Clustering Accuracy

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Abstract. In this short paper, we explain how to compute the clustering accuracy in general k clusters in Matlab.

Let y_i be the true classification label for the i-th data. Let $\widehat{y}_i$ be the estimate of y_i we determined from classification algorithms. Let $y = (y_1, \cdots, y_n)$ and $\widehat{y} = (\widehat{y}_1, \cdots, \widehat{y}_n)$. The classification accuracy $A(y, \widehat{y})$ is given by

$$A(\widehat{y}, y) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(\widehat{y} = y),$$

where $\mathbf{1}$ is the indicator function.

In clustering, there is no direct association between true clustering labels and predicted cluster labels. Given k clusters $C_1, \cdots, C_k$, its permutation $\pi(C_1), \cdots, \pi(C_k)$ is also a valid cluster for $\pi \in \mathbb{S}_k$, the permutation group of order k. Suppose [1 1 2 1 1 3 3] is the estimated cluster labels when the true labels are [1 1 1 2 2 3 3]. Then any permutation of estimated cluster labels such as [2 2 1 2 2 3 3] and [3 3 1 3 3 2 2] are other valid cluster labels. There are $k!$ possible permutations in $\mathbb{S}_k$ (Chung et al. 2019). Thus the clustering accuracy is modified as

$$A(\widehat{y}, y) = \frac{1}{n} \max_{\pi \in \mathbb{S}_k} \sum_{i=1}^{n} \mathbf{1}(\pi(\widehat{y}) = y).$$

This a modification to an assignment problem and can be solved using the Hungarian algorithm in $\mathcal{O}(k^3)$ run time (Edmonds & Karp 1972). In Matlab, it can be solved using `confusionmat.m`, which tabulates misclustering errors between the true cluster labels and predicted cluster labels. The confusion matrix $C(\widehat{y}, y)$ is a matrix of size $k \times k$ tabulating the correct number of clustering in each cluster. The diagonal entries show the correct number of clustering while the off-diagonal entries show the incorrect number of clusters. In Matlab, it can be computed using `confusionmat.m`:

```
ytrue = [ 1 1 1  2 2 3 3]
ypred = [ 1 1 2  1 1 3 3]
C = confusionmat(ypred, ytrue)

C =
```

```
      2     2     0
      1     0     0
      0     0     2
```

Alternately, we can compute the confusion matrix by simply counting the number of correct clustering:

```
C=zeros(k);
n=length(ytrue);
for i=1:n
    C(ypred(i),ytrue(i))=C(ypred(i),ytrue(i))+1;
end
```

To compute the clustering accuracy, we need to sum the diagonal entries. But the above matrix `C` is one possible confusion matrix. Under the permutation of cluster labels, we can get different confusion matrices. For large k, it is prohibitive expensive to search for all permutations. Thus we need to maximize the sum of diagonals of the confusion matrix under permutation with weight $C = (c_{ij})$:

$$\frac{1}{n} \max_{Q \in \mathbb{S}_k} \operatorname{tr}(QC) = \frac{1}{n} \max_{Q \in \mathbb{S}_k} \sum_{i,j} q_{ij} c_{ij}, \qquad (1)$$

where $Q = (q_{ij})$ is the permutation matrix consisting of entries 0 and 1 such that there is exactly single 1 in each row and each column. This is a linear sum assignment problem (LSAP), a special case of linear assignment problem (Bougleux & Brun 2016). LSAP is solved using `matchpairs.m` in Matlab (Duff & Koster 2001):

```
M=matchpairs(C, 0, 'max');

M =
      2     1
      1     2
      3     3

accuracy = sum(C(sub2ind(size(C), M(:,1), M(:,2))))/n

accuracy=
   0.7143
```

The whole procedure is packaged into a single Matlab function `clustering_accuracy.m`, which can be downloaded from http://pages.stat.wisc.edu/~mchung/dynamicTDA/matlab/clustering_accuracy.m.

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