Leaf clustering using circular densities

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Abstract

In the biology field of botany, leaf shape recognition is an important task. One way of characterising the leaf shape is through the centroid contour distances (CCD). Each CCD path might have different resolution, so normalisation is done by considering that they are circular densities. Densities are rotated by subtracting the mean preferred direction. Distance measures between densities are used to produce a hierarchical clustering method to classify the leaves. We illustrate our approach with a real dataset.

Keywords: Circular density, center contour distance, hierarchical clustering.

1 Introduction

The branch of biology that studies plants is botany, also called phytology. Historically, plant kingdom contained all living things that were not animals, however, nowadays fungi and algae are excluded (Mauseth 2019). There are more than three hundred thousand species of plants, so species identification has been an important task to define such a taxonomy of plants.

There are several ways of characterising a plant, but most of them concentrate on the features of their leaves, such as shape, vein, colour and texture. One way of characterising the shape is through a centroid contour distance (CCD) (Cope et al. 2012). CCD is a contour-based approach that consists in segmenting the silhouette of the leaf in a two dimensional image, and for each pixel, compute its distance to the centroid. CCD depends on the
resolution of the image, so different leaves might have different number of CCD points recorded.

CCD data has to be normalised in two aspects. First, the same leaf might lead to two different CCD representations based on the scale (closeness of the camera to the leaf), second, the starting point recorded for each leaf might not be the same, so reported data is subject to a rotation. Authors have proposed different ways of achieving this normalisation.

Wang et al. (2000) for example, do a subsampling of the contour points to get rid of the scale and do a shifting of the curve wrappedly, but to minimize the number of rotations they also perform a thinning to find a skeleton and simplify the computations in the matching process. Teng et al. (2009) simply divide by the maximum value to get rid of the scale and use a circular shift together with a similarity measure to match rotations. On the other hand, Kadir et al. (2011) uses normalised polar Fourier coefficients to get rid of the scale and rotation and they further use other shape, colour, vein and texture features in a probabilistic neural network to classify. Finally, Hasim et al. (2016) did a manual rotation to ensure that all leaves are in a vertical position and do not propose any scale correction arguing that their classification method is invariant under scale changes.

In this article we propose to characterise the CCD data as circular densities. By doing so the normalisation process is straightforward. Distances between densities are use to define a dissimilarity matrix and perform a hierarchical clustering to classify the leaves.

The contents of the rest of the paper is as follows: In Section 2 we characterise the CCD data as circular densities and propose a simple normalisation process to get rid of scale and rotation problems. In Section 3 we propose four types of distances to perform a hierarchical clustering. Data analysis is carried out along Sections 2 and 3. We finally conclude in Section 4.
2 CCD data as circular densities

Let us assume that each leaf \( i \) is characterised by a sequence of size \( n_i \) of center contour distances (CCD) \( y_i = (y_{i1}, \ldots, y_{in_i}) \), where \( y_{ij} \) is the CCD at location \( x_{ij} \) for \( j = 1, \ldots, n_i \) and \( i = 1, \ldots, m \) with \( m \) the number of leaves in the sample. Usually, locations \( x_{ij} \) are not available but it is assumed that the \( n_i \) measurements cover the entire contour of the leaf. We will assume that locations are uniformly spread angles around the circle \((0, 2\pi] \) in radians, therefore \( x_{i,j} = 2\pi j / n_i \).

We use \( y_i \) and \( x_i \) to characterise each leaf by a circular density \( f_i(t) \) (e.g. Jammalamadaka and SenGupta, 2001) in the following way:

\[
 f_i(t) = c_i \sum_{j=1}^{n_i} y_{ij} I_{[x_{i,j-1}, x_{ij}]}(t),
\]

for \( t \in (0, 2\pi] \) where \( x_{i,0} = 0 \) and \( c_i \) is a normalising constant such that \( \int f_i(t) dt = 1 \). It is straightforward to show that \( c_i = 1/(2\pi \bar{y}_i) \) with \( \bar{y}_i = (1/n_i) \sum_{j=1}^{n_i} y_{ij} \). By defining densities as in (1) we get rid of the scale of the CCD data that is not relevant for the classification.

Another confounding aspect of the CCD data is the rotation, the first available measure \( y_{i1} \) might not be made at the same location of the leaf for different \( i \)'s. Since we have arbitrarily defined the locations \( x_{ij} \) around the circle, we suggest to rotate the densities in the following way. If we let \( T_i \) be a random variable with probability density \( f_i(t) \), then the preferred (mean) angle \( \mu_i \) is defined via the first trigonometric moments as \( \mu_i = \arctan^*(\beta_i/\alpha_i) \) with \( \alpha_i = E(\cos T_i) \) and \( \beta_i = E(\sin T_i) \). Here, \( \arctan^*(\beta_i/\alpha_i) \) is an slightly modified function defined as \( \arctan(\beta_i/\alpha_i) \) if \( \beta_i > 0 \) and \( \alpha_i > 0 \), \( \arctan(\beta_i/\alpha_i) + \pi \) if \( \alpha_i < 0 \), and \( \arctan(\beta_i/\alpha_i) + 2\pi \) if \( \beta_i < 0 \) and \( \alpha_i > 0 \). Therefore, we define the rotated random variable \( T^*_i = T_i - \mu_i \), which has density

\[
 f^*_i(t) = \frac{1}{2\pi \bar{y}_i} \sum_{j=1}^{n_i} y_{ij} I_{[x^*_{i,j-1}, x^*_{ij}]}(t),
\]

where \( x^*_{ij} = x_{ij} - \mu_i \).
In principle, circular densities are defined for \( t \in \mathbb{R} \) and must satisfy the property \( f_t^*(t + 2\pi) = f_t^*(t) \). Density (2) is a perfectly defined circular density, which is better depicted around a circle. However, we are used to plot densities in a Cartesian system. Doing so might not be direct since rotated densities might have negative \( x_{ij}^* \) values. Considering the circular property, we can force the support to be constrained to \( t \in (0, 2\pi] \) by replacing negative \( x_{ij}^* \) values by \( x_{ij}^* + 2\pi \).

To illustrate how our normalisation and rotation proposal works, let us consider a dataset of size \( m = 10 \), for which the type of plant is already known. Three of them are FRS, two MOS, three AVS and two AGS. Available information consists of CCD measurements \( y_i \) of unequal sizes \( n_i \), for \( i = 1, \ldots, m \). In particular, vector sizes are

\[
n = (3603, 3392, 3293, 2649, 2270, 3633, 3623, 3791, 3864, 3035).
\]

In Figure [1] we show the unnormalised densities (1), i.e. assuming \( c_i = 1 \) in the left panel, and normalised and rotated densities (2) in the right panel. We have used different colour and line type for the four plants types. First note that in the left panel, vertical scale goes from 0 to 1000 and lines have different amplitudes, AVS leaves (red dotted-dashed lines) have small amplitude, whereas AGS leaves (yellow dashed lines) have huge amplitudes. For the FRS plants (blue solid lines) the raw data did not show a scale problem but a rotation in one of the three leaves, however for the AGS plants (yellow dashed lines), rotation is not the problem but a mismatch in the scales between the two leaves. Both problems were resolved with our proposal in the right panel.

Apart from representing each leaf as a circular density, we can plot the actual leaves by considering that the pairs \((x_{ij}, c_iy_{ij})\) in (1) or \((x_{ij}^*, c_iy_{ij})\) in (2), for \( j = 1, \ldots, n_i \) and \( i = 1, \ldots, n \), are points in polar coordinates where the abscissa corresponds to the angle and the ordinate to the radius or resultant length. We can then transform the polar coordinates to Cartesian coordinates by doing \( u_{ij} = c_iy_{ij}\cos(x_{ij}) \) and \( v_{ij} = c_iy_{ij}\sin(x_{ij}) \) and plot the
pairs \((u_{ij}, v_{ij})\) for \(j = 1, \ldots, n_i\) and \(i = 1, \ldots, n\).

In Figure 2 we show the three leaves of FRS type. In the top line we show the original orientation \(1\), where leaves FRS.003 and FRS.001 (first and third) have a horizontal orientation, whereas leaf FRS.016 appears in diagonal. After implementing our rotation correction \(2\), shown in the second row, all three leaves are facing towards the west. Finally, Figure 3 presents all ten leaves after normalisation, scale and rotation corrections.

### 3 Hierarchical clustering

So far, each leaf \(i\), originally defined by its CCD measurements \(y_i\), has been characterised by the circular density \(f_i^*(t)\) given in (2). To perform a hierarchical clustering (e.g. Johnson and Wichern 2007) we need a similarity/dissimilarity measure between any two densities \(f_i^*(t)\) and \(f_k^*(t)\), say \(D(f_i^*, f_k^*)\). There are several options to measure distances between densities, here we consider three of them that include the \(L_1\), the total variation and the Hellinger distances:

\[
D_1(f_i^*, f_k^*) = \int_0^{2\pi} |f_i^*(t) - f_k^*(t)|dt
\]

\[
D_2(f_i^*, f_k^*) = \sup_{t \in (0, 2\pi]} |f_i^*(t) - f_k^*(t)|
\]

\[
D_3(f_i^*, f_k^*) = \int_0^{2\pi} \left[ \{f_i^*(t)\}^{1/2} - \{f_k^*(t)\}^{1/2} \right]^2 dt
\]

Alternatively, each circular density \(f_i^*(t)\) can be entirely characterised by its trigonometric moments, these are \(\alpha_i(p) = E\{\cos(pT_i)\}\) and \(\beta_i(p) = E\{\sin(pT_i)\}\) for \(p = 1, 2, \ldots\). If we only consider the first \(2r\) moments, we can use euclidean distance as dissimilarity measure. We call this \(D_4(f_i^*(t), f_k^*(t))\). This latter approach is similar to Kadir et al. (2011) in the sense that they use normalised polar Fourier coefficients, but we do not require further normalisation as they do.

Once we have the distance function, we have to decide the link method to define the distances between clusters. In our experience, complete linkage provides good clusterings.
since it minimises the maximum distance within clusters (Glasbey, 1987). We will use this link.

Figure 4 shows the dendrograms obtained for the ten leaves dataset and for the four distances. In particular, for distance $D_4$ we used $r = 5$ to characterise the densities. Larger values of $r$ were also tested but provided no difference in the clustering obtained. We note that the vertical axes show different scales due to the different distances used. Recall that a longer vertical line in a dendrogram means that the individuals below are more dissimilar to the others. In all cases, the group of the two AGS plants is well identified. The group of three FRS plants is also identified by the four dendrograms, however, it is better separated (longer line) by the total variation distance ($D_2$), followed by the $L_1$ ($D_1$) and trigonometric moments ($D_4$) distances. The least clear job is made by the Hellinger ($D_3$) distance. Regarding plants MOS and AVS, all four distances mixed up the identification of the types. This is understandable since green and red densities in Figure 1 (right panel) are overlapped, and green and red leaves pictures in Figure 3 look very similar. $L_1$ ($D_1$) distance joins the two MOS leaves with leaf AVS.028 and put together the other two AVS.012 and AVS.002 leaves. Total variation ($D_2$) distance puts together MOS.015, AVS.028 and AVS.012 in one group and MOS.001 and AVS.002 in another. Hellinger ($D_3$) distance forms the same groups as the total variation distance, but perhaps in a less clear way (shorter vertical lines). Finally, trigonometric moments combined with euclidean distances ($D_4$) produces the same groups as the $L_1$ distance.

In summary, $D_1$ & $D_4$ and $D_2$ & $D_3$ produce the sample clusterings. In terms of errors, $D_1$ & $D_4$ only misplace one leaf, whereas $D_2$ & $D_3$ misplace two leaves. Visually judging the dendrograms, we believe that $D_1$ & $D_4$ are equally good and $D_2$ is preferred to $D_3$ in terms of clarity to identify the groups.
4 Conclusions

We have efficiently solved the leaf classification problem by resorting to the theory of circular densities and hierarchical clustering. As in most clustering problems, different procedures produce different groupings and the scientist has to select the clustering that better represents prior knowledge, is easier to interpret or minimises a classification error. With the four distances used in our particular dataset, we only produced two different clusterings, which by looking at the plots, both can be justified.

We argue that the key aspect of our proposal is the representation of each leaf by a circular density, where scaling and rotation are easily solved.

Data analysis presented here was implemented in R (R Core Team, 2021) and it only takes a few seconds to run. Both code and dataset are available under request.

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Figure 1: CCD data as circular densities. Without normalisation (left) and with normalisation and rotation (right).

Figure 2: FRS leaves plot. Before rotation (top) and after rotation (bottom).
Figure 3: Leaves plot after rotation.
Figure 4: Hierarchical clustering dendrograms for the four different distances.