KMeans Kernel Classifier

Course: Math Behind ML

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***Abstract*—The least squares SVM is a kernel method for non-linear regression and classification tasks. Here we combine KMeans clustering with the least squares SVM. First KMeans clustering is used to extract a set of representative vectors for each class, and then LS-SVM uses these representative vectors as a training dataset for the classification task**

I. Introduction

The kernel methods transform a given non-linear problem into a linear one by using a similarity kernel function $\Omega(x, x\prime)$. It is a similarity function defined over pairs of input data points $(x, x\prime)$. This way the input data is mapped into a higher dimensional feature space $\phi(x)$, where the inner product $\langle \cdot \ , \ \cdot \rangle$ can be calculated using Mercer's condition:

$$\Omega(x, x\prime) = \langle x \ , \ x\prime \rangle \tag{1}$$

Consider $\chi = \{x_n | n = 1, \ldots, N\}$ as training dataset.
Representer theorem: Any non-linear function $f : \chi \longrightarrow \mathbb{R}$ can be expressed as linear combination of kernel products on training dataset which was mentioned above earlier.

$$f(x) = \sum_{n=1}^{N} a_n \Omega(x, x_n) \tag{2}$$

Time complexity of LS-SVM is $O(N^3)$ where N is size of the training dataset which is too high and makes it unsuitable for large dataset. So for this reason we use KMeans clustering to extract a set of representative vectors for each class, and then LS-SVM uses these representative vectors as a training dataset for the classification task. This way we can reduce the time complexity of LS-SVM to $O((KQ)^3)$ where K is the number of classes and Q is number of centroids in each class. These representative vectors are also called as **centroids**. These are then used by LS-SVM to classify the test data. This KMeans-LS-SVM method has some advantages:

1) It is faster than LS-SVM.
2) It is more robust.
3) It is very easy to implement.

II. Kernel LS-SVM Classifer

We already know that in binary classification, kernel SVM method constructs a hyperplane with the maximal margin between the two classes in feature space $\phi(x)$. This can be represented as convex quadratic programming problem involving inequality constraints.

The kernel LS-SVM simplifies the optimization problem by considering equality constraints only, such that solution is obtained by solving a system of linear equations. Now this problem is similar to ridge regression problem which is formulated as follows:

$$\min_{w,b} \frac{1}{2} w^T w + \frac{\gamma}{2} \sum_{n=1}^{N} (\hat{y}_n - w^T \phi(x_n) - b)^2 \tag{3}$$

Assume that K classes are encoded using standard basis in $\mathbb{R}^K$, i.e, let $x_i \in C_k$, then output y_i is a vector with 1 in the k^{th} position and 0 elsewhere:

$$y_{ij} = \begin{cases} 1 & \text{if } x_i \in C_j \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

Consider input data $\{(x_i, yi) | x_i \in \mathbb{R}^{\mathbb{M}}, y_i \in \mathbb{R}^{\mathbb{K}}, i = 1, \ldots, N\}$ and the feature mapping function $\phi(x)$. The kernel LS-SVM is formulated as follows:

$$\min_{w,b} S(w, b, \epsilon) = \frac{1}{2} \sum_{j=1}^{K} w_j^T w_j + \frac{\gamma}{2} \sum_{i=1}^{N} \sum_{j=1}^{K} (\epsilon_{ij})^2 \tag{5}$$

subject to

$$\langle \phi(x)\ ,\ \omega_j \rangle + b_j = y_{ij} - \epsilon_{ij}, i = 1, \dots, N; j = 1, \dots, K \tag{6}$$

$$w_j^T \phi(x_i) + b_j = y_{ij} - \epsilon_{ij}, i = 1, \dots, N; j = 1, \dots, K \tag{7}$$

where $\epsilon_{ij} \geq 0$ are approximation errors, b_j is bias coefficient, $w^{(j)}$ is the vector of weights corresponding to the j^{th} class. The objective function S is a sum of least squares errors and the regularization term. This regularization parameter γ corresponds to a multi-dimensional version of the ridge regression problem.

In the primal weight space the multi class classifier takes the form:

$$x \in C_k, \Leftrightarrow k = arg \max_{j=1,\dots,K} g_j(x)$$

$$\text{where } g_j(x) = \frac{\exp(\langle \phi(x)\ ,\ w^{(j)} \rangle) + b_j)}{\sum_{i=1}^{K} \exp(\langle \phi(x)\ ,\ w^{(i)} \rangle) + b_i)}$$

Here g_j is the non-linear soft max function

Now applying Lagrangian to (5)

$$L(w, b, \epsilon, a) = S(w, b, \epsilon)$$
$$- \sum_{i=1}^{N} \sum_{j=1}^{K} a_{ij} [\langle \phi(x)\ ,\ \omega_j \rangle + b_j - y_{ij} + \epsilon_{ij}]$$

where $a_{ij} \in \mathbb{R}$ is the lagrange multiplier. Now applying KKT conditions:

$$\frac{\partial L}{\partial w^{(j)}} = 0 \implies w^{(j)} = \sum_{n=1}^{N} a_{nj} \phi(x_n) \tag{8}$$

$$\frac{\partial L}{\partial b_{(j)}} = 0 \implies \sum_{i=1}^{N} a_{ij} = 0 \tag{9}$$

$$\frac{\partial L}{\partial \epsilon_{(ij)}} = 0 \implies a_{ij} = \gamma \epsilon_{ij} \tag{10}$$

$$\frac{\partial L}{\partial a_{(ij)}} = 0 \implies \langle \phi(x)\ ,\ \omega_j \rangle + b_j - y_{ij} + \epsilon_{ij} = 0 \tag{11}$$

Now from eq(10) , eq(12) and eq(13):

$$\sum_{n=1}^{N} [\Omega(x_i, x_n) + \gamma^{-1} \delta_{in}] a_{nj} + bj = y_{ij}, \tag{12}$$

Here δ_{in} is the Kronecker delta function: where $\delta_{in} = 1$ if $i = n$ and 0 otherwise

As you can see in eq(14) there are K independent system of equations with binary labels y_{ij}. Now each system can be written in the matrix form as follows:

$$\begin{bmatrix} 0 & u^T \\ u & \Omega + \gamma^{-1} I \end{bmatrix} \begin{bmatrix} b_j \\ a^{(j)} \end{bmatrix} = \begin{bmatrix} 0 \\ y_j \end{bmatrix}, j = 1, \dots, K \tag{13}$$

Here $I_{N \times N}$ is the identity matrix, $u_{N \times 1} = [1, \dots, 1]^T$ is a vector of ones, $a_{N \times 1}^{(j)} = [a_{1j}, \dots, a_{Nj}]^T$ is weights and $y_j = [y_{1j}, \dots, y_{Nj}]^T$ is the vector of binary labels for the j^{th} class. Each system has $N+1$ linear equations with $N+1$ unknowns.

$$\Theta = \begin{bmatrix} 0 & u^T \\ u & \Omega + \gamma^{-1} I \end{bmatrix} \tag{14}$$

All the K systems can be written as:

$$\Theta W = Z \tag{15}$$

where

$$W_{(N+1) \times K} = \begin{bmatrix} b_1 & \dots & b_K \\ a^{(1)} & \dots & a^{(K)} \end{bmatrix}, Z_{(N+1) \times K} = \begin{bmatrix} 0 & \dots & 0 \\ y_1 & \dots & y_K \end{bmatrix}$$

Now once all the K systems are solved, we consider multi-class classifier in dual space(from eq (14)) as follows:

$$g_j(x) = \frac{\exp(\langle \phi(x)\ ,\ w^{(j)} \rangle) + b_j)}{\sum_{i=1}^{K} \exp(\langle \phi(x)\ ,\ w^{(i)} \rangle) + b_i)}$$

From eq(9) and eq(10), we get:

$$g_j(x) = \frac{\sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{nj} + b_j)}{\sum_{i=1}^{K} \sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{ni} + b_i)}$$

Now our problem becomes:

$$x \in C_k, \Leftrightarrow k = arg \max_{j=1,\dots,K} g_j(x)$$

$$\text{where } g_j(x) = \frac{\sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{nj} + b_j)}{\sum_{i=1}^{K} \sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{ni} + b_i)}$$

Here g_j is the non-linear soft max function

III. KMeans Clustering

First we use KMeans clustering algorithm to extract a set of representative vectors for each class. Now this representative vectors will be passed into LS-SVM kernel model as training dataset. KMeans clustering algorithm is as follows:

1) Take $\{x_i^k | x_i^k \in \mathbb{R}^{\mathbb{M}}, i = 1, \dots, N_k\}$ as training samples for class C_k where N_k is the number of training samples for the class C_k and $N = \sum_{k=1}^{K} N_k$ is the total number of training samples.
2) Take $\{\mu_q^k | \mu_q^k \in \mathbb{R}^{\mathbb{M}}, q = 1, \dots, Q\}$ as initial centroids for class C_k where $Q < N_K$ is the number of centroids for class C_k.

3) Build a matrix $X_k = [x^k_{im}]_{N_k \times M}$ where each row is a training sample for class C_k.
4) Build a matrix $\Xi_k = [\xi^k_{qm}]_{Q \times M}$ where each row is a randomly initialized centroid for class C_k.
5) Let $R_k = X_k \Xi_k^T = [r^k_{iq}]_{N_k \times Q}$
6) Let $\hat{R}_k = [r^{\hat{k}}_{iq}]_{N_k \times Q}$ be transformed sparse matrix of R_k where:

$$r^{\hat{k}}_{iq} = \begin{cases} 1 & \text{if } q = \arg\max_q r^k_{iq} \\ 0 & \text{otherwise} \end{cases} \quad i = 1, \ldots, N_k$$

Each sample is assigned to the nearest centroid.

7) $\hat{\Xi}_k = \hat{R}_k^T X_k = [\xi^{\hat{k}}_{qm}]_{Q \times M}$.
This is the new set of centroids.
8) Normalizing new set of centroids:

$$\xi^{\hat{k}}_q = \frac{\hat{\xi^k_q}}{||\hat{\xi^k_q}||} \qquad q = 1, \ldots, Q$$

9) Computing alignment deviation between new set and old set of centroids:

$$\delta = 1 - \frac{\sum_{q=1}^{Q} \langle \hat{\xi^k_q} \;\; \xi^k_q \rangle}{Q}$$

10) $\Xi_k = \hat{\Xi}_k$
11) Repeat steps 5 to 10 until $\delta < \beta$ where β is the tolerance.
12) Return Ξ_k

Here β is considered as small as possible.

IV. KMeans Kernel LS-SVM Classifier

After extracting a set of representative vectors for each class $C_k, k = 1, \ldots, K$ using KMeans clustering, we pass these KQ centroids into LS-SVM kernel model as training dataset. Training dataset for LS-SVM before KMeans clustering:

$$\{(x^k_i, y^k_i) | x^k_i \in \mathbb{R}^{\mathbb{M}}, y^k_i \in \mathbb{R}^{\mathbb{K}}, i = 1, \ldots, N\}$$

Training dataset for LS-SVM after KMeans clustering:

$$\{(\xi^k_q, y^k_q) | \xi^k_q \in \mathbb{R}^{\mathbb{M}}, y^k_q \in \mathbb{R}^{\mathbb{K}}, q = 1, \ldots, KQ\}$$

As you can see the training dataset size is reduced from N to KQ where $KQ < N$.

Previously there were $N + 1$ linear equations with $N + 1$ unknowns and $O(N^3)$ time complexity.

Now there are $KQ + 1$ linear equations with $KQ + 1$ unknowns and $O((KQ)^3)$ time complexity.

As we discussed earlier our problem previously was:

$$x \in C_k, \Leftrightarrow k = arg \max_{j=1,\ldots,K} g_j(x)$$

$$\text{where } g_j(x) = \frac{\sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{nj} + b_j)}{\sum_{i=1}^{K} \sum_{n=1}^{N} \exp(\Omega(x, x_n) a_{ni} + b_i)}$$

Now our problem becomes:

$$x \in C_k, \Leftrightarrow k = arg \max_{j=1,\ldots,K} g_j(x)$$

$$\text{where } g_j(x) = \frac{\sum_{n=1}^{KQ} \exp(\Omega(x, \xi^k_n) a_{nj} + b_j)}{\sum_{i=1}^{K} \sum_{n=1}^{KQ} \exp(\Omega(x, \xi^k_n) a_{ni} + b_i)}$$

Here g_j is the non-linear soft max function

V. Application

VI. Conclusion