall. The components overall offer baselines to address the question, "Does a particular category demonstrate a particular component intensively relative to the corresponding component overall?" Specifically, if $q'_j < Q'$, then the Quantity component for category j is less intensive than the Quantity component overall. If $q'_j = Q'$, then the Quantity component for category j is as intensive as the Quantity component overall. If $q'_j > Q'$, then the Quantity component for category j is more intensive than the Quantity component overall. Analogous relationships exist for Exchange and Shift. For example, if $e'_j > E'$, then the Exchange component for category j is more intensive than the Exchange component overall. If $s'_j > S'$, then the Shift component for category j is more intensive than the Shift component overall.

Fig. 1b shows how the component intensities of the categories relate to each other and to the components overall for the example in Table 1. The Quantity Overall line indicates that the Quantity component overall is 20% of the difference overall. The Quantity component for category 1 extends beyond the Quantity Overall line. Therefore, category 1 has a more intensive Quantity component relative to the Quantity component overall. The Quantity for category 2 ends before the Quantity Overall line. Therefore, category 2 has a less intensive Quantity component relative to the Quantity component overall. The Quantity for category 3 ends at the Quantity Overall line. Therefore, category 3 has a Quantity component as intensive as the Quantity component overall.

The Quantity + Exchange Overall line in Fig. 1b indicates that the sum of the Quantity and Exchange components overall is 60% of the difference overall. The difference between the lines in Fig. 1b is 40%, which equals the intensity of Exchange overall. Category 1 has more intensive Exchange relative to Exchange overall, while category 2 has less intensive Exchange relative to Exchange overall. Category 3 has Exchange equal in intensity to Exchange overall.

The Quantity + Exchange Overall line of 60% implies that the intensity of Shift overall is 40%, meaning 100% minus 60%. The Shift intensity for category 1 is entirely to the right of the Quantity + Exchange Overall line;

therefore, category 1 has less intensive Shift relative to Shift overall. Category 2 has more intensive Shift relative to Shift overall. Category 3 has Shift equal in intensity to Shift overall.

The concepts apply to the maps of temporal difference in Fig. 2, which derives from an overlay of maps at 2005 and 2013 (Ye and Pontius, 2018a,b). The spatial extent is a marsh, which is part of the Plum Island Ecosystems site in northeastern Massachusetts, USA. Both time points have four categories: Alterniflora, Patens, Water and Bare. Alterniflora and Patens refer to *spartina alterniflora* and *spartina patens* respectively, which are cordgrasses that require careful attention to distinguish via remotely sensed images, especially when tides vary between time points (Klemas and Victor, 2001). Each patch of temporal difference involves two categories: the losing category and the gaining category. Each pixel is 0.5 m on a side, meaning the spatial resolution is 50 cm.

3. Results

Table 3 records the temporal differences in the maps of Fig. 2. Analysis of Table 3 produces Fig. 3. Fig. 3a shows that Alterniflora and Patens account for the largest differences, and that their Exchange components are largest among their three components. Fig. 3b facilitates comparison among categories by presenting intensities by category and overall. The Quantity Overall line indicates that Quantity overall accounts for 31% of difference overall. Intensity of Exchange overall is the Quantity + Exchange Overall line minus the Quantity Overall line, which implies that Exchange accounts for 56% of the difference overall. The Quantity + Exchange Overall line implies that Shift accounts for 13% of difference overall. The Quantity component is smallest for Bare in size, but is more intensive for Bare than for Alterniflora and Patens. Patens does not have the smallest Quantity component size, but Patens is the only category that has a Quantity component less intensive than Quantity overall. Alterniflora and Patens have the largest Exchange components, and both are more intensive than Exchange overall. Patens and Bare are the only categories that have positive Shift components, and both are more intensive than Shift overall.

These results clarify the patterns visible in the maps of Fig. 2. The maps show that Alterniflora loses more than it gains, while the other categories gain more than they lose. Therefore, the Quantity components show net loss for Alterniflora and net gain for the other categories. The western side of the spatial extent shows linear features, which are drainage ditches. Those ditches contain Alterniflora surrounded by Patens at both time points. The ditches appear to move south from 2005 to 2013, perhaps due to image misregistration. This causes Exchange between Alterniflora and Patens, as Alterniflora loses to Patens while Alterniflora gains from Patens immediately to the south. It can be helpful to distinguish Exchange from other components of difference, because Exchange can alert scientists to systematic errors that cause confusion of two categories with each other. Misregistration and misclassification can cause Exchange. Small pixels
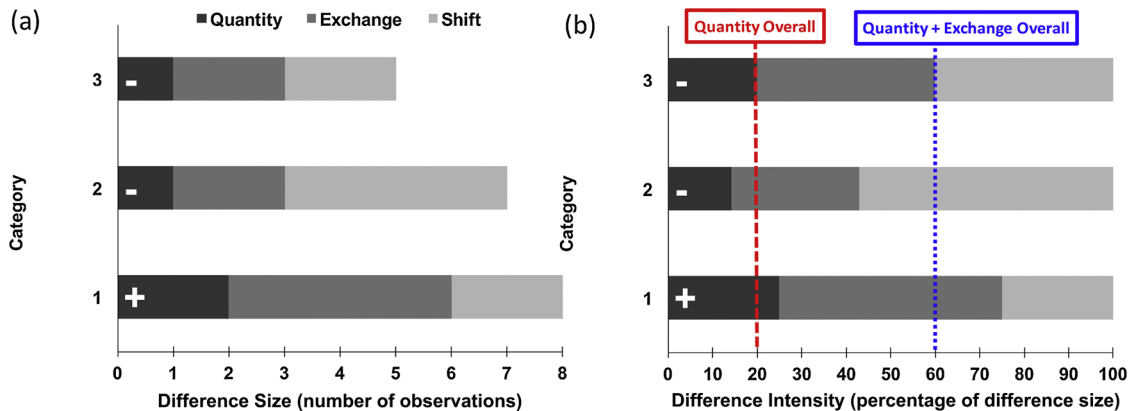

Fig. 1. (a) Size and (b) Intensity of differences for Table 1. A positive sign in the Quantity component denotes the column difference is greater than the row difference; a negative sign denotes the column difference is less than the row difference.
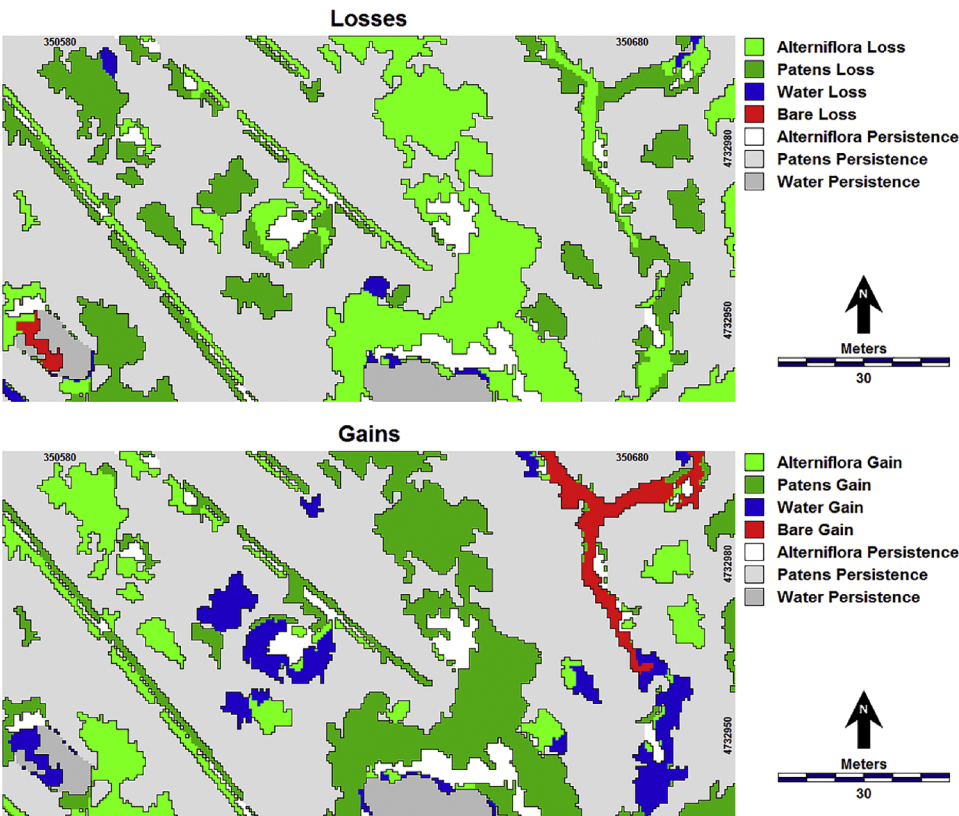
Fig. 2. Losses and Gains during 2005–2013 in a marsh of the Plum Island Ecosystems in northeastern Massachusetts, USA. Black lines outline patches of difference between 2005 and 2013.

Table 3

Transition matrix that shows change from 2005 in the rows to 2013 in the columns for the number of pixels in the maps in Fig. 2.

		2013					
		Alterniflora	Patens	Water	Bare	2005 Total	Loss
2005	Alterniflora	1,393	5,343	407	317	7,460	6,067
	Patens	2,737	20,023	1,056	367	24,183	4,160
	Water	87	111	803	14	1,015	212
	Bare	0	0	110	0	110	110
	2013 Total	4,217	25,477	2,376	698	32,768	
	Gain	2,824	5,454	1,573	698		10,549

demand precise georegistration of the maps from two time points; otherwise, misregistration can give the illusion of Exchange through time. Furthermore, various vegetation categories can have similar spectral signatures (Adam et al., 2010) and smaller pixels can decrease spectral separability (He et al., 2011), both of which can cause Exchange due to confusion of two categories with each other during classification. In contrast, Bare illustrates how Shift is distinct from Exchange. Bare has an intensive Shift component, as Bare loses to Water in the southwest corner while Bare gains from mostly Alterniflora and Patens in the northeast corner of the spatial extent. Some components reveal patterns that are not immediately obvious in the table or the maps. For example, Patens has a positive Shift component because Patens gains from Alterniflora more than Patens loses to Alterniflora, while Patens loses to Water and Bare more than Patens gains from Water and Bare. Alterniflora has zero Shift because Alterniflora loses more than Alterniflora gains with respect to each of the other categories. Water has zero
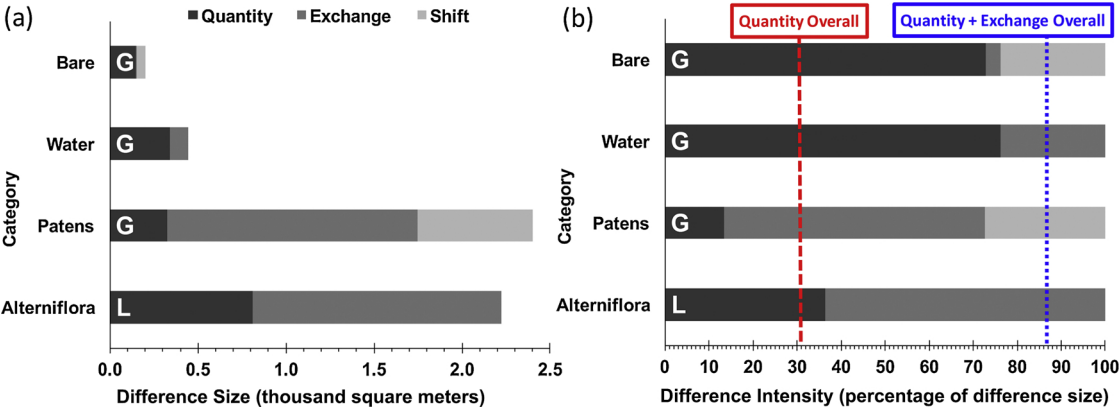

Fig. 3. (a) Size and (b) Intensity of differences for the Plum Island Ecosystems data. L denotes net loss and G denotes net gain.

Shift because Water loses less than Water gains with respect to each of the other categories.

4. Discussion

Recent literature shows how authors have adopted the components of Quantity, Exchange and Shift. Quan et al. (2018) used the components to analyze China's policy to maintain its size of cropland, which requires that cropland's gross gain compensate for cropland's gross loss. The Quantity component for cropland indicates whether the policy meets its goal. Exchange and Shift components for cropland can distinguish between ways to accomplish the goal. Exchange exists if cropland transitions to forest at some locations while forest transitions to cropland at other locations. Shift exists if the transition from built to cropland is less than the transition from cropland to built, while the transition from forest to cropland is greater than the transition from cropland to forest.

Whiteside and Bartolo (2015a) used the three components to compare the sizes of errors while mapping thirteen categories of aquatic vegetation. Their figure 11 has the same format as this article's Fig. 1a but not 1b. The sizes of their errors by category range from 2 to 16 percent of the their observations, so it is not immediately obvious how to compare the errors among their categories. This article's methods would have allowed them to enhance their interpretations by comparing the error for each category to the error for other categories and to the error overall in terms of intensities. Such an analysis would have allowed them to identify the categories that have a component that is more intensive compared to the corresponding component overall. A similar situation exists for Leiterer et al. (2018), who computed the sizes of the three components by category to characterize mapping errors. Their figures 10 and 12 are the format of this article's Fig. 1a but not 1b. This article's additional methods would have allowed them to specify the categories that experienced a component intensively relative to the corresponding component overall.

Other authors reported the sizes of three components overall but not by category. For example, García-Álvarez and Camacho Olmedo (2017) used the components overall to examine differences for two versions of the CORINE data. Sohl et al. (2016) showed that Exchange was the largest component of difference overall between modeled and observed land cover. Otero et al. (2016) showed that Exchange was the largest component overall for both of their algorithms to map land cover. Cissell et al. (2018) found that Exchange was the largest component overall in their mapping of land change. Whiteside and Bartolo (2015b) showed the three components overall to assess both classification error and temporal change. These authors could have enhanced interpretation by using this article's methods to show how difference by category relates to difference overall in terms of size and intensity. Furthermore, comparison of component intensities overall can facilitate comparison of one case study to another case study.

Some authors examined Quantity and Allocation by category and overall, but did not take the additional step to separate Allocation into Exchange and Shift (Camacho Olmedo et al., 2015). This article's concepts apply even for these cases that focus on the components of Quantity and Allocation. For such cases, the Quantity Overall line in Figs. 1 and 3 is relevant. For example, Malek and Verburg (2017) compared the sizes of Quantity and Allocation for 21 categories. This article's methods could have helped them detect the categories that had a Quantity component that was more intensive than Quantity overall. Montereale-Gavazzi et al. (2017) reported the sizes of Quantity and Allocation of temporal change in a seafloor by category and overall. They showed that Allocation was larger than Quantity for all of their categories. If they would have used this article's methods, then they would have been able to gain additional insights that Shift existed for only one category, which was the only category where Quantity was more intensive than Quantity overall.

Some authors gave overall Quantity and Allocation, but did not analyze behavior of individual categories. For such situations, readers cannot tell which categories contributed to which components overall (Colkesen and Kavzoglu, 2017). Fox et al. (2017) presented an application where Exchange would have been helpful to compute, as they

reported, "Gross (class) changes at the landscape level were dominated by exchange between woodland and shrubland …" If they had applied this article's methods, then they could have reported how the Exchange between woodland and shrubland contributed to difference overall.

This article's concepts apply even for applications that involve only two categories. If an application has exactly two categories, then Allocation difference is entirely Exchange, while Shift does not exist. For example, Skowno et al. (2017) compared Grassland and Woodland at 1990 and 2013. They found it helpful to report that Quantity was greater than Allocation to describe classification error, while Quantity was less than Allocation to describe temporal change. Kganyago et al. (2018) reported that Exchange was larger than Quantity for the errors in the data from both Landsat 8 and SPOT 6 concerning detection of a non-native plant. Malinowski et al. (2015) reported Quantity and Allocation components to measure the errors in maps of a binary variable for 12 classification methods. The classification methods had various sizes of overall error, therefore it would have been helpful to have the insights that component intensities would have offered.

Other equations exist that are similar to but not identical to this article's equations. Warrens (2015) gave equations to compute relative Quantity disagreement and relative Allocation disagreement. Those relative metrics are ratios that include agreement in their denominators, thus are not identical to this article's intensities of differences. Specifically, Eq. (15) gives Warrens' relative Quantity disagreement for category i.

$$\phi_i = \left| \sum_{j=1}^{J} (C_{ij} - C_{ji}) \right| \Big/ \left[\sum_{j=1}^{J} (C_{ij} + C_{ji}) \right] \tag{15}$$

The summation in the numerator of ϕ_i for category i is analogous to the summation in the numerator of q'_j for category j. However, ϕ_i has a denominator that is larger than the denominator of q'_j because the denominator of ϕ_i includes two times the agreement for category i. Warrens' relative metrics can facilitate comparison of each category to other categories. It is not immediately clear how Warrens' relative metrics could compare each category to the difference overall, because Warrens does not give relative Quantity and Allocation disagreements overall. Ayala-Izurieta et al. (2017) use the equations of Warrens and give an additional equation for ϕ^*_i which is equivalent to Eq. (16).

$$\phi_i^* = q_i' / 100\% \tag{16}$$

Table 10 in Ayala-Izurieta et al. (2017) contains results that appear inconsistent with their equation for ϕ^*_i. The caption of their table 10 claims to give the relative components of Warrens, but the authors confirmed that the numbers in their table 10 are the components of Pontius and Santacruz (2014).

Readers can compute the three components by category and overall using two types of software. First, the *diffeR* package in R computes the sizes of components at multiple resolutions (Pontius and Santacruz, 2015). Multiple resolution analysis allows one to quantify the distances over which Exchange and Shift occur. The *diffeR* package does not yet compute component intensities. Second, the *PontiusMatrix* spreadsheet computes component sizes and intensities to produce figures of the format in this article. The spreadsheet's documentation and videos give instructions concerning how to customize the figures. The spreadsheet can convert a sample confusion matrix to an estimated population confusion matrix, which is essential for stratified sampling designs where the sampling density varies among the row categories.

5. Conclusions

This article presents concepts to interpret differences that derive from a square contingency table, such as a confusion matrix or a transition matrix. Previous work showed how to express the difference size as the sum of three components: Quantity, Exchange and Shift. This article introduces an additional procedure to compute each component's intensity as the component's size divided by the difference's size.

Comparison of intensities facilitates comparison among categories that have various sizes of differences. Users of the software R can use the package *diffeR* to compute the sizes of the components. Readers can compute both sizes and intensities of the components by entering their matrix into the *PontiusMatrix* spreadsheet, which they can obtain for free from www.clarku.edu/~rpontius.

Declarations of interest

None.

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