A New Family of Graph Representation Matrices: Application to Graph and Signal Classification

T. Averty, A. O. Boudraa (*Senior Member, IEEE*) and D. Daré-Emzivat

***Abstract*—Most natural matrices that incorporate information about a graph are the adjacency and the Laplacian matrices. These algebraic representations govern the fundamental concepts and tools in graph signal processing even though they reveal information in different ways. Furthermore, in the context of spectral graph classification, the problem of cospectrality may arise and it is not well handled by these matrices. Thus, the question of finding the best graph representation matrix still stands. In this letter, a new family of representations that well captures information about graphs and also allows to find the standard representation matrices, is introduced. This family of unified matrices well captures the graph information and extends the recent works of the literature. Two properties are proven, namely its positive semidefiniteness and the monotonicity of their eigenvalues. Reported experimental results of spectral graph classification highlight the potential and the added value of this new family of matrices, and evidence that the best representation depends upon the structure of the underlying graph.**

***Index Terms*—Graph representation, adjacency matrix, Laplacian matrix, spectral graph theory, graph signal processing**

I. Introduction

NETWORK data are generated from varying sources and arise naturally in diverse fields such as social media, physics, chemistry, biology or information systems [1], [2]. Data structures of such networks are well captured by graphs, which are powerful models for relational data representation that comprise a set of nodes (vertices) and weighted edges. To describe the connections between vertices in a graph, a matrix representation is used. A great deal of information about the graph's structural properties can be retrieved from it: degree distribution, node centralities or molecular indices. Salient features can also be revealed from eigenvalues of the matrix representation [2]–[4]. There are two natural matrices to conveniently represent a graph, namely adjacency matrix $\mathbf{A}$ and Laplacian matrix $\mathbf{L}$. Study of these matrices constitutes a significant topic in both algebraic graph theory and graph signal processing (GSP) [1], [3], [5]. In recent domain of GSP, fundamental concepts on graphs based on these two matrices are defined, but the difference in their foundation leads to different definitions and techniques for signal analysis and processing [6]–[8]. Overall, graphs study can be divided into two main schools of thought : adjacency-based and Laplacian-based. In the first one, we can quote the work of Sandryhaila *et al.* where the matrix $\mathbf{A}$ is adopted as the shift operator and concepts of impulse and frequency response, convolution, filtering, and Fourier transform are developed [7], [9]. In the second school, consider the work of Shuman *et al.* which defines a generic framework for processing data on graphs, where operations such as filtering, translation, modulation, dilation, and downsampling are defined using the Laplacian matrix $\mathbf{L}$ [6], [10], [11]. They also put forward a suitable interpretation of the eigenvalues (resp. eigenvectors) of matrix $\mathbf{L}$ as frequencies (resp. vibratory modes) of the graph under study. Of course, other representation matrices have also been used, such as the degree matrix $\mathbf{D}$, the signless Laplacian $\mathbf{Q}$ [12] and the normalized Laplacian $\boldsymbol{\mathcal{L}}$ [4]. This raises a legitimate question: Which is better to use, matrix $\mathbf{A}$ or matrix $\mathbf{L}$? Or an other ? On this point, the debate remains open. The answer depends upon the target applications and what operations to be performed on the graph. This being said, one may think about an other way, where matrices are combined to form a single matrix representation.

It has been shown by Bay-Ahmed *et al.* that, in spite of the linear relationship between matrices $\mathbf{A}$ and $\mathbf{L}$, these two matrices reveal informations of graph in different ways [13]. The authors highlight the graph's representation disparity between both of them illustrated *via* entropy, connectivity and complexity measures [13]. These findings strengthens the idea to combine the two matrices to better reveal the structural and spectral properties of the graph. In the same spirit, Nikiforov unifies the study of matrices $\mathbf{A}$ and $\mathbf{Q}$ in order to highlight the differences and similarities between those two matrices [14]. This work gives rise to α–adjacency matrix $\mathbf{A}_\alpha$ which, for particular values of α, recovers the classical representation matrices $\mathbf{A}, \mathbf{Q}$ and $\mathbf{D}$ [15]. However, matrix $\mathbf{L}$ cannot be obtained from the matrix $\mathbf{A}_\alpha$. Using the same strategy, Wang *et al.* proposed a family of graph representations $\mathbf{L}_\alpha$ called α–Laplacian [16] which, unlike Nikiforov's approach, allows recovery of matrix $\mathbf{L}$ but fails to obtain exactly matrix $\mathbf{A}$.

Based on our previous work [13] and inspired by the families of graph representations $\mathbf{A}_\alpha$ and $\mathbf{L}_\alpha$, we extend the work of Nikiforov *et al.* [14] and Wang *et al.* [16] that includes both the matrix $\mathbf{A}$ and matrix $\mathbf{L}$, which are the two main graph representations, particularly in GSP. Matrices $\mathbf{Q}$ and $\mathbf{D}$ can also be retrieved from the proposed graph representations, thus completing the list of classic representation matrices.

II. Preliminaries & Related Works

This section covers some graph preliminaries and the related works about generalized representation matrices. First, we recall that a simple undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a pair of sets: the set $\mathcal{V}$ consisting of n vertices, called order of G, and the set $\mathcal{E} \subseteq \{\{i,j\} : (i,j) \in \mathcal{V}^2, i \neq j\}$ of m edges. Weights w_{ij} can be added to edge to signify importance of a link between two nodes in a network. In the unweighted case, matrix $\mathbf{A}$ is binary, where the coefficient $\mathbf{A}_{ij}$ is 1 if there exists an edge $\{i,j\}$ and 0 otherwise. For weighted graph, the 1 is replaced by the weight w_{ij}. Another matrix is the

The authors are with the Arts et Métiers Institute of Technology, École navale, IRENav (EA 3634), BCRM Brest, CC 600, 29240 Brest Cedex 9, France ([tristan.averty, delphine.dare, abdel.boudraa]@ecole-navale.fr)

diagonal degree matrix $\mathbf{D}$ which contains information about the degree of each vertex $\deg(i) = \sum_{j=1}^{n} \mathbf{A}_{ij}$ defined as the number of edges attached to each vertex in the unweighted case. The last conventional matrix is the Laplacian matrix $\mathbf{L} := \mathbf{D} - \mathbf{A}$ defined as a combination of the two former. This matrix is used particularly in spectral graph theory, since it has a physical meaning insofar as a quadratic form can be defined from it, which measures the smoothness of a function defined on the graph [4]. Variants of the matrix $\mathbf{L}$ exist such as the normalized Laplacian $\boldsymbol{\mathcal{L}} := \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$ [4] or the signless Laplacian $\mathbf{Q} := \mathbf{D} + \mathbf{A}$ [17].

The idea behind this work came from the observation that GSP, a fairly recent field that takes advantage of graph spectral theory, was seeing two theories "competing" with each other as mentioned above: the one for which the graph Fourier transform is defined using matrix $\mathbf{A}$ [7], and the other defined using matrix $\mathbf{L}$ [6]. So the idea is to think of a parametric representation that can be used to study several of them at once, in particular their spectral aspects. Indeed, the spectral graph theory is an aspect very rich for the study of graphs. If $\lambda_1 \leq \cdots \leq \lambda_n$ denote the eigenvalues of $\mathbf{A}$ and $0 = \mu_1 \leq \cdots \leq \mu_n$ denote the eigenvalues of $\mathbf{L}$, then some properties can be established on these spectra that allow us to retrieve structural attributes [4]. With this in mind, classical similarity measures based on structural attributes, such as the shortest path (SP), random walk (RW), graphlet count kernel (GK) or the Weisfeiler-Lehman isomorphism test (WL), are gradually giving way to spectral similarity measures which compare the spectra of the representation matrices of the graphs studied [13], [18], [19]. Thus, one can calculate the Euclidean distance between $\mathbf{A}$–spectra (or $\mathbf{L}$). This would not be a rigorous distance, because a zero distance between spectra does not imply that the graphs are identical: this is the cospectrality problem [17], [20]. In fact, two structurally different graphs with the same spectra (with respect to a chosen representation matrix) can be found or constructed. To tackle this problem, Joint Spectral Similarity (JSS) between two graphs G_1 and G_2 was introduced in [13]:

$$\mathrm{JSS}_\beta(G_1, G_2) = \beta \mathrm{SS}_{\mathbf{L}}(G_1, G_2) + (1-\beta)\mathrm{SS}_{\mathbf{A}}(G_1, G_2) \quad (1)$$

where

$$\mathrm{SS}_{\mathbf{A}}(G_1, G_2) = \sum_{\ell=1}^{N} \left(\lambda_\ell^{(1)} - \lambda_\ell^{(2)}\right)^2$$
$$\mathrm{SS}_{\mathbf{L}}(G_1, G_2) = \sum_{\ell=1}^{N} \left(\mu_\ell^{(1)} - \mu_\ell^{(2)}\right)^2$$

with a parameter β varying from 0 to 1, $N = \min(n_1, n_2)$ with n_1 (resp. n_2) the order of G_1 (resp. G_2), where $\lambda_\ell^{(1)}$ (resp. $\lambda_\ell^{(2)}$) represents the ℓ^{th} eigenvalue of the matrix $\mathbf{A}$ of G_1 (resp. G_2) and where $\mu_\ell^{(1)}$ (resp. $\mu_\ell^{(2)}$) represents the ℓ^{th} eigenvalue of the matrix $\mathbf{L}$ of G_1 (resp. G_2). A limitation of this measure is the need to calculate two spectra. So, to take this into account, as well as cospectrality, we can think about a combination of matrices that allows us to cover traditional ones. One can quote the generalized adjacency matrix $\mathbf{G} = a\mathbf{A} + b\mathbf{I} + c\mathbf{J}$ and the universal one $\mathbf{U} = \mathbf{G} + d\mathbf{D}$ (with $a, b, c, d \in \mathbb{R}, a \neq 0, \mathbf{I}$ the identity matrix and $\mathbf{J}$ the one matrix) introduced by van Dam *et al.* [21], [22]. However, these two matrices have too many parameters which prevent intuitive and visual analysis. This is why, Nikiforov [14] introduced the α–adjacency matrix $\mathbf{A}_\alpha = \alpha\mathbf{D} + (1-\alpha)\mathbf{A}$ for $\alpha \in [0, 1]$. But the matrix $\mathbf{L}$ can not be recovered from $\mathbf{A}_\alpha$. So Wang *et al.* [16] defined the α–Laplacian $\mathbf{L}_\alpha = \alpha\mathbf{D} + (\alpha - 1)\mathbf{A}$ with $\alpha \in [0, 1]$. This matrix passes through $\mathbf{L}$ but also by $-\mathbf{A}$ which does not seem to be much of a problem, since the spectra of $\mathbf{L}$ and $\mathbf{A}$ should be studied in polarity inversion, *i.e.* the largest eigenvalue of matrix $\mathbf{A}$ corresponds to the smallest eigenvalue of $\mathbf{L}$ [23], [24]. Also, one can cite the $\mathbf{T}_\alpha$ representation matrix defined by $\mathbf{T}_\alpha := \alpha\mathbf{D} + (1 - 2\alpha)\mathbf{A}$ for $\alpha \in [0, 1]$ introduced by Averty *et al.* [25]. In the same work, a new measure of spectral similarity based on a correlation between $\mathbf{T}_\alpha$ spectra is proposed [25]. Let G_1 and G_2 be two graphs of order n. If $\widetilde{\boldsymbol{\nu}}_1^{(\alpha)}$ (resp. $\widetilde{\boldsymbol{\nu}}_2^{(\alpha)}$) represents the standardized spectrum of the matrix $\mathbf{T}_\alpha(G_1)$ (resp. $\mathbf{T}_\alpha(G_2)$), then the similarity measure is defined by

$$\mathrm{SCor}_{\mathbf{T}_\alpha}(G_1, G_2) := \sqrt{1 - \left(\frac{1}{n}\left\langle \widetilde{\boldsymbol{\nu}}_1^{(\alpha)}, \widetilde{\boldsymbol{\nu}}_2^{(\alpha)} \right\rangle\right)^2} \quad (2)$$

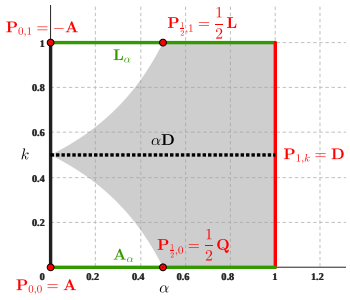
where $\langle \cdot, \cdot \rangle$ is the inner product. It has been shown that promising classification results can be obtained with this measure integrated into a SVM kernel in comparison with the structural kernels previously discussed [25]. Main limitation of the latter measure is that it requires graphs of the same size. If this is not the case, a node-padding can be done [26].

III. Proposed Representation Matrix

With regard to all that was written earlier, and if we want to gather all the desired advantages, including the fact that we need to include matrix $\mathbf{Q}$ as it has the advantage of encountering fewer cospectral graphs (for $n \geq 7$) [17], a novel parametric representation of graphs has to be defined. A first, relatively naive way of doing this is to concatenate the $\mathbf{A}_\alpha$ and $\mathbf{L}_\alpha$ matrices, which can be done by introducing a matrix $\mathbf{S}_\gamma := (1 - |\gamma|)\mathbf{D} + \gamma\mathbf{A}$ for a parameter $\gamma \in [-1, 1]$. Indeed, for $\gamma \leq 0$, the γ–Laplacian can be retrieved and for $\gamma \geq 0$, it is the γ–adjacency. But this intuitive manner does not give enough space as we are interested in whether there is a "best" representation by combining all these previous matrices. To do this, the following representation plan is constructed:

$$\mathbf{P}_{\alpha,k} := \alpha\mathbf{D} + (2k - 1)(\alpha - 1)\mathbf{A}, \quad \alpha, k \in [0, 1]. \quad (3)$$

As illustrated in Fig. 1, most representation matrices can be recovered from $\mathbf{P}_{\alpha,k}$. Thus, we can study the gradual changes



Matrices $\mathbf{P}_{\alpha,k}$	Classical matrices
$\mathbf{P}_{0,0}$	$\mathbf{A}$
$2\mathbf{P}_{\frac{1}{2},1}$	$\mathbf{L}$
$\mathbf{P}_{0,1}$	$-\mathbf{A}$
$2\mathbf{P}_{\frac{1}{2},0}$	$\mathbf{Q}$
$\mathbf{P}_{\alpha,\frac{1}{2}}$	$\alpha\mathbf{D}$
$\mathbf{P}_{1,k}$	$\mathbf{D}$
$\mathbf{P}_{\alpha,0}$	$\mathbf{A}_\alpha$
$\mathbf{P}_{\alpha,1}$	$\mathbf{L}_\alpha$

Fig. 1. Representation plan $\mathbf{P}_{\alpha,k}$ for $\alpha, k \in [0, 1]$. Standard representation matrices are in red on the figure although the matrices of Nikiforov and Wang are green. These matrix equalities are listed in the table on the right.

of $\mathbf{P}_{\alpha,k}$ between $\mathbf{A}$ and $\mathbf{D}$, passing through $\mathbf{Q}$ and $\mathbf{L}$. In the following, we present two important properties of $\mathbf{P}_{\alpha,k}$, namely the positive semidefiniteness and the monotonicity of their eigenvalues in α.

Prop 1. *Let G be a graph with $\mathbf{P}_{\alpha,k}$ its representation plan. Then $\mathbf{P}_{\alpha,k}$ is positive semidefinite if $\frac{2\alpha-1}{2(\alpha-1)} \leq k \leq \frac{1}{2(1-\alpha)}$.*

Proof. Since $\mathbf{A} = \mathbf{D} - \mathbf{L}$, the expression of $\mathbf{P}_{\alpha,k}$ can be written as:

$$\mathbf{P}_{\alpha,k} = [\alpha + (2k-1)(\alpha-1)]\,\mathbf{D} + (2k-1)(1-\alpha)\mathbf{L}.$$

As $\mathbf{D}$ and $\mathbf{L}$ are two positive semidefinite matrices and using the fact that the sum of two positive semidefinite matrices is positive semidefinite, then both conditions $\alpha + (2k-1)(\alpha-1) \geq 0$ and $(2k-1)(1-\alpha) \geq 0$ are needed to get the positive semidefiniteness of $\mathbf{P}_{\alpha,k}$. Thus, it is necessary to have $\frac{1}{2} \leq k \leq \frac{1}{2(1-\alpha)}$. Secondly, generalizing what Nikiforov did for $\mathbf{A}_\alpha$ to the plan $\mathbf{P}_{\alpha,k}$ [14]:

$$\begin{aligned}\langle \mathbf{P}_{\alpha,k}\mathbf{x}, \mathbf{x}\rangle = [\alpha - (2k-1)(\alpha-1)] \sum_{i\in\mathcal{V}} x_i^2 \deg(i) \\ + (2k-1)(\alpha-1) \sum_{(i,j)\in\mathcal{E}} (x_i + x_j)^2\end{aligned}$$

where x_i is i^{th} component of the vector $\mathbf{x} \in \mathbb{R}^n$. For any edge $\{i,j\}$,

$$\begin{aligned}\langle \mathbf{P}_{\alpha,k}\mathbf{x}, \mathbf{x}\rangle \geq [\alpha - (2k-1)(\alpha-1)]\,(x_i^2 + x_j^2) \\ + (2k-1)(\alpha-1)(x_i + x_j)^2.\end{aligned}$$

Then, an other condition to get the positive semidefiniteness of $\mathbf{P}_{\alpha,k}$ is to have $\alpha - (2k-1)(\alpha-1) \geq 0$ and $(2k-1)(\alpha-1) \geq 0$ which implies $\frac{2\alpha-1}{2(\alpha-1)} \leq k \leq \frac{1}{2}$. Finally, by grouping all the conditions together, we obtain a necessary condition: if $\frac{2\alpha-1}{2(\alpha-1)} \leq k \leq \frac{1}{2(1-\alpha)}$, then $\mathbf{P}_{\alpha,k}$ is positive semidefinite. ■

Fig. 1 also presents an illustration of the Prop 1's necessary conditions: matrices defined in the shaded area are necessarily positive semidefinite. Actually, it may be conjectured thanks to the Theorem 3.5 of Wang *et al.* [16] that the condition of positive semidefiniteness $\frac{1}{2} \leq k \leq \frac{1}{2(1-\alpha)}$ is necessary and sufficient *i.e.* it does not exist a couple (α^*, k^*) in the domain $\left[0, \frac{1}{2}\right] \times \left[\frac{1}{2(1-\alpha)}, 1\right]$ for which the matrix $\mathbf{P}_{\alpha^*,k^*}$ is positive semidefinite. This conjecture is illustrated on two graphs (the comet and the twoballs graphs) by Fig. 2. Elsewhere, Prop 1 points to a condition that is only necessary. Indeed, like Nikiforov's work, determining the domain in which the condition becomes necessary and sufficient seems to be an arduous task and must obviously depend on the structure of the graph under study. For this reason, an open question is: for which graphs does the assertion of Prop 1 become reciprocal? To illustrate, and as shown by Fig. 2, the comet graph seems to have a positive semidefinite representation plan in the aforementioned domain and nowhere else whereas for the twoballs graph, the condition is only necessary. Indeed, as an example for this graph, the $\mathbf{P}_{0.25,0.25}$ matrix is positive semidefinite even though the point is outside the proven domain of Prop 1.

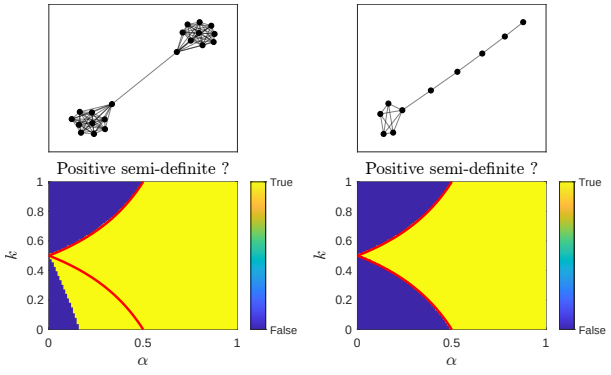


Fig. 2. Graphs (Left : Twoballs / Right : Comet) and positive semidefiniteness of their $\mathbf{P}_{\alpha,k}$ representation matrices with respect to α and k (yellow for true, blue for false). The red curves correspond to the condition of Prop 1.

In the sequel, let us denote $\nu_\ell^{(\alpha,k)}$ the ℓ^{th} eigenvalue of the matrix $\mathbf{P}_{\alpha,k}$. Another interesting result is the generalization of Nikiforov's Proposition 3 in [14] on the monotonicity of $\nu_\ell^{(\alpha,k)}$ in α (and not in k), formalized by the following proposition.

Prop 2. *Let G be a graph, $\alpha \in [0,1]$ and $\alpha' \in [\alpha, 1]$. Then,*

$$\nu_\ell^{(\alpha,k)} \leq \nu_\ell^{(\alpha',k)}, \quad \forall k \in [0,1]$$

Proof. Let $\alpha \in [0,1]$ and $\alpha' \in [\alpha,1]$. The same proof scheme as Nikiforov [14] is used so the following expression needs to be written

$$\mathbf{P}_{\alpha',k} - \mathbf{P}_{\alpha,k} = (\alpha' - \alpha)\,[\mathbf{D} - (2k-1)\mathbf{A}]$$

Thanks to a simplified version of the Weyl theorem [27], it follows

$$\nu_\ell(\mathbf{P}_{\alpha',k}) - \nu_\ell(\mathbf{P}_{\alpha,k}) \geq (\alpha' - \alpha)\nu_1(\mathbf{D} - (2k-1)\mathbf{A}) \geq 0$$

where $\nu_1(\mathbf{D} - (2k-1)\mathbf{A})$, which denotes the smallest eigenvalue of the matrix $\mathbf{M} := \mathbf{D} - (2k-1)\mathbf{A}$, is non-negative. To prove it, let us show that $\mathbf{M}$ is positive semidefinite. Let $\mathbf{x}$ be a vector of $\mathbb{R}^n$:

$$\begin{aligned}\langle \mathbf{M}\mathbf{x}, \mathbf{x}\rangle &= \sum_{i\in\mathcal{V}} x_i^2 d_i - 2(2k-1) \sum_{(i,j)\in\mathcal{E}} x_i x_j \\ &= 2(1-k) \sum_{i\in\mathcal{V}} x_i^2 d_i + (2k-1) \sum_{(i,j)\in\mathcal{E}} (x_i - x_j)^2 \quad (4) \\ &= 2k \sum_{i\in\mathcal{V}} x_i^2 d_i + (1-2k) \sum_{(i,j)\in\mathcal{E}} (x_i + x_j)^2. \quad (5)\end{aligned}$$

We use the expression (5) for $0 \leq k \leq 1/2$ and (4) for $1/2 \leq k \leq 1$ to prove that $\langle \mathbf{M}\mathbf{x}, \mathbf{x}\rangle \geq 0$. All eigenvalues of $\mathbf{M}$, in particular the smallest, are thus non-negative which completes the proof. ■

This result lends theoretical support to the definition of this representation plan and allows conjectures to be made about possible results, since it is known in advance that spectra will stack according to α for any k chosen between 0 and 1.

IV. Graph Spectral Classification

A. Motivations & Classification strategy

As an application of this new representation matrix, this section is dedicated to a spectral classification of graphs. This $\mathbf{P}_{\alpha,k}$ matrix plan should be seen as a tool for highlighting how spectral information evolves "between" classical representation matrices. Therefore, we adopt a SVM classification method to show that there are intermediate matrices containing more discriminating spectral information for graph classification. In our SVM classification, the kernel is defined as a variant of Eq. (2) in the sense that the standardized spectra of the $\mathbf{T}_\alpha$ matrices are replaced by the standardized spectra of the $\mathbf{P}_{\alpha,k}$ matrices, *i.e.* the Gram matrix $\mathbf{K}$ will be defined with the following coefficients

$$[\mathbf{K}]_{ij} = \exp\left(-\,\mathrm{SCor}_{\mathbf{P}_{\alpha,k}}(G_i, G_j)\right). \quad (6)$$

B. Graph & Signal datasets

To show the interest of the family $\mathbf{P}_{\alpha,k}$ for graphs representation, five well known databases containing graphs or signals of very different origins are used for classification purpose. Databases **MUTAG** [28] and **PTC_MR** [29] contain respectively 188 and 344 chemical compounds labeled according to their mutagenic effect on a bacterium and carcinogenicity on male rats respectively. The **IMDB-BINARY** and **IMDB-MULTI** [30] movie collaboration datasets are used and consist of the ego-networks of respectively 1000 and 1500 actors/actresses who played roles in movies in IMDb divided into respectively two and three genres. The **ItalyPowerDemand** [31], [32] dataset contains 1096 pieces of a twelve monthly electrical power demand time series from Italy. The classification task is to distinguish days from Oct to March from Apr to Sept. These signals are converted into graphs thanks to the well-known horizontal visibility algorithm [33], [34]. Since the structures embedded in the graphs are different, it is expected that the results will differ from one database to another. Consequently, the "best" matrix for spectral classification will differ as well.

C. Results & Discussions

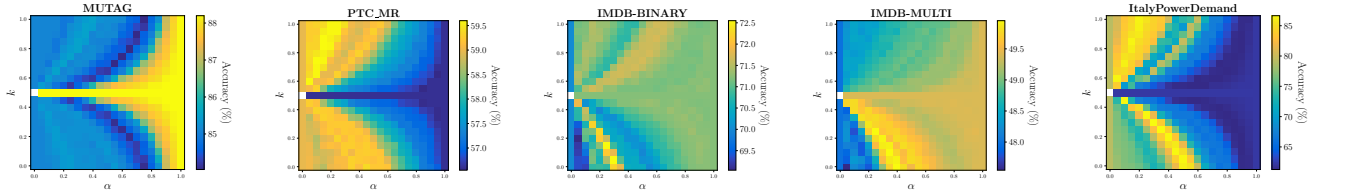
The SVM classifier is trained with a 10-fold stratified cross-validation. Graphical results and the associated accuracy values, averaged over 10 iterations, are shown in Fig. 3. Parameters α and k of the plan $\mathbf{P}_{\alpha,k}$ are taken between 0 and 1 by step 0.05. As depicted in Fig. 3, "maps" that represent classification accuracies are different from one database to another. This highlights the fact that a sole representation does not fit well all the databases. That is to say, it is not the spectral content of a single matrix that allows the best classification for all databases. On the other hand, the optimal matrices in terms of classification accuracies differ greatly from one database to the next as it can be read on the table of Fig. 3. Indeed, it is the matrix $\mathbf{P}_{1,k} = \mathbf{D}$ for MUTAG with an accuracy of 88.2% exceeding the others by nearly 3%. For PTC_MR, the matrix $\mathbf{P}_{0.1,0.75}$, with an accuracy of 59.6%, is slightly ahead (+0.5%) of the results obtained with the classic matrices $\mathbf{L}$ and $\mathbf{Q}$. It is again a non-standard matrix ($\mathbf{P}_{0.3,0.05}$) for IMDB-BINARY that reaches a 72.55% classification accuracy and for ItalyPowerDemand, it is the matrix $\mathbf{P}_{0.35,0.25}$ that performs best a little higher than the result with the matrix $\mathbf{Q}$. The reasons why it is these parameters that produce the best results must be investigated. What these results show is that in 4 out of 5 cases it is not a standard representation matrix ($\mathbf{A}$, $\mathbf{L}$, $\mathbf{D}$ or $\mathbf{Q}$) which provides the best spectral classification to be carried out. For the same classification method, we highlight here that the optimal spectral content differs from one matrix to another and does not reside in the classic matrices but in a combination of the latter. Even if the main objective was not classification, but graph representation, the accuracy results (Fig. 3) obtained with the SCor kernel are comparable to those of SP and WL structural kernels and the JSS spectral kernel. However, for the ItalyPowerDemand database, the accuracy reached by WL is the best. In terms of computation times listed in Table I of kernel matrices on entire databases, the SCor kernel is better than the computationally-intensive RW and GK kernels, as well as the JSS kernel, which requires two spectra computation. The SP and WL kernels require less computation time, as they are dependent on the structures in the graphs. Since our method only depends on the number of vertices, it will be better suited to dense graphs, unlike the SP and WL kernels, which are better suited to sparse graphs.

	SCor	JSS	SP	RW	GK	WL
MUTAG	0.25	0.31	0.30	6.83	1.52	0.06
PTC_MR	0.68	0.68	0.45	19.52	1.76	0.09
IMDB-BINARY	5.69	7.41	3.73	215	> 900	0.72
IMDB-MULTI	10.01	10.41	3.02	235	> 900	0.80
ItalyPowerDemand	4.93	13.04	2.95	No convergence	24.79	0.62

TABLE I
AVERAGED COMPUTATION TIMES OF DIFFERENT KERNELS (IN SECONDS).

V. CONCLUSION & PERSPECTIVES

In this letter, a new family of representation matrices generalizing most of the traditional ones, noted $\mathbf{P}_{\alpha,k}$, that well captures information about a graph is introduced. This family has at least two properties, namely the positive semidefiniteness and the monotonicity of the eigenvalues in parameter α. In addition, we report graph classification results using a spectral correlation kernel on real data from the literature that highlight the added value of this family of matrices by showing that classification accuracies are similar or even better than other traditional kernels. As future work, we plan to investigate more properties of $\mathbf{P}_{\alpha,k}$ and potential concepts of digital signal processing such as filtering or frequency response based on $\mathbf{P}_{\alpha,k}$. Another natural extension will be to develop a strategy to estimate the best parameters (α, k) of the representation that incorporates information about the graph under study.



	Best matrices	SCor kernel with classical matrices				Other kernels		
		$\mathbf{A} = \mathbf{P}_{0,0}$	$\mathbf{D} = \mathbf{P}_{1,k}$	$\mathbf{L} = 2\mathbf{P}_{0.5,1}$	$\mathbf{Q} = 2\mathbf{P}_{0.5,0}$	JSS	SP	WL
MUTAG	$88.2 \pm 0.4\%$ ($\mathbf{P}_{1,k}$)	$85.1 \pm 0.1\%$	$88.2 \pm 0.4\%$	$85.2 \pm 0.4\%$	$85.1 \pm 0.6\%$	$84.3 \pm 1.1\%$	$83.6 \pm 1.2\%$	$85.6 \pm 0.9\%$
PTC_MR	$59.6 \pm 0.7\%$ ($\mathbf{P}_{0.1,0.75}$)	$59.0 \pm 1.2\%$	$56.6 \pm 0.7\%$	$59.1 \pm 0.8\%$	$59.2 \pm 0.5\%$	$57.8 \pm 2.1\%$	$58.2 \pm 1.9\%$	$62.3 \pm 1.0\%$
IMDB-BINARY	$72.6 \pm 0.5\%$ ($\mathbf{P}_{0.3,0.05}$)	$70.0 \pm 0.8\%$	$71.2 \pm 0.5\%$	$71.1 \pm 0.6\%$	$70.5 \pm 0.6\%$	$67.5 \pm 0.9\%$	$69.8 \pm 1.3\%$	$72.7 \pm 1.2\%$
IMDB-MULTI	$50.0 \pm 0.5\%$ ($\mathbf{P}_{0.35,0.1}$)	$48.0 \pm 0.4\%$	$49.4 \pm 0.3\%$	$48.9 \pm 0.2\%$	$49.5 \pm 0.4\%$	$48.3 \pm 0.4\%$	$49.3 \pm 0.6\%$	$50.8 \pm 0.5\%$
ItalyPowerDemand	$86.7 \pm 0.2\%$ ($\mathbf{P}_{0.35,0.25}$)	$79.1 \pm 0.2\%$	$62.2 \pm 0.4\%$	$73.6 \pm 0.4\%$	$86.0 \pm 0.2\%$	$92.3 \pm 0.2\%$	$91.6 \pm 0.5\%$	$96.1 \pm 0.1\%$

Fig. 3. Figures on the top depict classification accuracies for 5 graph datasets and for different values of α and k defining $\mathbf{P}_{\alpha,k}$. In the table, accuracies reached by SCor kernel for the best $\mathbf{P}_{\alpha,k}$ matrix and for classical ones ($\mathbf{A}, \mathbf{D}, \mathbf{L}, \mathbf{Q}$) as well as accuracies obtained with other kernels (JSS, SP and WL).

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