DEVELOPMENT OF AN INTELLIGENT SYSTEM USING KERNEL-BASED LEARNING METHODS FOR PREDICTING OIL-PALM YIELD

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Abstract:

Intelligent systems based on machine learning techniques, such as classification, clustering, are gaining wide spread popularity in real world applications. This paper presents our work on developing an intelligent system for predicting crop yield, for example oil-palm yield, from climate and plantation data. At the core of our system is a method for unsupervised partitioning of data for finding spatio-temporal patterns in climate data using kernel methods which offer strength to deal with complex data non-linearly separable in input space. This work gets inspiration from the notion that a non-linear data transformation into some high dimensional feature space increases the possibility of linear separability of the patterns in the transformed space. Therefore, it simplifies exploration of the associated structure in the data. Kernel methods implicitly perform a non-linear mapping of the input data into a high dimensional feature space by replacing the inner products with an appropriate positive definite function. In this paper we present a robust weighted kernel k-means algorithm incorporating spatial constraints for clustering climate data. The proposed algorithm can effectively handle noise, outliers and auto-correlation in the spatial data, for effective and efficient data analysis by exploring patterns and structures in the data, and thus can be used for predicting oil-palm yield by analyzing various factors affecting oil-palm yield.

Keywords: Pattern analysis, clustering, kernel methods, spatial data, oil-palm yield

1. Introduction

Oil-palm has become an important crop in Malaysia. However, oil-palm production potential is reduced when trees are exposed to stressful weather conditions. Low moisture is the most common stressful condition oil-palm faces, so monitoring rainfall and other related parameters (e.g. temperature, pressure, soil moisture, sun-shine duration, humidity, etc) is useful in predicting oil palm yield levels. The lagged effect of weather in Malaysia has implications for global vegetable oil prices in general and for the palm oil market in particular. Moreover, not enough is known about the daily patterns of rainfall or sunshine illumination levels to determine what may mitigate the expected negative effects of the heavy or below-normal rainfall [26]. Keeping this importance in view, this study is aimed at investigating the impacts of hydrological and meteorological conditions on oil-palm plantation using computational machine learning techniques. It is hoped that machine learning techniques would be very useful for analyzing the relationships between agro-hydrological parameters. Resulting improved understanding of the factors affecting oil-palm yield would not only help in accurately predicting yield levels but would also help substantially in looking for mitigating solutions.

Data clustering, a class of unsupervised learning algorithms, is an important and applications-oriented branch of machine learning. Its goal is to estimate the structure or density of a set of data without a training signal. It has a wide range of general and scientific applications such as data compression, unsupervised classification, image segmentation, anomaly detection, etc. There are many approaches to data clustering that vary in their complexity and effectiveness, due to the wide number of applications that these algorithms have. While there has been a large amount of research into the task of clustering, currently popular clustering methods often fail to find high-quality clusters.

A number of kernel-based learning methods have been proposed in recent years [3, 7, 8, 9, 15, 16, 21]. However, much research effort is being put up for improving these techniques and in applying these techniques to various application domains. Generally speaking, kernel function implicitly defines a non-linear transformation that maps the data from their original space to a high dimensional space where the data are expected to be more separable. Consequently, the kernel methods may achieve better performance by working in the new space. While powerful kernel methods have been proposed for supervised classification and regression problems, the development of effective kernel method for clustering, aside from a few tentative solutions [4, 9, 17], needs further investigation.

Finding good quality clusters in spatial data (e.g, temperature, precipitation, pressure, etc) is more challenging because of its peculiar characteristics such as auto-correlation, non-linear separability, outliers, noise, high-dimensionality, and when the data has clusters of widely differing shapes and sizes [11, 18, 22]. With this in view, we present a weighted kernel k-means clustering algorithm incorporating spatial constraints bearing spatial neighborhood information in order to handle spatial auto-correlation, outliers and noise in the spatial data.

This paper is organized as follows. In the next section, a brief overview of the problem area is given. In section 3, it is pointed out how kernel-based methods can be useful for clustering non-linearly separable and high-dimensional spatial (climate) data. Two currently proposed kernel-based algorithms are briefly reviewed in the next section. In section 5, a weighted kernel k-means algorithm with spatial constraints is presented which could be useful for handling noise, outliers and auto-correlation in the spatial data. In order to speed up computations, use of triangular inequality is described in section 6. Finally in section 8, brief discussion and conclusion are given.

2. Application Area and Methods

This work is focusing on clustering spatial data, e.g. for finding patterns in rainfall, temperature, pressure data so that their impact on other objects like vegetation (specifically oil-palm yield) etc could be explored. A very simplified view of the problem domain might look like as shown in Figure 1. The data for the problem domain might consist of a sequence of snapshots of the earth areas taken at various points in time, as shown in the figure. Each snapshot might consist of

measurement values for a number of variables e.g., temperature, pressure, precipitation, etc. All attribute data within a snapshot is represented using spatial frameworks, i.e., a partitioning of the study region into a set of mutually disjoint divisions which collectively cover the entire study region. This way we would be dealing with spatial time series data.

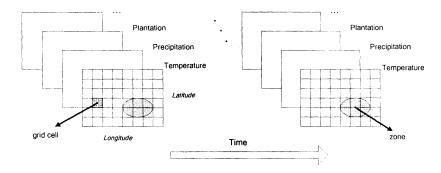


Figure 1. A simplified view of the problem domain

Clustering, often better known as spatial zone formation in this context, segments land into smaller pieces that are relatively homogeneous in some sense. While these zones can be specified directly by researchers, clustering provides a general data mining approach for automatically creating zones. Thus, our basic approach is to treat the zone creation problem as a cluster analysis problem. Cluster analysis groups objects (grid cells) so that the objects in a group are similar to one another and different from the objects in other groups. A goal of the work is to use clustering to divide areas of the land into disjoint regions in an automatic, but meaningful way that enables us to identify regions of the land whose constituent points have similar short-term and long-term characteristics. Given relatively uniform clusters we can then identify how various phenomena or parameters, such as precipitation, influence the climate and oil-palm produce (for example) of different areas.

The spatial and temporal nature of our target data poses a number of challenges. For instance, such type of earth science data is noisy. In addition, such data displays autocorrelation (i.e., measured values that are close in time and space tend to be highly correlated, or similar), high dimensionality (for example, if we consider monthly precipitation values at 1000 spatial points for 12 years, then each time series would be 144 dimensional vector), clusters of non-convex shapes, outliers.

If we apply a clustering algorithm to cluster time series associated with points on the land, we obtain clusters that represent land regions with relatively homogeneous behavior. The centroids of these clusters are time series that summarize the behavior of these land areas, and can be represented as indices. Consequently, clustering is an initial and key step in using data mining for the discovery of indices. Afterwards, the correlation between the clusters we have found can be analyzed.

Next, the influence of potential indices on land points can be evaluated. Specifically, we are interested in using a time series (cluster centroid, or otherwise) as indices if it can be used to

explain the behavior of a well-defined region of the land, especially with respect to oil-palm yield. One way of evaluating impact of indices on the land is to compute the correlation of each cluster centroid with each land point, where the behavior of a land point is described by a time series which captures the time dependent behavior of some variable (e.g., precipitation, temperature, pressure, humidity, oil-palm yield) associated with the land point. In this fashion, we can determine, for each land point, the cluster centroid with which it is most highly correlated.

3. System Overview and Architecture

For this application, the yield values of oil-palm plantation areas over a span of time constitute time series. The analysis of these and other time series (e.g., precipitation, temperature, pressure, etc) can be conducted using clustering technique. Clustering can be helpful in analyzing the impact of various hydrological and meteorological variables on the oil-palm plantation. Clustering enables us to identify regions of the land whose constituent points have similar short-term and long-term characteristics. Given relatively uniform clusters we can then identify how various parameters, such as precipitation, temperature etc, influence the climate and oil-palm produce of different areas using correlation. This way clustering can better help in detailed analysis of our problem.

In this application, the data consist of various agro-hydrological and meteorological parameters such as: rainfall, evaporation, air temperature, pressure, relative humidity, sunshine duration, soil temperature, oil-palm yield, etc. The objects (observations, events) in a particular agro-hydrologic environment may have certain temporal and spatial relationships. And, the objects are non-static and undergo some change with time. The rate of change varies from object to object. The nature of change may also vary. For example, an object may change in terms of its spatial configuration or location and may also change in terms of attributes. For example, one data set contains 1 year long time series of daily precipitation (365 observations total) for 100 climate divisions located in a specified region. A "climate division" is an (usually small) area comprising one or more meteorological stations. The data matrix is 365 (days) by 100 (objects). Cluster analysis can be performed on these data. The intent here is to create "component objects" or object clusters that emphasize raw spatial and temporal similarity. This way we can get indices values for various parameters on which we can perform correlation analysis. It will further assist in pattern discovery and analysis of data, thus enabling us to study the impact of various parameters on vegetation, e.g., on oil-palm yield and also to predict oil-palm yield from the available data.

With the steps outlined above, a simplified architecture of the agro-hydrological system look like as shown below:

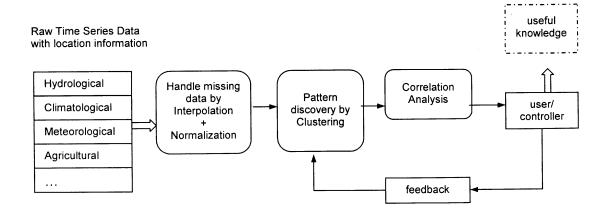


Figure 2: A simplified architecture for the system

4. Kernel-Based Methods

The kernel methods are among the most researched subjects within machine-learning community in recent years and has been widely applied to pattern recognition and function approximation. Typical examples are support vector machines [2, 6, 20], kernel Fisher linear discriminant analysis [14], kernel principal component analysis [17], kernel perceptron algorithm [5], just to name a few. The fundamental idea of the kernel methods is to first transform the original low-dimensional inner-product input space into a higher dimensional feature space through some nonlinear mapping where complex nonlinear problems in the original low-dimensional space can more likely be linearly treated and solved in the transformed space according to the well-known Cover's theorem. However, usually such mapping into high-dimensional feature space will undoubtedly lead to an exponential increase of computational time, i.e., so-called curse of dimensionality. Fortunately, adopting kernel functions to substitute an inner product in the original space, which exactly corresponds to mapping the space into higher-dimensional feature space, is a favorable option. Therefore, the inner product form leads us to applying the kernel methods to cluster complex data [9, 15].

Let a nonlinear transformation function ϕ maps the data into a higher dimensional space. Suppose there exists a function K, called a kernel function, such that,

$$K(x_i, x_j) = \phi(x_i) \cdot \phi(x_j)$$

A kernel function is substituted for the dot product of the transformed vectors, and the explicit form of the transformation function ϕ is not necessarily known. In this way, kernels allow large non-linear feature spaces to be explored while avoiding curse of dimensionality. Further, the use of the kernel function is less computationally intensive. The formulation of the kernel function from the dot product is a special case of Mercer's theorem [16].

Examples of some well-known kernel functions are given below:

- Polynomial: $K(x_i, x_j) = \langle x_i, x_j \rangle^d$
- Radial Basis Function (RBF): $K(x_i, x_j) = \exp(-\|x_i x_j\|^2 / 2\sigma^2)$
- Sigmoid: $K(x_i, x_j) = \tanh(\alpha < x_i, x_j > +\beta)$

5. Proposed Weighted Kernel K-Means with Spatial Constraints

Clustering has received a significant amount of renewed attention with the advent of nonlinear clustering methods based on kernels as it provides a common means of identifying structure in complex data [2, 4, 9, 15].

We first fix the notation: let $X = \{x_i\}_{i=1,\dots,n}$ be a data set with $x_i \in \mathbb{R}^N$. We call codebook the set $W = \{w_j\}_{j=1,\dots,k}$ with $w_j \in \mathbb{R}^N$ and k << n. The Voronoi set (V_j) of the codevector w_j is the set of all vectors in X for which w_j is the nearest vector, i.e.

$$V_j = \{x_i \in X | j = arg \min_{i=1,...,k} ||x_i - w_j||\}$$

For a fixed training set X the quantization error E(W) associated to the Voronoi tessellation induced by the codebook W can be written as

$$E(W) = \sum_{j=1}^{k} \sum_{x_i \in V_i} \left\| x_i - w_j \right\|^2$$
 (1)

K-means is an iterative method for minimizing the quantization error E(W) by repeatedly moving all codevectors to the arithmetic mean of their Voronoi sets. In the case of finite data set X and Euclidean distance, the centroid condition reduces to

$$w_j = \frac{1}{|V_j|} \sum_{x_i \in V_j} x_i \tag{2}$$

where $|V_j|$ denotes the cardinality of V_j . Therefore, k-means is guaranteed to find a local minimum for the quantization error.

The k-means clustering algorithm can be enhanced by the use of a kernel function; by using an appropriate nonlinear mapping from the original (input) space to a higher dimensional feature space, one can extract clusters that are non-linearly separable in input space. Usually the extension from k-means to kernel k-means is realised by expressing the distance in the form of kernel function [16]. The kernel k-means algorithm can be generalized by introducing a weight for each point x, denoted by u(x) [24]. This generalization would be powerful for making the algorithm more robust to noise and useful for handling auto-correlation in the spatial data. Using the non-linear function ϕ , the objective function of weighted kernel k-means can be defined as:

$$E(W) = \sum_{j=1}^{k} \sum_{x_i \in V_j} u(x_i) \| \phi(x_i) - w_j \|^2$$
(3)

$$w_j = \frac{\sum_{x_j \in \mathcal{V}_j} u(x_j) \phi(x_j)}{\sum_{x_j \in \mathcal{V}_j} u(x_j)}$$
(4)

The Euclidean distance from $\phi(x)$ to center w_j is given by (all computations in the form of inner products can be replaced by entries of the kernel matrix) the following eq.

$$\left\| \phi(x_i) - \frac{\sum_{x_j \in V_j} u(x_j) \phi(x_j)}{\sum_{x_j \in V_j} u(x_j)} \right\|^2 = K(x_i, x_i) - 2 \frac{\sum_{x_j \in V_j} u(x_j) K(x_i, x_j)}{\sum_{x_j \in V_j} u(x_j)} + \frac{\sum_{x_j, x_i \in V_j} u(x_j) u(x_i) K(x_j, x_i)}{\left(\sum_{x_j \in V_j} u(x_j)\right)^2}$$
(5)

In the above expression, the last term is needed to be calculated once per each iteration of the algorithm, and is representative of cluster centroids. If we write

$$C_{k} = \frac{\sum_{x_{j}, x_{i} \in V_{j}} u(x_{j})u(x_{l})K(x_{j}, x_{l})}{\left(\sum_{x_{j} \in V_{j}} u(x_{j})\right)^{2}}$$
(6)

With this substitution, eq (5) can be re-written as

$$\left\| \phi(x_i) - \frac{\sum_{x_j \in V_j} u(x_j) \phi(x_j)}{\sum_{x_j \in V_j} u(x_j)} \right\|^2 = K(x_i, x_i) - 2 \frac{\sum_{x_j \in V_j} u(x_j) K(x_i, x_j)}{\sum_{x_j \in V_j} u(x_j)} + C_k$$
(7)

For increasing the robustness of fuzzy c-means to noise, an approach is proposed in [1]. Here we propose a modification to the weighted kernel k-means to increase the robustness to noise and to account for spatial autocorrelation in the spatial data. It can be achieved by a modification to eq. (3) by introducing a penalty term containing spatial neighborhood information. This penalty term acts as a regularizer and biases the solution toward piecewise-homogeneous labeling. Such regularization is also helpful in finding clusters in the data corrupted by noise. The objective function (3) can, thus, be written as:

$$E(W) = \sum_{j=1}^{k} \sum_{x_i \in V_i} u(x_i) \| \phi(x_i) - w_j \|^2 + \frac{\gamma}{N_R} \sum_{j=1}^{k} \sum_{x_i \in V_i} u(x_i) \sum_{r \in N_k} \| \phi(x_r) - w_j \|^2$$
(8)

where N_k stands for the set of neighbors that exist in a window around x_i and N_R is the cardinality of N_k . The parameter γ controls the effect of the penalty term. The relative importance of the regularizing term is inversely proportional to the accuracy of clustering results.

For kernel functions, the following can be written

$$\|\phi(x_i) - w_j\|^2 = K(x_i, x_i) - 2K(x_i, w_j) + K(w_j, w_j)$$

If we adopt the Gaussian radial basis function (RBF), viz.

$$K(x_i, x_j) = \exp\left(-\frac{\left\|x_i - x_j\right\|^2}{2\sigma^2}\right)$$

then K(x, x) = 1, so eq. (8) can be simplified as

$$E(W) = 2\sum_{j=1}^{k} \sum_{x_i \in V_j} u(x_i) (1 - K(x_i, w_j)) + \frac{\gamma}{N_R} \sum_{j=1}^{k} \sum_{x_i \in V_j} u(x_i) \sum_{r \in N_k} (1 - K(x_r, w_j))$$
(9)

The distance in the last term of eq. (8), can be calculated as

$$\left\| \phi(x_r) - \frac{\sum_{x_j \in V_j} u(x_j) \phi(x_j)}{\sum_{x_j \in V_j} u(x_j)} \right\|^2 = 1 - 2 \frac{\sum_{x_j \in V_j} u(x_j) K(x_r, x_j)}{\sum_{x_j \in V_j} u(x_j)} + \frac{\sum_{x_j, x_j \in V_j} u(x_j) u(x_l) K(x_j, x_l)}{\left(\sum_{x_j \in V_j} u(x_j)\right)^2}$$
(10)

As first term of the above equation does not play any role for finding minimum distance, so it can be omitted, however.

$$\left\| \phi(x_r) - \frac{\sum_{x_j \in V_j} u(x_j) \phi(x_j)}{\sum_{x_j \in V_j} u(x_j)} \right\|^2 = 1 - 2 \frac{\sum_{x_j \in V_j} u(x_j) K(x_r, x_j)}{\sum_{x_j \in V_j} u(x_j)} + C_k = 1 - \beta_r + C_k$$
(11)

For RBF, eq. (5) can be written as

$$\left\| \phi(x_i) - \frac{\sum_{x_j \in V_j} u(x_j) \phi(x_j)}{\sum_{x_j \in V_j} u(x_j)} \right\|^2 = 1 - 2 \frac{\sum_{x_j \in V_j} u(x_j) K(x_i, x_j)}{\sum_{x_j \in V_j} u(x_j)} + C_k$$
(12)

As first term of the above equation does not play any role for finding minimum distance, so it can be omitted..

We have to calculate the distance from each point to every cluster representative. This can be obtained from eq. (8) after incorporating the penalty term containing spatial neighborhood information by using eq. (11) and (12). Hence, the effective minimum distance can be calculated using the expression:

$$-2\frac{\sum_{x_{j}\in V_{j}}u(x_{j})K(x_{i},x_{j})}{\sum_{x_{i}\in V_{k}}u(x_{j})}+C_{k}+\frac{\gamma}{N_{R}}\sum_{r\in N_{k}}(\beta_{r}+C_{k})$$
(13)

Now, the algorithm, weighted kernel k-means with spatial constraints, can be written as follows.

Algorithm SWK-means: Spatial Weighted Kernel k-means (weighted kernel k-means with spatial constraints)

SWK means
$$(K, k, u, N, \gamma, \varepsilon)$$

Input: K: kernel matrix, k: number of clusters, u: weights for each point, set $\varepsilon > 0$ to a very small value for termination, N: information about the set of neighbors around a point, γ : penalty term parameter,

Output: $w_1, ..., w_k$: partitioning of the points

- 1. Initialize the k clusters: $w_1=0, \ldots, w_k=0$
- 2. Set i = 0.
- 3. For each cluster, compute C(k) using expression (6)
- 4. For each point x, find its new cluster index as

$$j(x) = \arg\min_{j} \|\phi(x) - w_{j}\|^{2}$$
 using expression (13),

5. Compute the updated clusters as

$$w_i^{(i+1)} = \{x : j(x) = j\}$$

6. Repeat steps 3-4 until the following termination criterion is met:

$$\left\|W_{new} - W_{old}\right\| < \varepsilon$$

where, $W = \{w_1, w_1, w_1, \dots, w_k\}$ are the vectors of cluster centroids.

6. Handling Outliers

This section briefly discusses about spatial outliers, i.e., observations which appear to be inconsistent with their neighborhoods. Detecting spatial outliers is useful in many applications of geographic information systems and spatial databases, including transportation, ecology, public safety, public health, climatology, location-based services, and severe weather prediction. Informally, a spatial outlier is a local instability (in values of non-spatial attributes) or a spatially referenced object whose non-spatial attributes are extreme relative to its neighbors, even though the attributes may not be significantly different from the entire population.

We can examine how eq. (10) makes the algorithm robust to outliers. As $K(x_i, x_j)$ measures the similarity between x_i and x_j , and when x_i is an outlier, i.e., x_i is far from the other data points, then $K(x_i, x_j)$ will be very small. So, the second term in the above expression will get very low value or, in other words, the weighted sum of data points will be suppressed. The total expression will get higher value and hence results in robustness by not assigning the point to the cluster.

7. Scalability Issue

The pruning procedure used in [23, 25] can be adapted to speed up the distance computations in the weighted kernel k-means algorithm. The acceleration scheme is based on the idea that we can use the triangle inequality to avoid unnecessary computations. According to the triangle inequality, for a point x_i , we can write, $d(x_i, w_i^n) \ge d(x_i, w_i^o) - d(w_i^o, w_i^n)$. The distances between the corresponding new and old centers, $d(w_i^o, w_i^n)$ for all j, can be computed. And this information can be stored in a $k \times k$ matrix. Similarly, another $k \times n$ matrix can be kept that contains lower bounds for the distances from each point to each center. The distance from a point to its cluster centre is exact in the matrix for lower bounds. Suppose, after a single iteration, all distances between each point and each center, $d(x_i, w_i^o)$, are computed. In the next iteration, after the centers are updated, we can estimate the lower bounds from each point x_i to the new cluster center, w_i^n , using $d(w_i^o, w_i^n)$ calculations and the distances from the previous iteration, i.e., we calculate the lower bounds as $d(x_i, w_i^o) - d(w_i^o, w_i^n)$. The distance from x_i to w_i^n is computed only if the estimation is smaller than distance from x_i to its cluster center. This estimation results in sufficient saving in computational time. Once we have computed lower bounds and begin to compute exact distances, the lower bound allows us to determine whether or not to determine remaining distances exactly.

8. Conclusions

In this paper, a few challenges especially related to clustering spatial data are pointed out. Among these, the important issues/problems that need to be addressed are: i) non-linear separability of data in input space, ii) outliers and noise, iii) auto-correlation in spatial data, iv) high dimensionality of data.

The strengths of kernel methods are outlined, which are helpful for clustering complex and high dimensional data that is non-linearly separable in input space. With regard to addressing these problems, and consequently developing a prediction engine for oil-palm yield, we presented weighted kernel k-means incorporating spatial constraints. The proposed algorithm has the mechanism to handle spatial autocorrelation, noise and outliers in the spatial data. We are getting promising results on our test data sets. It is very much hoped that the algorithm would prove to be robust and effective for spatial (climate) data analysis, and it would be very useful for oil-palm yield prediction by working at the core of the prediction system. In future we plan to investigate the estimation of optimal number of clusters automatically.

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