Context-dependent kernel design for object matching and recognition

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Abstract

The success of kernel methods including support vector networks (SVMs) strongly depends on the design of appropriate kernels. While initially kernels were designed in order to handle fixed-length data, their extension to unordered, variable-length data became more than necessary for real pattern recognition problems such as object recognition and bioinformatics.

We focus in this paper on object recognition using a new type of kernel referred to as “context-dependent”. Objects, seen as constellations of local features (interest points, regions, etc.), are matched by minimizing an energy function mixing (1) a fidelity term which measures the quality of feature matching, (2) a neighborhood criteria which captures the object geometry and (3) a regularization term. We will show that the fixed-point of this energy is a “context-dependent” kernel (“CDK”) which also satisfies the Mercer condition. Experiments conducted on object recognition show that when plugging our kernel in SVMs, we clearly outperform SVMs with “context-free” kernels.

1. Introduction

Object recognition is one of the biggest challenges in vision and its interest is still growing [10]. Among existing methods, those based on machine learning (ML), show a particular interest as they are performant and theoretically well grounded [5]. ML approaches, such as the popular support vector networks [6], basically require the design of similarity measures, also referred to as kernels, which should provide high values when two objects share similar structures/appearances and should be invariant, as much as possible, to the linear and non-linear transformations. Kernel-based object recognition methods were initially holistic, i.e., each object is mapped into one or multiple fixed-length vectors and a similarity, based on color, texture or shape [29, 8], is then defined. Local kernels, i.e., those based on bags or local sets were introduced in order to represent data which cannot be represented by ordered and fixed-length feature vectors, such as graphs, trees, interest points, etc [11]. It is well known that both holistic and local kernels should satisfy certain properties among them the positive definiteness, low complexity for evaluation, flexibility in order to handle variable-length data and also invariance. Holistic kernels have the advantage of being simple to evaluate, discriminating but less flexible than local kernels in order to handle invariance\(^1\). While the design of kernels gathering flexibility, invariance and low complexity is a challenging task; the proof of their positive definiteness is sometimes harder [9]. This property also known as the Mercer condition ensures, according to Vapnik’s SVM theory [30], optimal generalization performance and also the uniqueness of the SVM solution.

Consider a database of objects (images), each one seen as a constellation of local features, for instance interest points [24, 19, 18], extracted using any suitable filter [13]. Again, original holistic kernels explicitly (or implicitly) map objects into fixed-length feature vectors and take the similarity as a decreasing function of any well-defined distance [3]. In contrast to holistic kernels, local ones are designed in order to handle variable-length and unordered data. Two families of local kernels can be found in the literature; those based on statistical “length-insensitive” measures such as the Kullback Leibler divergence, and those which require a preliminary step of alignment. In the first family, the authors in [17, 21] estimate for each object (constellation of local features) a probability distribution and compute the similarity between two objects (two distributions) using the “Kullback Leibler divergence” in [21] and the “Bhattacharyya affinity” in [17]. Only the function in [17] satisfies the Mercer condition and both kernels were applied for image recognition tasks. In [33], the authors discuss a new type of kernel referred to as “principal angles” which is positive definite. Its definition is based on the computation of the principal angles between two linear

\(^1\)In case of object recognition, invariance means robustness to occlusion, geometric transformations and illumination.
subspaces under an orthogonality constraint. The authors demonstrate the validity of their method on visual recognition tasks including classification of motion trajectory and face recognition. An extension to subsets of varying cardinality is proposed in [26]. In this first family of kernels, the main drawback, in some methods, resides is the strong assumption about the used probabilistic models in order to approximate the set of local features which may not hold true in practice.

In the second family, the “max” kernel [32] considers the similarity function, between two feature sets, as the sum of their matching scores and unlike discussed in [32] this kernel is actually not Mercer [2]. In [20], the authors introduced the “circular-shift” kernel defined as a weighted combination of Mercer kernels using an exponent. The latter is chosen in order to give more prominence to the largest terms so the resulting similarity function approximates the “max” and also satisfies the Mercer condition. The authors combined local features and their relative angles in order to make their kernel rotation invariant and they show its performance for the particular task of object recognition. In [7], the authors introduced the “intermediate” matching kernel, for object recognition, which uses virtual local features in order to approximate the “max” while satisfying the Mercer condition. Recently, [12] introduced the “pyramid-match” kernel, for object recognition, which uses a multi-resolution histogram representation and computes the similarity using a weighted histogram intersection. The authors showed that their function is positive definite and can be computed linearly with respect to the number of local features. Other matching kernels include the “dynamic programming” function which provides, in [2], an effective matching strategy for handwritten character recognition, nevertheless the Mercer condition is not guaranteed.

<table>
<thead>
<tr>
<th>Naive matching</th>
<th>'H'</th>
<th>'I'</th>
<th>'S'</th>
<th>'T'</th>
<th>'R'</th>
</tr>
</thead>
<tbody>
<tr>
<td>'S'</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>'T'</td>
<td>0</td>
<td>1</td>
<td>-1</td>
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<td>0</td>
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<tr>
<td>'R'</td>
<td>0</td>
<td>0</td>
<td>-0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Context-dependent</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 1. This table shows a simple comparison between similarity measures when using naive matching (upper table) and context-dependent matching (lower table).

1.1. Motivation and Contribution

The success of the second family of local kernels strongly depends on the quality of alignments which are difficult to obtain mainly when images contain redundant and repeatable structures. Regardless the Mercer condition, a naive matching kernel (such as the “max”), which looks for all the possible alignments and sums the best ones, will certainly fail and results into many false matches (see Figures 1 and 2, left). The same argument is supported in [24], for the general problem of visual features matching, about the strong spatial correlation between interest points and the corresponding close local features in the image space. This limitation also appears in closely related areas such as text analysis, and particularly string alignment. A simple example, of aligning two strings (“Sir” and “Hi Sir”) using a simple similarity measure \( I_{\{c_1=c_2\}} \) between any two characters \( c_1 \) and \( c_2 \), shows that without any extra information about the context (i.e., the sub-string) surrounding each character in (“Sir” and “Hi Sir”), the alignment process results into false matches (See Table 1). Hence, it is necessary to consider the context as a part of the alignment process when designing kernels.

In this paper, we introduce a new kernel, called “context-dependent” (or “CDK”) and defined as the fixed-point of an energy function which balances an “alignment quality” term and a “neighborhood” criteria. The alignment quality is inversely proportional to the expectation of the Euclidean distance between the most likely aligned features (see Section 2) while the neighborhood criteria measures the spatial coherence of the alignments; given a pair of features \((f_p, f_q)\) with a high alignment quality, the neighborhood criteria is proportional to the alignment quality of all the pairs close\(^2\) to \((f_p, f_q)\). The general form of “CDK” captures the similarity between any two features by incorporating also their context, i.e., the similarity of the surrounding features. Our proposed kernel can be

\[ 2\text{The closeness is defined in Section 2.} \]
viewed as a variant of “dynamic programming” kernel [2] where instead of using the ordering assumption we consider a neighborhood assumption which states that two points match if they have similar features and if they satisfy a neighborhood criteria i.e., their neighbors match too. This also appears in other well studied kernels such as Fisher [15], which implements the conditional dependency between data using the Markov assumption. “CDK” also implements such dependency with an extra advantage of being the fixed-point and the (sub)optimal solution of an energy function closely related to the goal of our application. This goal is to gather the properties of flexibility, invariance and mainly discrimination by allowing each local feature to consider its context in the matching process. Notice that the goal of this paper is not to extend local features to be global and doing so (as in [22, 1]) makes local features less invariant, but rather to design a similarity kernel (“CDK”) which captures the context while being invariant. Even though we investigate “CDK” in the particular task of object recognition, we can easily extend it to handle closely related areas in machine learning such as text alignment for documents retrieval [23], machine translation [28] and bioinformatics [25].

In the remainder of this paper we consider the following terminology and notation. A feature refers to a local interest point \( x_i \) which is a unique indicator which provides the class or the subset \( x \) or \( x_i \) as a symmetric function which, for instance the 128 coefficients of the SIFT[19]. We define \( \mathcal{X} \) as the set of all possible features taken from all the possible images in the world and \( \mathcal{X} \) is a random variable standing for a sample in \( \mathcal{X} \). We also consider \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) as a symmetric function which, given two samples \( \{x_i, x_j\} \), provides a similarity measure. Other notations will be introduced as we go along through different sections of this paper which is organized as follows. We first introduce in Section 2, our energy function which makes it possible to design our context-dependent kernel and we show that this kernel satisfies the Mercer condition so we can use it for support vector machine training and other kernel methods. In Section 3 we show the application of this kernel in object recognition. We discuss in Section 4 the advantages and weaknesses of this kernel and the possible extensions in order to handle other tasks such as string matching and machine translation. We conclude in Section 5 and we provide some future research directions.

2. Kernel Design

Define \( \mathcal{X} = \cup_{p \in \mathbb{N}^+} \mathcal{S}_p \) as the set of all possible interest points taken from all the possible objects in the world. We assume that all the objects are sampled with a given cardinality i.e., \( |\mathcal{S}_p| = n, |\mathcal{S}_q| = m, \forall \ p, q \in \mathbb{N}^+ \) (and \( m \) might be different). Our goal is to design a kernel \( k \) which provides the similarity between any two objects (subsets) \( \mathcal{S}_p, \mathcal{S}_q \) in \( \mathcal{X} \).

Definition 1 (Subset Kernels) let \( \mathcal{X} \) be an input space, and consider \( \mathcal{S}_p, \mathcal{S}_q \subseteq \mathcal{X} \) as two finite subsets of \( \mathcal{X} \). We define the similarity function or kernel \( K \) between \( \mathcal{S}_p = \{x_1, \ldots, x_n\} \) and \( \mathcal{S}_q = \{x_1, \ldots, x_m\} \) as

\[
K(\mathcal{S}_p, \mathcal{S}_q) = \sum_{i,j}^n \sum_{j}^m k(x_i^p, x_j^q),
\]

where \( k \) is symmetric and continuous on \( \mathcal{X} \times \mathcal{X} \), so \( K \) will also be continuous and symmetric. Since \( K \) is defined as the cross-similarity \( k \) between all the possible sample pairs taken from \( \mathcal{S}_p \times \mathcal{S}_q \), it is obvious that \( K \) has the big advantage of not requiring any (hard) alignment between the samples of \( \mathcal{S}_p \) and \( \mathcal{S}_q \). Nevertheless, for a given \( \mathcal{S}_p, \mathcal{S}_q \), the value of \( K(\mathcal{S}_p, \mathcal{S}_q) \) should be dominated by \( \max_{i,j} k(x_i^p, x_j^q) \), so \( k \) should be appropriately designed (see Section 2.1). Let \( X \) be a random variable standing for samples taken from \( \mathcal{S}_p \) and \( X' \) is defined in a similar way for the subset \( \mathcal{S}_q \). We design our kernel \( k(x_i^p, x_j^q) = P(X' = x_j^q, X = x_i^p) \) as the joint probability that \( x_j^q \) matches \( x_i^p \). Again, it is clear enough (see Figures 1,2 and Table 1) that when this joint probability is estimated using only the sample coordinates (without their contexts), this may result into many false matches and wrong estimate of \( P(X' = x_j^q, X = x_i^p) \).

Before describing the whole design of \( k \), we start with our definition of context-dependent kernels.

Definition 2 (Context-Dependent Kernels) we define a context-dependent kernel \( k \) as any symmetric, continuous and recursive function \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) such that \( k(x_i^p, x_j^q) \) is equal to

\[
c(x_i^p, x_j^q) \times h \left( \sum_{k,l} k(x_k^p, x_l^q) \forall (x_k^p, x_i^p, x_j^q) \right),
\]

where \( c \) is a positive (semi) definite and context-free (non-recursive) kernel, \( V(x, x', y, y') \) is a monotonic decreasing function of any (pseudo) distance involving \( (x, x', y, y') \) and \( h(x) \) is monotonically increasing.

2.1. Approach

We consider the issue of designing \( k \) using a variational framework. Let \( \mathcal{I}_p = \{1, \ldots, n\}, \mathcal{I}_q = \{1, \ldots, m\}, \mu = \{k(x_i^p, x_j^q)\}, d(x_i^p, x_j^q) = ||\psi_f(x_i^p) - \psi_f(x_j^q)||_2 \) and \( N_p(x_i^p) = \{x_k^p \in \mathcal{S}_p : k \neq i, \|\psi_g(x_i^p) - \psi_g(x_k^p)\|_2 \leq \epsilon_p \} \).
\( \epsilon_p \) defines a neighborhood and \( \mathcal{N}_q \) is defined in the same way for \( \mathcal{S}_q \). Consider \( \alpha, \beta \geq 0, \mu = \{k(x_i^p, x_j^q)\} \) is found by solving

\[
\min_{\mu} \beta \sum_{i \in \mathcal{I}_p, j \in \mathcal{I}_q} k(x_i^p, x_j^q) \log(k(x_i^p, x_j^q)) + \alpha \sum_{i \in \mathcal{I}_p, j \in \mathcal{I}_q} k(x_i^p, x_j^q) \left( - \sum_{x_k^p \in \mathcal{N}_p(x_i^p)} k(x_k^p, x_j^q) \right)
\]

\text{s.t.} \quad k(x_i^p, x_j^q) \in [0,1] \quad i \in \mathcal{I}_p, \quad j \in \mathcal{I}_q

\text{and results. Let} \( \mathcal{X} \) be an input space and let \( k_t : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) be symmetric and continuous. \( k_t \) is Mercer, i.e., positive (semi) definite, if and only if any Gram (kernel scalar product) matrix built by restricting \( k_t \) to any finite subset of \( \mathcal{X} \) is positive (semi) definite. A Mercer kernel \( k_t \) guarantees the existence of a reproducing kernel Hilbert space \( \mathcal{H} \) where \( k_t \) can be written as a dot product i.e., \( \exists \Phi_t : \mathcal{X} \rightarrow \mathcal{H} \) such that \( \forall x, x' \in \mathcal{X}, k_t(x, x') = \langle \Phi_t(x), \Phi_t(x') \rangle \).

**Proposition 2 (Closure[27])** the sum and the product of any two Mercer kernels is a Mercer kernel. The exponential of any Mercer kernel is also a Mercer kernel.

**Proposition 3** let \( \mathcal{V}(x_i^p, x_j^q) = g(x_i^p, x_j^q)x_k^p, x_j^q \) consider \( g : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) and \( k_0 \) positive definite. The kernel \( k_t \) is then positive definite.

\[
\exp \left( - \sum_{y \in \mathcal{Y}} p(x, y) y' \right) k_t(x, y) \geq 0
\]
We have
\[
(*) = \sum_{i,j} c_i c_j \sum_{y,y'} g(x_i,y) g(x_j,y') k_{t-1}(y,y') \\
= \sum_{y,y'} \left( \sum_i c_i g(x_i,y) \right) \times \left( \sum_j c_j g(x_j,y') \right) k_{t-1}(y,y') \\
= \sum_{y,y'} \gamma_y \gamma_{y'} k_{t-1}(y,y') \\
= \| \sum_y \gamma_y \Phi_{t-1}(y) \|_H \geq 0. \quad \Box
\]

(6)

Corollary 1 \textit{K defined in (1) is also a Mercer kernel.}

\textbf{Proof.} the proof is straightforward for the particular case \( n = m \). As \( k_t(x_i^p, x_j^q) = \langle \Phi_t(x_i^p), \Phi_t(x_j^q) \rangle \), we can write \( K(S_p, S_q) = \sum_{i,j} \langle \Phi_t(x_i^p), \Phi_t(x_j^q) \rangle = \langle \sum_i \Phi_t(x_i^p), \sum_j \Phi_t(x_j^q) \rangle \) and this corresponds to a dot product in some Hilbert space. The proof can be found in [27, 14] for the general case of finite subsets of any length.

\[ \Box \]

2.3. Algorithm and Setting

The factor \( \beta \), in \( k_t \), acts as a scale parameter and it is selected using
\[
\beta \leftarrow \mathbb{E}_r \left[ \mathbb{E}_{(X_i^r, X_j^r) \leq t} [d(X_i^r, X_j^r)] \right] \tag{7}
\]
here \( \mathbb{E} \) denotes the expectation and \( X_i^r \) (also \( X_j^r \)) denotes a random variable standing for samples in \( S_r \). The coefficient \( \alpha \) controls the tradeoff between the alignment quality and the neighborhood criteria. It is selected by cross-validation and it should guarantee \( k_t(x_i^p, x_j^q) \in [0,1] \).

If \( A = \sup_{i,j} \sum_{k,l} g(x_i^p, x_k^p) \times g(x_j^q, x_l^q) \), \( \alpha \) should then be selected in \([0, \frac{\beta}{2A}]\) (see. appendix).

Let \( P_{i,j} \) denotes the \( i^{th} \) row of the \( j^{th} \) column of \( P \). Consider \( P, Q \) as the intrinsic adjacency matrices of \( S_p \) and \( S_q \), respectively defined as \( P_{i,k} = g(x_i^p, x_k^p), Q_{j,t} = g(x_j^q, x_t^q) \). Let \( U \) denotes the unit matrix and consider \( D_{i,j} = d(x_i^p, x_j^q), \mu_{i,j}^{(t)} = k_i(x_i^p, x_j^q) \). Now, \( \mu_{i,j}^{(t)} \) is iteratively found using Algorithm (“CDK”) (see table 2) and converges to a fixed point (see. appendix).

3. Performance

3.1. Databases

Experiments were conducted on the Swedish set (15 classes, 75 images per category) and a random subset of

![Figure 2](image-url)

Figure 2. This figure shows a comparison of the matching results when using a naive matching strategy without geometry and our “context-dependent” kernel matching. (Top figures) show the distribution of the kernel values \( k(x_i, x_j) \), \( i \in I_q \) using a context-free kernel (left) and our “CDK” kernel (right). We can clearly see that the highest value changes its location so the matching results are now corrected (as shown in middle figures). (Bottom) other matching results.

<table>
<thead>
<tr>
<th>Algorithm (CDK)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Initialization:</strong></td>
</tr>
<tr>
<td>Set ( \beta ) using (7) and ( \alpha \in [0, \frac{\beta}{2A}] )</td>
</tr>
<tr>
<td>Set ( \mu^{(0)} \leftarrow k_0, t \leftarrow 0 )</td>
</tr>
<tr>
<td><strong>Repeat</strong> until ( t \to T_{\text{max}} ) or ( | \mu^{(t)} - \mu^{(t-1)} |_2 \to 0 )</td>
</tr>
<tr>
<td>( \mu^{(t)} \leftarrow \exp \left( -D/\beta + \frac{2\alpha}{\beta} P \mu^{(t-1)} Q - U \right) )</td>
</tr>
</tbody>
</table>

Table 2. The “CDK” kernel evaluation.
M N I S T digit database (10 classes, 200 images per category). Each class in Swedish (resp. MNIST) is split into 50 + 25 (resp. 100 + 100) contours for training and testing. Interest points were sampled from each contour in MNIST (resp. Swedish) and encoded using the 60 (resp. 16) coefficients of the shape-context descriptor [4].

3.2. Generalization and Comparison

We evaluate \( k_t, t \in \mathbb{N}^+ \) using two initializations: (i) linear \( k_0(x,x') = k_t(x,x') = (x,x') \) (ii) and polynomial \( k_0(x,x') = k_p(x,x') = ((x,x')+1)^2 \). Our goal is to show the improvement brought when using \( k_t, t \in \mathbb{N}^+ \), so we tested it against the standard context-free kernels \( k_l \) and \( k_p \) (i.e., \( k_t, t = 0 \)). For this purpose, we train a “one-versus-all” SVM classifier for each class in both MNIST and Swedish using the subset kernel \( K(S_p, S_q) = \sum_{x \in S_p, x' \in S_q} k_t(x,x') \). The performance are measured, on different test sets, using \( n \)-fold cross-validation (\( n = 5 \)).

We remind that \( \beta \) is set using (7) as the left-hand side of \( k_t \) corresponds to the Gaussian kernel with scale \( \beta \). In practice, \( \beta = 0.1 \). The influence (and the performance) of the right-hand side of \( k_t \) increases as \( \alpha \) increases (see. Figure 3), nevertheless and as shown in the appendix, the convergence of \( k_t \) to a fixed point is guaranteed only if \( \alpha \in [0, \frac{\beta}{2\|A\|}] \). Therefore, it is obvious that \( \alpha \) should be set to \( \frac{\beta}{2\|A\|} \) where \( A = \sup_{i,j} \sum_{k \in \mathbb{N}} g(x_i^k, x_i^k) \times g(x_j^q, x_j^q) \) (in practice, \( 0 \leq g \leq 1 \) and \( A = 1 \)).

Tables (3, 4), show the 5-fold cross validation errors on MNIST and Swedish for different iterations; we clearly see the out-performance and the improvement of the “CDK” kernel \( h_t, t \in \mathbb{N}^+ \) with respect to the context-free kernels used for initialization \( (k_0 = k_l \text{ and } k_0 = k_p) \).

4. Remarks and Discussion

The adjacency matrix \( P \), in \( k_t \), provides the intrinsic properties and also characterizes the geometry of an object \( S_p \). Let us remind \( \mathcal{N}_p(x_i^p) = \{ x_k^p \in S_p : k \neq i, \| \psi_g(x_i^p) - \psi_g(x_k^p) \|_2 \leq \epsilon_p \} \) and \( P_{i,j} = \mathbb{1}_{\{ x_j^q \in \mathcal{N}_p(x_i^p) \}} \).

It is easy to see that \( P \) is translation and rotation invariant and can also be make scale invariant when \( \epsilon_p \) is adapted to the scale of \( \psi_g(x_i^p) \). It follows that the right-hand side of our kernel is invariant to any 2D similarity transformation. Notice, also, that the left-hand side of \( k_t \) involves similarity invariant descriptors \( \psi_f(x_i^p) \), \( \psi_f(x_j^q) \) so \( k_t \) (and \( K \)) is similarity invariant.

The out-performance of our kernel comes essentially from the inclusion of the context. This strongly improves the precision and helps including the intrinsic properties (geometry) of objects. Even though tested only on visual object recognition, our kernel can be extended to many other pattern analysis problems such as bioinformatics.
speech and text. For instance, in text analysis and particularity machine translation [28], the design of a similarity kernel between words in two different languages, can be achieved using any standard dictionary (for instance WordNet). Of course, the latter defines similarity between any two words \((w_e, w_f)\) independently from their bilingual training text (or bitext), i.e., the phrases where \((w_e, w_f)\) might appear and this results into bad translation performances. A better estimate of similarity between two words \((w_e, w_f)\), can be achieved using their context i.e., the set of words which cooccur frequently with \((w_e, w_f)\) [16].

Finally, one current limitation of our kernel \(k_t\) resides in its evaluation complexity. Assuming \(k_{t-1}\) known, for a given pair \(x^p_i, x^q_j\), this complexity is \(O(\max(N^2, s))\), where \(s\) is the dimension of \(\psi_f(x^p)\) and \(N = \max_{i,p} \#\{N_p(x^p)\}\). It is clear enough that when \(N < \sqrt{s}\), the complexity of evaluating our kernel is strictly equivalent to that of usual kernels such as the linear. Nevertheless, the worst case \((N \gg \sqrt{s})\) makes our kernel evaluation prohibitive and this is mainly due to the right-hand side of \(k_t(x^p_i, x^q_j)\) which requires the evaluation of kernel sums in a hypercube of dimension 4. A simple and straightforward generalization of the integral image (see for instance [31]) will reduce this complexity to \(O(s)\).

5. Conclusion

We introduced in this paper a new type of kernels referred to as context-dependent. Its strength resides in the improvement of the alignments between interest points which is considered as a preliminary step in order to increase the robustness and the precision of object recognition.

We have also shown that our kernel is Mercer and applicable to SVM learning. The latter is achieved for shape recognition problems and has better performance than SVM with context-free kernels. Future work includes the comparison of our kernel with other context-free kernels and its application in scene and object understanding using more challenges and databases.

Appendix

Proposition 1 (cont.)

Proof. Let us consider

\[
\mu = \{k(x^p_i, x^q_j) = \exp(-U^2_{ij}), U_{ij} \in \mathbb{R}, i \in \mathcal{I}_p, j \in \mathcal{I}_q\}, \quad \text{and} \quad U = \{U_{ij}\}.
\]

Per definition the bounds on \(\{k(x^p_i, x^q_j)\}\) are satisfied. Now, the objective function (3) can be rewritten as

\[
\min_{U, \lambda} \sum_{i,j} \exp(-U^2_{ij}) d(x^p_i, x^q_j) - \beta \sum_{i,j} \exp(-U^2_{ij}) U^2_{ij} -
\alpha \sum_{i,j,k,l} \beta U_{ij} \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij}) (8)
\]

s.t.

\[
\sum_{j} \exp(-U^2_{ij}) = 1, \quad \forall i \in \mathcal{I}_p
\]

By introducing Lagrange coefficients \(\lambda\) for the equality constraint \(\sum_{i,j} \exp(-U^2_{ij}) = 1\), the above constrained minimization problem can now be rewritten:

\[
\min_{U, \lambda} \mathcal{L}(U, \lambda) =
\min_{U, \lambda} \sum_{i,j} \exp(-U^2_{ij}) d(x^p_i, x^q_j) - \beta \sum_{i,j} \exp(-U^2_{ij}) U^2_{ij} -
\alpha \sum_{i,j,k,l} \beta U_{ij} \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij}) (9)
\]

The conditions for optimality, i.e., when the gradient with respect to \(U_{ij}\) and \(\lambda\) vanishes, lead to:

\[
-2 \ U_{ij} \exp(-U^2_{ij}) \ d(x^p_i, x^q_j) + 2 \beta \ U_{ij} \ U^2_{ij} - 2 \ \beta \ U_{ij} \ \exp(-U^2_{ij}) -
4 \ \alpha \ \exp(-U^2_{ij}) \ U_{ij} \exp(-U^2_{ij}) +
4 \ \alpha \ \sum_{k,l} \ \exp(-U^2_{ij}) \ \exp(-U^2_{kl}) \ \exp(-U^2_{ij}) = 0 (10)
\]

and

\[
\sum_{i,j} \exp(-U^2_{ij}) = 1
\]

\[
\frac{\partial \mathcal{L}}{\partial U_{ij}} = 0 \text{ implies:}
\]

\[
-2 \ U_{ij} \exp(-U^2_{ij}) \ d(x^p_i, x^q_j) + 2 \beta \ U_{ij} \ U^2_{ij} - 2 \ \beta \ U_{ij} \ \exp(-U^2_{ij}) -
2 \alpha \ \sum_{k,l} \ \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij})
\]

so

\[
k(x^p_i, x^q_j) = \exp(-U^2_{ij})
\]

\[
= \exp\left(-\frac{d(x^p_i, x^q_j)}{\beta}\right) \exp(-1) \times
\exp\left(\frac{2 \alpha}{\beta} \sum_{k,l} \ \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij})\right) \times
\exp\left(-\frac{2 \alpha}{\beta} \ \exp(-U^2_{ij}) \exp(-U^2_{ij})\right)
\]

It is easy to see that \(\exp\left(-\frac{2 \alpha}{\beta} \ \exp(-U^2_{ij}) \exp(-U^2_{ij})\right)\) is constant (i.e., independent from \(i, j\)). Now \(\frac{\partial \mathcal{L}}{\partial \lambda} = 0\), implies \(\exp(-\lambda) = \exp(1) / \sum_{i,j} Z_{ij}\)

with \(Z_{ij} = \exp(-\frac{d(x^p_i, x^q_j)}{\beta}) + \frac{2 \alpha}{\beta} \sum_{k,l} \ \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij}) k(x^p_i, x^q_j)\)

By plugging the above two equations into (12), the global form of the solution \(\{k_t(x^p_i, x^q_j)\}\) which minimizes the constrained minimization problem (3) is:

\[
\frac{1}{Z_i} \ \exp\left(-\frac{d(x^p_i, x^q_j)}{\beta}\right) \times \exp\left(\frac{2 \alpha}{\beta} \sum_{k,l} \ \exp(-U^2_{ij}) \exp(-U^2_{kl}) \exp(-U^2_{ij})\right) (13)
\]

where \(Z_i = \sum_{j} Z^{(i)}_{ij}\). The solution of (3) corresponds to a fixed-point which is found iteratively \(\mathcal{U}\).

Convergence

Let us assume \(0 \leq g \leq 1\), and remind \(\mu^{(t)} \in \mathbb{R}^{n \times m}\) be the vector of components \(\mu^{(t)}_{i,j} = k_t(x^p_i, x^q_j)\). Introduce the mapping \(f : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^{n \times m}\) defined by its component

\[
f_{i,j}(\nu) = \exp\left(-\frac{d(x^p_i, x^q_j)}{\beta} + \frac{2 \alpha}{\beta} \sum_{k,l} g(x^p_i, x^q_k)g(x^q_j, x^q_l)\nu_{k,l}\right) (14)
\]
By construction of the kernel $k_1$, we have $\mu^{(t)} = f(\mu^{(t-1)})$. Let $A$ and $B$ satisfy
\[ \sup_{1 \leq i \leq n, 1 \leq j \leq m} \sum_{k, \ell} g(x^i_k, x^j_\ell)g(x^{i'}_k, x^{j'}_\ell) \leq A \] \[ \sum_{i, j} \exp \left( -1 - \frac{d(x^i_k, x^{j'}_\ell)}{\beta} \right) \leq B \]

Consider $L = 2\exp \left( \frac{2\alpha}{\beta} \right)$, and let $B = \{ v \in \mathbb{R}^{n \times m} : \forall 1 \leq i \leq n, 1 \leq j \leq m, |v_{i,j}| \leq 1 \}$ be the $\ell_\infty$-ball of radius 1. Finally, let $\| \cdot \|$ denote the $L_1$-norm on $\mathbb{R}^{n \times m}$: $\|u\|_1 = \sum_{1 \leq i \leq n, 1 \leq j \leq m} |u_{i,j}|$.

**Proposition 4** If $\mu^{(0)} \leq 1$ and $2\alpha A \leq \beta$, then we have $f(B) \subseteq B$, and on $B$, $f$ is $L$-Lipschitz for the norm $\| \cdot \|_1$.

In particular, if $L < 1$, then there exists a unique $\tilde{v} \in B$ such that $f(\tilde{v}) = \tilde{v}$, and the sequence $(\mu^{(t)})$ satisfies
\[ \|\mu^{(t)} - \tilde{v}\|_1 \leq L \|\mu^{(0)} - \tilde{v}\|_1 \xrightarrow{t \to +\infty} 0. \]

**Proof.** The first assertion is proved by induction by checking that for $\|v\|_1 \leq 1$, we have
\[ f_{i,j}(v) \leq \exp \left( -1 + \frac{2\alpha}{\beta} \sum_{k, \ell} g(x^i_k, x^j_\ell)g(x^{i'}_k, x^{j'}_\ell)K_{v_k, \ell} \right) \] \[ \leq \exp \left( -1 + \frac{2\alpha}{\beta} A \right) \leq 1. \]

For the second assertion, note that for any $v \in B$, we have $|\partial f_{i,j}/\partial x^i_k(v)| \leq \exp \left( -1 - \frac{d(x^i_k, x^{i'}_k)}{\beta} \right)$ for any $v, v' \in B$, we have
\[ \|f(v) - f(v')\|_1 = \sum_{i, j} |f_{i,j}(v) - f_{i,j}(v')| = (**) \]

\[ \leq \sum_{i, j} \exp \left( -1 - \frac{d(x^i_k, x^{i'}_k)}{\beta} \right) \frac{2\alpha}{\beta} \exp \left( \frac{2\alpha}{\beta} A \right) \]
\[ \times \sum_{k, \ell} g(x^i_k, x^j_\ell)g(x^{i'}_k, x^{j'}_\ell)K_{v_k, \ell} - \sum_{k, \ell} g(x^i_k, x^j_\ell)g(x^{i'}_k, x^{j'}_\ell)K_{v_k, \ell} \]
\[ \leq \sum_{i, j} \exp \left( -1 - \frac{d(x^i_k, x^{j'}_\ell)}{\beta} \right) \frac{2\alpha}{\beta} \exp \left( \frac{2\alpha}{\beta} A \right) \|v - v'\|_2^2 \]
\[ \leq L \|v - v'\|_1. \]

which proves the second assertion. The last assertion directly comes from the fixed-point theorem.

**References**


