Pattern Recognition 85 (2019) 70–77

Contents lists available at ScienceDirect

Pattern Recognition

journal homepage: www.elsevier.com/locate/patcog

Exploiting multiplex data relationships in Support Vector Machines

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ARTICLE INFO

Article history:
Received 25 August 2017
Revised 30 May 2018
Accepted 31 July 2018
Available online 1 August 2018

Keywords:
Multiplex data relationships
Support Vector Machine
Graph-based regularization
Multiple Kernel Learning

ABSTRACT

In this paper, a novel method for introducing multiplex data relationships to the SVM optimization process is presented. Different properties about the training data are encoded in graph structures, in the form of pairwise data relationships. Then, they are incorporated to the SVM optimization problem, as modified graph-regularized basekernels, each highlighting a different property about the training data. The contribution of each graph-regularized kernel to the SVM classification problem, is estimated automatically. Thereby, the solution of the proposed modified SVM optimization problem lies in a regularized space, where data similarity is expressed by a linear combination of multiple single-graph regularized kernels. The proposed method exploits and extends the findings of Multiple Kernel Learning and graph-based SVM method families. It is shown that the available kernel options for the former can be broadened, and the exhaustive parameter tuning for the latter can be eliminated. Moreover, both method families can be considered as special cases of the proposed formulation, hereafter. Our experimental evaluation in visual data classification problems denote the superiority of the proposed method. The obtained classification performance gains can be explained by the exploitation of multiplex data relationships, during the classifier optimization process.

1. Introduction

Computer vision/visual analysis methods have found industrial applications in several areas such as in robotic systems e.g., unmanned aerial vehicles and virtual reality, and their growth over the past few years have been immense. Such visual analysis applications including face recognition, object recognition, human action recognition, human/object tracking and many other applications, are commonly addressed as classification problems [1,2]. One of the most widely studied classification methods in visual analysis applications is the Support Vector Machines (SVM) classifier. SVM-based methods and extensions have been employed in mathematical/engineering problems including one-class and multiclass classification, regression and semi-supervised learning [3–6]. In its simplest form, SVM learns from labeled data examples originating from two classes, the hyperplane that separates them with the maximum margin, at the training data input (or feature) space. After its first proposal, SVM has been extended to determine decision functions in feature spaces obtained by employing non-linear data mappings, where data similarity is implicitly expressed by a kernel function. The explicit data mapping is not required to be known, if the adopted kernel function satisfies Mercer conditions [7]. Common practices for determining a feature space where SVM provides satisfactory performance to a given classification/regression problem, involve selecting a kernel function from a set of widely adopted kernel functions e.g., polynomial, sigmoid, Radial Basis Function (RBF), and thereby tuning the corresponding hyperparameters using e.g., cross validation, based on previous knowledge about the problem at hand. In every case, the performance of SVM heavily depends on the adopted kernel function choice, since the optimal solution for each problem might lie in unknown feature spaces.

In order to determine the optimal feature space for SVM operation, Multiple Kernel Learning (MKL) methods have been proposed. Their basic assumption is that the optimal underlying data mapping, i.e., the optimal kernel function, is a weighted combination (either linear or non-linear) of Multiple Kernel functions, the so-called basekernels [8–11]. The participation of each kernel to the optimal solution is determined by a parameter vector, i.e., the basekernel weights. The weights of the basekernels are estimated in an automated fashion along with the SVM hyperplane, by following an additional optimization procedure (e.g., single-step sequential optimization, two-step optimization). Standard MKL methods employ L_p or L_1 loss functions for determining the kernel weights, with the latter producing sparse solutions and the former providing fast convergence [12,13]. Besides the important theoretical advancements of MKL methods, only few basekernel combinations have found to be successful in realistic applications, i.e.,

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https://doi.org/10.1016/j.patcog.2018.07.032
0031-3203/

MKL methods method might suffer from overfitting issues or limited performance gains [11–13].

A alternative approach for improving classification performance, are methods that introduce additional optimization options to the standard SVM optimization problem, exploiting discriminant/manifold learning criteria [6]. That is, slightly modified SVM-based optimization problems have been proposed, that lead to standard SVM solutions in regularized spaces, expressed by a geometric transformation of the derived SVM hyperplane with the adopted criteria. For example, employing discriminant learning information e.g., within-class variance information [14], promotes SVM hyperplanes that span along low data variance directions [15,16]. Alternatively, SVM-based methods have been proposed for semi-supervised learning case, by integrating SVM with manifold learning [6], by exploiting kNN graphs as additional regularization criteria. It has been shown that exploiting such criteria at the fully supervised learning case is also beneficial to the classification performance. Since advances in graph-theory allow several manifold/discriminant learning criteria to be expressed using generic graph-based representation [17], methods incorporating the underlying data geometry in the SVM optimization problem can be implemented through graph-based SVM methods [18–20]. The adoption of generic graph structures within the SVM optimization process, containing e.g., intrinsic (within-class), or between-class data relationships, promotes solutions that are less prone to over-fitting. The disadvantage of graph-based SVM methods is that deriving the optimal classification space requires the evaluation of different graph settings, as well as tuning the additional introduced hyperparameters.

In visual analysis applications, MKL and graph-based SVM methods have been successfully employed over the past few years. Their success can be mainly attributed to the exploitation of the multimodal/multiplex structure of images and video data [21], related to e.g., spatial and temporal information, information extracted by multiple descriptor types, or even noise generated by camera movement, multiple viewing angles and illumination changes. All this information cannot be efficiently encoded with a single kernel matrix. Our work was inspired by the successful exploitation of multiple graphs in related application scenarios, e.g., label propagation [22–26]. Therefore, we have devised a classification method that introduces multiple graphs to the SVM optimization problem, by exploiting the intuitions of both MKL and graph-based SVM method families.

In this paper, a novel classification method that incorporates multiplex data relationships to the SVM optimization process, is presented. Multiplex data relationships are encoded in the form of multiple graph structures, containing pairwise data relationships, each corresponding to a specific data property. We propose a modified SVM optimization problem, that incorporates this information. As an effect, the generated SVM hyperplane is driven to directions where the most discriminant training data properties are highlighted. From our derivations, it is shown that the solution of the proposed optimization problem lies in a modified space, where data similarity is explicitly determined by a linear combination of graph-regularized kernel matrices. Moreover, it is proven that both Multiple Kernel Learning and Graph-based SVM method families method families can be formulated as special cases of the proposed method, hereafter. Finally, the proposed method exploits and extends the findings of Multiple Kernel Learning and graph-based SVM method families, by broadening the available kernel options for the former, and eliminating exhaustive parameter tuning for the latter.

2. Related work

In this section, we overview the preliminary material required to introduce the proposed method. Section 2.1 contains the description of the generic MKL–SVM optimization problem and Section 2.2 contains an overview of the recently proposed Graph-Embedded Support Vector Machines, exploiting a single graph in its optimization problem for regularization purposes.

2.1. Multiple Kernel learning support vector machines

Let a set of labeled data $\mathcal{S} = \{\boldsymbol{x}_i, y_i\}, i = 1, \ldots, N$ sampled from $\mathcal{X} \times \mathcal{Y}$, where $\mathcal{X} \in \mathbb{R}^D$ and $\mathcal{Y} \in \{-1, 1\}$, that is employed in order to train an SVM classifier. MKL–SVM methods optimize for implicitly determining the optimal feature space for solving the SVM optimization problem. Similarity in that space is reproduced by a linear or non-linear combination of Multiple Kernel functions [10,13,27–30]. Let M mapping functions $\phi_m(\cdot) \mapsto \mathcal{H}^m, m = 1, \ldots, M$ that have been employed as base data mappings. Similarity in the respective spaces is reproduced by the associated basekernel function $\kappa_m(\cdot, \cdot) = \phi_m(\cdot)^T \phi_m(\cdot)$, and $\mathcal{H}^m$ is a Reproducing Kernel Hilbert Space (RKHS). Assuming M basekernels have been linearly combined, then the obtained space $\mathcal{H}$ is also a RKHS, reproduced by kernel $\kappa(\cdot, \cdot)$. Similarity in that space can be calculated explicitly by a weighted summation of the basekernels, as follows:

$$\kappa(\cdot, \cdot) = \sum_{m=1}^{M} \mu_m \kappa_m(\cdot, \cdot), \tag{1}$$

where κ_m is the mth kernel function weighted by a parameter $\mu_m \geq 0$.

In order to learn the kernel weighting parameters μ_m and the optimal SVM hyperplane at the same time, the MKL–SVM optimization problem is formed as a max-min optimization problem:

$$\max_{\boldsymbol{\alpha}} \min_{\boldsymbol{\mu}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \sum_{m=1}^{M} \mu_m \kappa_m(\boldsymbol{x}_i, \boldsymbol{x}_j)$$
$$\text{s.t.} \quad 0 \leq \alpha_i \leq c \quad \text{and} \quad \sum_{m=1}^{M} \mu_m^p = 1, \tag{2}$$

where $\boldsymbol{a}$ is the support vector coefficient vector and $p \geq 1$ is a parameter that affects the sparsity of the obtained basekernel combination. The above defined optimization problem can be solved sequentially or in an iterative manner, keeping $\boldsymbol{a}$ or $\boldsymbol{\mu}$ as constants in the respective optimization steps. Assuming that the kernel weighting parameters $\boldsymbol{\mu}$ have been determined, then $\boldsymbol{K} = \sum_{m=1}^{M} \mu_m \boldsymbol{K}_m$ is the kernel matrix that can be employed for solving the standard SVM classification problem. According to Representer Theorem [7], the relevant SVM hyperplane $\boldsymbol{w} = \boldsymbol{\Phi a}$ that lies in the RKHS $\mathcal{H}$, can be reconstructed by the determined support vector coefficient vector $\boldsymbol{a}$ and the arbitrary training data representations $\boldsymbol{\Phi} \in \mathcal{H}$. Data similarity in that space can only be reproduced by the basekernel combination, since the kernel $\boldsymbol{K}$ cannot be calculated, otherwise.

After training the classifier, a test sample $\boldsymbol{x}$ is classified to the positive or negative training class, according to the outputs of the following decision function:

$$f(\boldsymbol{x}) = \sum_{i=1}^{N} y_i \alpha_i \sum_{m=1}^{M} \mu_m \kappa_m(\boldsymbol{x}_i, \boldsymbol{x}) + b, \tag{3}$$

where b is the standard SVM bias term. Finally, the test sample is classified to the positive class if $sign(f(\boldsymbol{x})) \geq 0$ or the negative class, otherwise.

2.2. Support Vector Machines exploiting geometric data relationships

Graph-based SVM methods exploit data relationships expressed by a single graph in the SVM optimization problem [18,20]. To this end, it is assumed that the training data $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ have been embedded in an undirected weighted graph $\mathcal{G} = \{\mathcal{X}, \mathbf{W}\}$, where $\boldsymbol{W} \in \mathbb{R}^{N \times N}$ is the graph weight matrix. It should be noted that non-linear data relationships might be expressed as well, by

employing the explicit data mappings in a feature space i.e., $\mathcal{X} = \{\phi(\boldsymbol{x}_1), \ldots, \phi(\boldsymbol{x}_N)\}$, where $\phi(\cdot) : \mathbb{R}^D \mapsto \mathcal{H}$ is mapping function. In either case, the matrix $\boldsymbol{S}$ can be employed to preserve data relationships expressed by $\mathcal{G}$, in the feature space $\mathcal{H}$. The definition of $\boldsymbol{S}$ is the following:

$$\boldsymbol{S} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} W_{ij}\big(\phi(\boldsymbol{x}_i) - \phi(\boldsymbol{x}_j)\big)\big(\phi(\boldsymbol{x}_i) - \phi(\boldsymbol{x}_j)\big)^T = \boldsymbol{\Phi}\boldsymbol{L}\boldsymbol{\Phi}^T, \quad (4)$$

where $\boldsymbol{L} \in \mathbb{R}^{N\times N}$ is the graph Laplacian matrix defined by $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{W}$, where $\boldsymbol{D} \in \mathbb{R}^{N\times N}$ is the (diagonal) degree matrix having elements $[\boldsymbol{D}]_{ii} = \sum_{i\neq j}[\boldsymbol{W}]_{ij}$, $i = 1, \ldots, N$, and $\boldsymbol{\Phi}$ is a matrix containing the data representations in $\mathcal{H}$. Depending on the exploited graph type [17], $\boldsymbol{L}$ can be used in order to describe geometric data relationships employed in several dimensionality reduction and manifold learning techniques, such as Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), Clustering-based Discriminant Analysis (CDA), Laplacian Eigenmap (LE) and Locally Linear Embedding (LLE) [17,19,20]. Finally, the Graph-Embedded SVM (GE-SVM) optimization problem is defined as follows [18,20]:

$$\begin{aligned} \min_{\boldsymbol{w},\boldsymbol{\xi},b} \quad & \frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{\lambda}{2}\boldsymbol{w}^T\boldsymbol{S}\boldsymbol{w} + c\sum_{i=1}^{N}\xi_i + b, \\ \text{s.t.} \quad & y_i\big(\boldsymbol{w}^T\phi(\boldsymbol{x}_i) + b\big) \leq 1 - \xi_i, i = 1, \ldots, N, \\ & \xi_i \geq 0, \end{aligned} \quad (5)$$

while an additional constraint $\boldsymbol{w}^T\boldsymbol{S}\boldsymbol{w} > 0$ is also imposed demanding that the matrix $\boldsymbol{S}$ is positive semi-definite. Compared to standard SVM, an additional parameter $\lambda \geq 0$ is introduced, that controls the amount of regularization introduced by the second term. GE-SVM can be considered a generalization of other SVM-based methods, e.g., given a value of $\lambda = 0$, the method degenerates to standard SVM. Depending on the definition of $\boldsymbol{S}$, GE-SVM is equivalent to previously devised regularized SVM methods such as the Minimum Variance SVM [15] or Laplacian SVM [6].

The equivalent dual problem is defined as follows:

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \quad & \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \phi(\boldsymbol{x}_i)^T(\boldsymbol{I} + \lambda\boldsymbol{S})^{-1}\phi(\boldsymbol{x}_j), \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq c. \end{aligned} \quad (6)$$

Finally, in order to classify a test sample, the standard SVM decision function is employed, by employing a regularized kernel of the following form:

$$\tilde{\kappa}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi(\boldsymbol{x}_i)^T(\boldsymbol{I} + \lambda\boldsymbol{S})^{-1}\phi(\boldsymbol{x}_j). \quad (7)$$

GE-SVM can be solved using standard SVM implementations, by replacing the standard kernel matrix with the one defined above. As have been shown in recent work, GE-SVM outperforms the standard SVM [18,20], in almost every SVM classification task, including one-class classification [19], and in some cases by a large extent. However, the increased classification performance comes with the cost of increased computational complexity, related to inefficient parameter tuning. The required parameters to be tuned include the standard SVM parameter c and the introduced parameter λ, and moreover, depending on the adopted graph type, even more hyperparameters are required to be tuned as well, e.g., k for the kNN graph case. Graph-hyperparameter selection is even more complex for the state-of-the-art performing positive and negative graph exploitation case [20]. The demanding computational complexity of GE-SVM limit its exploitation options in realistic application scenarios.

3. Multiplex data relationships in Support Vector Machines

In this Section, we describe in detail the proposed method, which extends the standard SVM problem, by incorporating additional optimization criteria, in addition to maximizing the classification margin. These criteria include incorporating geometric or semantic information about the training data, e.g., within-class variance information, local geometric data relationships information, expressed with multiple graph structures, i.e., multiplex data relationships. Their detailed mathematical description is given in Section 3.1. The introduced terms have the effect of projecting the SVM hyperplane in such directions, where the respective information of each additional term is emphasized. Moreover, a weighting parameter is introduced, that determines the contribution of each term to the final solution. From our derivations, analytically described in Section 3.2, it is proven that each of the proposed additional optimization term can also be expressed with a separate regularized kernel matrix. Thus, the proposed optimization problem can be solved using standard MKL–SVM methods, only by employing graph-regularized kernel matrices as basekernels, instead of standard ones, while the optimal weighting parameters are optimally estimated. Finally, computational complexity of the proposed method, as well as its generalization properties are discussed in Section 3.3.

3.1. Multiplex data relationships

Multiplex data relationships can be expressed by using a set of graphs, each describing a different pairwise property about the training set. Pairwise properties of the training data may include e.g., local geometric data information (encoded by kNN graphs) or global geometric data information (encoded in fully connected graphs). In addition, hand-crafted graph types or graphs that might be introduced in the future could be employed, as well. Let us denote by $\mathcal{G}^m = \{\mathcal{X}, \boldsymbol{W}^m\}, m = 1, \ldots, M$ the mth graph with $\boldsymbol{W}^m$ its corresponding graph weight matrix, containing the weights of the connections between the graph vertices $\mathcal{X} = \{\phi(\boldsymbol{x}_1), \ldots, \phi(\boldsymbol{x}_N)\}$.

In order to express local geometric data information for our multiplex graph paradigm, let us denote by $\mathcal{G}^l$ a kNN graph. Also let $\mathcal{N}_i$ be the neighborhood of each vertex, connecting it with the k most similar vectors. Then, the corresponding graph weights can be initiated with a heat kernel function:

$$W_{ij}^l = \begin{cases} exp\big(-\gamma||\boldsymbol{x}_i - \boldsymbol{x}_j||_2^2\big), & \text{if } \boldsymbol{x}_j \in \mathcal{N}_i \\ 0, & \text{otherwise,} \end{cases} \quad (8)$$

where γ is a free parameter that scales the Euclidean distances between the graph vertices $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$. Let $\boldsymbol{S}_l$ encode the local geometry of the training data, defined in a similar manner as in (4):

$$\boldsymbol{S}_l = \boldsymbol{\Phi}\boldsymbol{L}_l\boldsymbol{\Phi}^T, \quad (9)$$

where $\boldsymbol{L}_l$ is the corresponding Laplacian matrix.

In order to encode the global geometry of the training data, fully connected graphs ($k = N$) of similar definition could be employed. Alternatively, we exploit a different fully connected graph type definition. From a discriminant analysis point of view [17], we would require that items belonging to the same class (e.g., class $c, c = 1, \ldots, C$) to be connected with equal weights, expressed in the graph $\mathcal{G}^w$, using the following weight matrix:

$$W_{ij}^w = 1/N_c, \quad \text{if } y_i = y_j = c, \quad (10)$$

where N_c is the number of items belonging to the cth class. In fact, the corresponding matrix $\boldsymbol{S}_w$ that expresses global geometric data relationships as in Eq. (4), is the within-class scatter matrix, as can be shown below:

$$\begin{aligned} \boldsymbol{S}_w &= \sum_{c=1}^{C}\sum_{i=1}^{N_c}(\boldsymbol{\phi}_i^c - \bar{\boldsymbol{\phi}}^c)(\boldsymbol{\phi}_i^c - \bar{\boldsymbol{\phi}}^c)^T \\ &= \boldsymbol{\Phi}\left(\boldsymbol{I} - \sum_{c=1}^{C}\frac{1}{N_c}\boldsymbol{e}_c\boldsymbol{e}_c^T\right)\boldsymbol{\Phi}^T = \boldsymbol{\Phi}\boldsymbol{L}_w\boldsymbol{\Phi}^T, \end{aligned} \quad (11)$$

where c is an index denoting the class of sample $\boldsymbol{x}_i$, $\boldsymbol{\phi}_i$ is a shorthand for $\phi(\boldsymbol{x}_i)$, $\bar{\boldsymbol{\phi}}^c$ is the mean sample of class c in the feature space, $\boldsymbol{e}_c \in \mathbb{R}^N$ is a vector of ones in the positions where $y_i = c$, or zeros, otherwise, and $\boldsymbol{L}_w$ is the corresponding graph Laplacian matrix.

In the following Subsection, we describe how multiplex data relationships are introduced to the SVM optimization problem.

3.2. Proposed method

The proposed method aims at generating a decision function in a space where multiplex data relationships are emphasized. In order to model the multiple data relationships, we employ the matrices $\boldsymbol{S}_m, m = 1, \ldots, M$, where the mth matrix encode the data properties that are described by the mth graph type. Then, a decision function can be obtained, by combining SVM hyperplanes $\boldsymbol{w}_m$ that have been regularized with the corresponding matrix $\boldsymbol{S}_m$. The introduced regularization effect is controlled by the parameters $\lambda_m > 0$. Finally, multiplex data relationships are weighted according to their effect in the final decision function with the parameters μ_m. In order to determine the weighting parameters μ_m, and obtain the decision function at the same time, we propose the following optimization problem:

$$\begin{aligned} \min_{\{\boldsymbol{w}\},\boldsymbol{\xi},b,\boldsymbol{\mu}} \quad & \frac{1}{2}\sum_{m=1}^{M}\mu_m^{-p}\left(\|\boldsymbol{w}_m\|^2 + \lambda_m \boldsymbol{w}_m^T \boldsymbol{S}_m \boldsymbol{w}_m\right) + c\sum_{i=1}^{N}\xi_i + b, \\ \text{s.t.} \quad & \sum_{m=1}^{M} y_i\left(\boldsymbol{w}_m^T\phi_m(\boldsymbol{x}_i) + b\right) \le 1 - \xi_i, i = 1, \ldots, N, \\ & \xi_i \ge 0, \ \sum_{m=1}^{M}\mu_m^p = 1, \mu_m > 0, \end{aligned} \tag{12}$$

where each hyperplane $\boldsymbol{w}_m$, as well as each of the matrices $\boldsymbol{S}_m$ are defined in the feature space $\mathcal{H}_m$, and $p \ge 1$ is a parameter that affects the sparsity of the final solution, similar to MKL methods. For simplicity reasons, we consider the case where $p = 1$, hereafter. The Lagrangian function corresponding to the proposed optimization problem is of the following form:

$$\begin{aligned} L = \frac{1}{2}\sum_{m=1}^{M}\frac{1}{\mu_m}\boldsymbol{w}_m^T(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)\boldsymbol{w}_m + b - \sum_{i=1}^{N}\alpha_i\left(\sum_{m=1}^{M} y_i\left(\boldsymbol{w}_m^T\phi_m(\boldsymbol{x}_i)\right.\right. \\ \left.\left. + b\right) - 1 + \xi_i\right) + \sum_{i=1}^{N}(c - \beta_i)\xi_i - \sum_{m=1}^{M}\gamma_m\mu_m - \delta\left(\sum_{m=1}^{M}\mu_m - 1\right), \end{aligned} \tag{13}$$

where α_i, β_i, γ_m and δ are the Lagrange multipliers corresponding to the constraints of (12) and $\boldsymbol{I}$ is an identity matrix of appropriate dimensions.

By setting the partial derivative of the Lagrangian with respect to each hyperplane equal to zero, $\frac{\partial L}{\partial \boldsymbol{w}_m} = 0$, we obtain:

$$\frac{1}{\mu_m}(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)\boldsymbol{w}_m = \sum_{i=1}^{N}\alpha_i y_i \phi(\boldsymbol{x}_i). \tag{14}$$

By setting the partial derivatives of L with respect to ξ_i and β equal to zero, i.e., $\frac{\partial L}{\partial \boldsymbol{\xi}} = 0$ and $\frac{\partial L}{\partial \boldsymbol{b}} = 0$, we obtain $\beta_i = c - \alpha_i$ and $\sum_{i=1}^{N}\alpha_i y_i = 1$, respectively. Then, by replacing back in the Lagrangian, the proposed optimization problem takes the following form:

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \ \min_{\boldsymbol{\mu}} & \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j\left(\sum_{m=1}^{M}\mu_m\phi_m(\boldsymbol{x}_i)^T(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)^{-1}\phi_m(\boldsymbol{x}_j)\right) \\ \text{s.t.} \quad & 0 \le \alpha_i \le c \ \text{ and } \ \sum_{m=1}^{M}\mu_m = 1. \end{aligned} \tag{15}$$

We observe that the above defined optimization problem is similar to the standard SVM optimization problem, if we employ a kernel $q(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{m=1}^{M}\mu_m\phi_m(\boldsymbol{x}_i)^T(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)^{-1}\phi_m(\boldsymbol{x}_j)$. This kernel can be explicitly determined by a linear combination of multiple basekernels $\tilde{\kappa}_m$, weighted by parameters μ_m, such that:

$$q(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{m=1}^{M}\mu_m\tilde{\kappa}_m(\boldsymbol{x}_i, \boldsymbol{x}_j), \tag{16}$$

where $\tilde{\kappa}_m(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi_m(\boldsymbol{x}_i)^T(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)^{-1}\phi_m(\boldsymbol{x}_j)$ contains data similarity in the space where the $m-$th training data property is emphasized. We recall that $\boldsymbol{S}_m = \boldsymbol{\Phi}\boldsymbol{L}_m\boldsymbol{\Phi}^T$, where $\boldsymbol{L}_m$ is the Laplacian matrix of the mth graph. In order to obtain the basekernel matrix, we first calculate the inversion $(\boldsymbol{I} + \lambda_m\boldsymbol{S}_m)^{-1}$, by exploiting the Woodbury matrix inversion identity [31]:

$$\left(\boldsymbol{I} + \lambda_m\boldsymbol{\Phi}\boldsymbol{L}_m\boldsymbol{\Phi}^T\right)^{-1} = \boldsymbol{I} - \boldsymbol{\Phi}\left(\frac{1}{\lambda_m}\boldsymbol{L}_m^{-1} + \boldsymbol{\Phi}^T\boldsymbol{\Phi}\right)^{-1}\boldsymbol{\Phi}^T, \tag{17}$$

where $\boldsymbol{\Phi}^T\boldsymbol{\Phi} = \boldsymbol{K}$, which is a Kernel matrix that expresses similarity in the space associated with the employed mapping function. Moreover, this formula can be further simplified by exploiting the Searle matrix inversion identity [31]:

$$\left(\frac{1}{\lambda_m}\boldsymbol{L}_m^{-1} + \boldsymbol{K}\right)^{-1} = \boldsymbol{K}^{-1}\left(\lambda_m\boldsymbol{L}_m + \boldsymbol{K}^{-1}\right)^{-1}\lambda_m\boldsymbol{L}_m, \tag{18}$$

Finally, each regularized kernel matrix can be explicitly calculated as follows:

$$\begin{aligned} \tilde{\boldsymbol{K}}_m &= \boldsymbol{\Phi}^T\left[\boldsymbol{I} - \boldsymbol{\Phi}\boldsymbol{K}^{-1}\left(\lambda_m\boldsymbol{L}_m + \boldsymbol{K}^{-1}\right)^{-1}\lambda_m\boldsymbol{L}\boldsymbol{\Phi}^T\right]\boldsymbol{\Phi} \\ &= \boldsymbol{K} - \left(\lambda_m\boldsymbol{L}_m + \boldsymbol{K}^{-1}\right)^{-1}\lambda_m\boldsymbol{L}_m\boldsymbol{K} \\ &= \left[\boldsymbol{I} - \left(\lambda_m\boldsymbol{L}_m + \boldsymbol{K}^{-1}\right)^{-1}\lambda_m\boldsymbol{L}_m\right]\boldsymbol{K}. \end{aligned} \tag{19}$$

By replacing the calculated basekernels back to the Lagrangian, we obtain a MKL–SVM optimization problem:

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \ \min_{\boldsymbol{\mu}} & \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j\sum_{m=1}^{M}\mu_m\tilde{\kappa}_m(\boldsymbol{x}_i, \boldsymbol{x}_j) \\ \text{s.t.} \quad & 0 \le \alpha_i \le c \ \text{ and } \ \sum_{m=1}^{M}\mu_m = 1, \end{aligned} \tag{20}$$

which is similar to the optimization problem defined in (2), only by replacing the basekernels $\boldsymbol{K}_m$ with $\tilde{\boldsymbol{K}}_m$. In order to solve this optimization problem, any MKL–SVM method can be employed [12]. To this end, we have employed the recently proposed soft-margin MKL–SVM method [11] in all our experiments, since it outperforms other widely adopted MKL methods [32,33] in video classification problems, by providing an efficient compromise between sparse solutions and fast convergence. That is, the min–max optimization problem is broken into two quadratic programming optimization problems that are solved sequentially, one for the standard SVM, and a separate soft-margin optimization one for determining the parameters μ_m. Finally, in order to classify a test sample, we employ the MKL decision function (3), using the appropriate matrices.

3.3. Discussion

The proposed method employs multiple graphs for regularization purposes, in the form of multiple single-graph regularized kernels. The optimization problem is formulated as a MKL–SVM optimization problem. The advantage of this approach is the elimination of exhaustive parameter fine-tuning, related to estimating the graph-hyperparameters. Their effect, along with the parameter λ, can be implicitly determined only by optimally determining the base kernel weights μ_m. In order to demonstrate how important

is this property, let us consider the related GE-SVM case. Let a set of M kNN graphs that can be derived from Eq. (9), to be employed for regularization purposes. The graph hyperparameters that require tuning for each graph include the number of nearest neighbors k and the RBF parameter γ_k. Along with these, an additional RBF γ parameter for creating the standard SVM kernel function that will be regularized using the graphs, is also required to be tuned. Finally, tuning is required for determining the amount of the introduced regularization effect λ, as well as the standard SVM parameter c, totaling 5 parameters. Without an optimization procedure for these, i.e., the proposed approach, determining the optimal parameter combination with traditional methods, e.g., grid search, is computationally intensive.

On the other hand, we consider the complexity of the proposed method. Since the proposed method can be solved using any MKL–SVM solver, its computational complexity in the training phase is equal to the complexity of the solver, along with the complexity required to calculate the regularized basekernels using Eq. (19). Let us consider that all of the employed kernels are regularized versions of the same standard basekernel $\boldsymbol{K}$ (e.g., RBF), having size equal to $N \times N$, where N is the number of the employed training data. First, the basekernels need to calculated and inverted. Then, in order to obtain each regularized basekernel version, a Laplacian matrix $\boldsymbol{L}_m$ of size $N \times N$ needs to be determined. Then, an additional inversion of the quantity inside the parenthesis of size $N \times N$ is required. Finally, this quantity is multiplied with $\boldsymbol{L}_m$, and this result is then saved and stored, since this result will be employed for deriving the regularized basekernel at the inference stage, as well. Therefore, the complexity of the training stage is equal to the complexity of the MKL–SVM solver, plus two inversions of size $N \times N$, the calculation of the Laplacian matrix and two matrix multiplications of size $N \times N$ for each basekernel. In the inference stage, the computational complexity is equal to standard MKL–SVM, plus one matrix multiplication for each of the resulted basekernels. Thus, assuming hardware restrictions e.g., embedded systems, adopting sparse solutions is preferred.

Finally, another aspect of the proposed method includes its generalization features. The proposed formulation is generic, since related methods may be presented as special cases of the proposed method, hereafter. That can be achieved by changing the basekernel matrix combination. For example, replacing the derived kernel matrix $\boldsymbol{Q}$ with the standard SVM kernel matrix $\boldsymbol{K}$ and $\mu = 1$, the proposed method degenerates to standard SVM. Using a set of standard SVM kernel matrices derived by employing several mapping functions, or similar mapping functions with different parameters, the proposed method represents the basic MKL formulation. Finally, introducing a single graph regularized kernel matrix (i.e., $\mu = 1$) in the SVM optimization process, the proposed method degenerates to GE-SVM.

4. Experiments

In order to evaluate the performance of the proposed method, we have conducted experiments in visual analysis classification problems. To this end, we have employed publicly available datasets for face recognition, object classification and human action recognition. The employed datasets were carefully selected to demonstrate the effectiveness of the proposed method in various classification problems. For each of the employed datasets, different descriptor types we employed, including pre-extracted feature vectors, deep features, pre-computed kernel matrices, feature vectors minimal pre-processing i.e., pixel luminosities and advanced hand-crafted features. Since all employed datasets are well balanced in terms of instances per class, for both training and testing purposes, the Classification Rate (CR) was employed as performance metric.

Along with the proposed method, we have also implemented the standard SVM [5], the GE-SVM [18] and MKL–SVM [11]. Our experimental platform was a PC with 32GB of RAM on a i7 processor, using a Matlab implementation. For comparison fairness, the same SVM solver was employed for all methods [34], and the parameter settings were also set to be equal for all methods, where applicable. The SVM parameter c was set equal to 10^{ℓ} , $\ell = -2, \ldots, 6$ for all methods. In all our experiments, we have employed the kernel versions of the competing algorithms for each experiment, by employing the RBF kernel:

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = exp\left(-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|_2^2\right), \tag{21}$$

where $\gamma = 1/2a\sigma^2$, σ^2 is the standard deviation of the training data, which is the normal scaling factor and the optimal γ was determined from a range of different values of a, equal to $a = -1, 0, 0.5, 1, 5, 10$. All the constructed RBF kernel matrices that were employed for standard SVM were also employed as basekernels in MKL–SVM. In order to construct the kernel matrices that were used for GE-SVM, we employed the regularized version of the kernel matrices using two types of regularizers, i.e., $\boldsymbol{S}_l$ from Eq. (9) and $\boldsymbol{S}_w$ from Eq. (11). The additional parameter λ was set equal to $10^s, s = -3, \ldots, 3$. The kNN graph being employed in $\boldsymbol{S}_l$ was containing local geometric data relationships from $k = 5, 10, 15$ neighbors. In GE-SVM, the best performing regularized kernel during cross validation was employed for testing the classifier. The same regularized kernels constructed for GE-SVM were employed as basekernels in the proposed method, with the difference that only a value $\lambda_m = 10^{-1}$ was used, since its effects can be implicitly simulated by optimally solving for the kernel weights μ_m. The optimal parameter settings for standard SVM and GE-SVM methods were determined using grid search, using a 5−fold cross validation procedure on the training set. The parameter μ of MKL–SVM and the proposed method was determined from solving the optimization problem.

Detailed description for the experimental protocol followed for each classification problem is analytically described in Sections 4.1, 4.2 and 4.3, respectively. Finally, we describe the conducted significance analysis of the obtained results in Section 4.4.

4.1. Experiments in face recognition

In our experiments in face recognition, we have employed the PubFig+LFW [35], AR [36], Yale [37] and ORL [38] datasets. The PubFig+LFW [35] is a benchmark dataset for open-universe face identification, consisting of 13, 002 facial images representing 83 individuals from PubFig83, divided into 2/3 training (8720 faces) and 1/3 testing set (4282 faces), as well as 12, 066 images representing over 5000 faces which form the distractor set from LFW. For each facial image, the extracted features include the Histogram of Oriented Gradients (HOG), Local Binary Patterns (LBP) and Gabor wavelet features. The extracted features were reduced to 2048 dimensions with Principal Component Analysis (PCA), from which we only employed the first 1536 dimensions, as advised by the dataset providers [35].

Moreover, we have also employed classic face recognition datasets, i.e. the AR [36], Yale [37] and ORL [38] datasets, containing 2600, and 2432 and 400 frontal facial images belonging to 100, 38 and 40 subjects, respectively. As feature vectors, we have employed the grayscale resized images to 40×30 pixels, and vectorized them so that to produce a $D = 1200$ dimensional vector for each facial image. Since no standard experimental protocol have been defined on these datasets, we have performed a 5−fold cross-validation procedure and report the average obtained performance among the folds.

Experimental results are drawn in Table 1. As can be seen, the proposed method outperformed all competing methods in every

Table 1
Classification rates (CR) in face recognition datasets.

Algorithm/dataset	PubFig+LFW	ORL	AR	Yale
SVM	36.24	98.75	99.11	97.94
GE-SVM	34.35	98.75	99.19	97.94
MKL–SVM	84.17	98.75	90.57	96.08
PROPOSED	**88.77**	**99.25**	**99.42**	**98.06**

Table 2
Classification rates (CR) in object recognition datasets.

Algorithm/dataset	CIFAR-100	Caltech101
SVM	73.20	66.17
GE-SVM	72.30	66.56
MKL–SVM	75.40	72.42
PROPOSED	**79.80**	**73.39**

case, in terms of classification accuracy. More specifically, by observing the performance of all competing methods in PubFig+LFW dataset, whose feature vectors include information from handcrafted descriptors, employing Multiple Kernel matrices seem to have been beneficial to classification performance. This can be explained by the fact that the extracted features may lie in multiple distributions, not modeled adequately by a single normal distribution (i.e., the standard SVM case), or even a regularized one (i.e., the GE-SVM case). The performance of MKL–SVM denoted that exploiting multiple distributions for modeling data similarity was beneficial to performance. In every case, the proposed method outperformed the competition, by exploiting the additional global and local geometric particularities of each class, modeled by the added graph structures. This information acted as an advanced regularizer to the solution, offering more accurate feature representation, in comparison with the competition.

In our experiments on classic face recognition datasets, we have observed that employing the MKL–SVM, seem to have not influenced positively the classification performance, maybe related to over-fitting issues. This effect is supported by the performance of GE-SVM, which outperformed the standard SVM and MKL–SVM, by having one graph regularizing the classification space. However, the proposed method was able to alleviate the negative overfitting effects, by optimally determining the most efficient regularized kernel combination.

4.2. Experiments in object classification

In our experiments on object classification, we have employed the CIFAR-100 [39] and Caltech101 [40] datasets. In CIFAR-100 dataset, we have employed pre-extracted features [41]. That is, the feature vectors were computed by performing a forward pass to a pre-trained CNN network from the fully connected layer 'fc2', having feature dimensionality $D = 255$, based on a Hadamard coding pre-processing [41,42]. We have employed the small dataset version, which includes 5000 training and 1000 testing samples, belonging to 10 classes, corresponding to ones predefined by the dataset providers [39]. We have constructed the RBF kernel matrices by employing the above mentioned features, and employed them to the SVM and MKL–SVM methods. Their regularized alternatives were employed for the GE-SVM and the proposed method. In Caltech101 dataset, we have employed 10 pre-computed kernel matrices [43], derived from employing the Geometric blur [44], dense visual words [45] and Self-similarity [46] descriptors.

In standard SVM, we have reported the maximum performance obtained by employing each of the 10 pre-computed kernel matrices. In GE-SVM, we have employed the regularized kernel alternatives, by employing $\boldsymbol{S}_l$ with $k = 5, 10, 15$ neighbors and $\boldsymbol{S}_w$ with $\lambda_m = 10^{-1}$, leading to a total of 40 kernel matrices. Finally, these kernel matrices were employed by proposed method, as well. Classification rates on both datasets is shown in Table 2. As can be seen in both cases, the proposed method greatly outperformed the competition. The proposed method outperformed MKL–SVM by 1.5%. This demonstrates the effectiveness of the proposed method, for the case where pre-computed kernel matrices have been employed.

Table 3
Classification rates (CR) in human action recognition datasets.

Algorithm/dataset	I3DPost	IMPART	Olympic sports	Hollywood 3D
SVM	94.39	85.32	73.13	29.87
GE-SVM	94.87	**86.47**	**74.63**	29.87
MKL–SVM	94.39	85.33	73.88	30.52
PROPOSED	**95.51**	85.75	**74.63**	**32.14**

4.3. Experiments in human action recognition

In our experiments in human action recognition, we have employed the i3DPost multi-view action database [47], the IMPART Multi-modal/Multi-view Dataset [48], the Olympic Sports [49] and the Hollywood3D [50] publicly available datasets. In i3DPost and IMPART datasets, we have employed a 3-fold cross validation procedure, where we have split the datasets in 3 mutually exclusive sets, having 6/8 people for training purposes, and 2/8 for testing in i3DPost dataset, and 2/3 and 1/3 in IMPART dataset, respectively. The reported performance is the average obtained classification rate among the 3 folds. In Hollywood 3D and Olympic Sports datasets, we employed the standard training and test videos, provided by the dataset providers [49–51].

In order to obtain vectorial video representations for each video segment depicting each action, we have employed the dense trajectory-based video description [52]. This video description calculates five descriptor types on the trajectories of densely-sampled video frame interest points that are tracked for a number of consecutive video frames, namely the Histogram of Oriented Gradients, Histogram of Optical Flow, Motion Boundary Histograms along directions x, y and the normalized trajectory coordinates. Video segment representations are thereby obtained by using the Bag-of-Words model [53,54], creating a video description of having 5 descriptors of 100, 500, 4000 and 4000 dimensions, for i3DPost, IMPART, Olympic sports and Hollywood3D, respectively. In standard SVM and GE-SVM methods, information from the 5 descriptor types was fused with kernel methods as in [55], i.e.,: $k(\mathcal{X}_i, \mathcal{X}_j) = \exp(-\frac{1}{d}\gamma_d \sum_d \|\mathbf{x}_i^d - \mathbf{x}_j^d\|_2^2)$, $\boldsymbol{x}_i^d \in \mathbb{R}^D$ is a video feature vector for $d = 5$ (number of descriptor types) and $\gamma_d = 2\sigma_d^2$ is a parameter scaling the Euclidean distance between $\boldsymbol{x}_i^d$ and $\boldsymbol{x}_j^d$. In MKL–SVM and the proposed method, besides the fused kernel matrix, each separate kernel matrix containing data similarity derived for each descriptor type was employed.

Experimental results in human action recognition are drawn in Table 3. As can be observed, the proposed method outperformed the competition in almost every case. Using MKL–SVM for fusing information from the specific descriptor types provided slightly improved classification performance in comparison with standard SVM. In addition, by observing the performance of GE-SVM, employing graph-based regularization provided furthermore increased classification performance. The proposed method outperformed both GE-SVM and MKL–SVM, by exploiting multiple regularized basekernels, i.e., combining the performance gains of both MKL and GE-SVM approaches.

Table 4
Statistical test details.

Mean ranks	SVM	GE-SVM	MKL–SVM	Proposed
	3.35	2.65	2.85	1.15
Posthoc procedure	Nemenyi		Bergman–Hommel's	
α	0.05		0.0083	
CD	1.48		1.38	

4.4. Significance analysis

After obtaining the performance of the competing methods in all experiments, we determined whether the observed differences of the proposed method with the competition are statistically significant, or not [56–58]. To this end, we have tested the null hypotheses that all classifiers perform the same, using the Friedman's test. The mean ranks for each algorithm according to their performance in all classification problems are shown in Table 4. By employing 10 datasets and 4 classifiers, the degrees of freedom is equal to 27. The Friedman statistic is equal to $\chi_F^2 = 16.14$, and the critical value was 7.81. Therefore, the null hypotheses that all classifiers perform the same, was rejected. After employing the Nemenyi post-hoc procedure for pairwise comparison, using a significance level of 95%, i.e., $a = 0.05$, the Critical Distance (CD) was found at 1.48, which means that the proposed method performed significantly better than all competing methods. Moreover, we have also used the Bergman–Hommel's posthoc procedure, which amplifies the test power by using an exhaustive sets of hypothesis, i.e hypothesis that can be true at the same time. The critical distance was calculated at 1.38. Therefore, the proposed method performs significantly better than the competition.

5. Conclusion

We have presented a novel method for introducing multiplex data relationships to the SVM optimization process, by exploiting pairwise data information expressed in multiple graph structures. Our experiments denoted that the proposed method provided consistently increased classification performance against the competition, in different visual data classification problems. The improved classification accuracy was mainly achieved, due to the exploitation of advanced graph-based regularization settings in an optimal fashion, effectively representing the multimodal/multiplex image and video data characteristics. Since the proposed method provided enhanced classification performance using various descriptor settings, including simple pixel luminosities, advanced handcrafted feature types and deep representations, it should be expected that it will perform well in other standard classification problems, as well.

Moreover, since the proposed method is a generic formulation for Graph-based SVM methods and Multiple Kernel methods, evolution in both fields shall favor the proposed method as well. That is, novel advanced regularization settings using graph types unknown at the present, perhaps exploiting deep learning architectures, could be integrated with the proposed formulations. In addition, advanced Multiple Kernel Learning solvers that will be introduced in the future can be employed for solving the proposed optimization problem. Evolution in both domains can serve as a feature research direction.

Acknowledgment

This work has received funding from the European Union's European Union Seventh Framework Programme (FP7/2007-2013) under grant agreement number 316564 (IMPART) and Horizon 2020 research and innovation programme under grant agreement number 731667 (MULTIDRONE). This publication reflects only the authors' views. The European Commission is not responsible for any use that may be made of the information it contains.

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