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Donatello Conte

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# 1 **Graphs in pattern recognition: successes, shortcomings and new** 2 **perspectives**

3 **Donatello Conte**<sup>a,\*</sup>

4 <sup>a</sup>Université de Tours, Laboratoire d'Informatique Fondamentale et Appliquée de Tours (LIFAT - EA6300), Tours,  
5 France

6 **Abstract.** Graphs in Pattern Recognition have been studied starting from the late seventies with alternating events of  
7 successes and failures. Far from wanting to propose a new survey on the subject, this paper aims to present the areas  
8 in which graphs have been shown to be effective, and to illustrate the problems still open in this research domain, with  
9 a focus on recent developments moving in the direction of Deep Learning. The paper intends to arouse the interest of  
10 neophytes to this interesting domain that is the representation of the world through graphs.

11 **Keywords:** Graphs in Pattern Recognition, Graph matching, Graph Topology, Graph Embedding, Graph Neural Net-  
12 works.

13 \*Donatello Conte, [donatello.conte@univ-tours.fr](mailto:donatello.conte@univ-tours.fr)

## 14 **1 Introduction**

15 Graphs are powerful data structures that represent mainly relationships between entities.

16 Graph representation is very common in many application contexts, from social networks to  
17 chemo-informatics and transportation systems. But graphs have been effectively used in many  
18 other contexts, in particular image processing and computer vision.

19 Pattern Recognition methods using graphs have been proposed since early 90's (see<sup>1</sup> for a sur-  
20 vey on first papers discussing graph-based representation in Pattern Recognition). In this early  
21 period, until about 2010, researchers focused on problems of graph matching,<sup>2</sup> graph embedding  
22 (<sup>3-5</sup>), and graph topology (<sup>6,7</sup>). After there was an explosion of interest in deep learning tech-  
23 niques, and the use of graphs in neural networks (<sup>8,9</sup>). Recent trends can be found in some recent  
24 surveys<sup>10,11</sup> and a dozen other surveys are present in the literature.

25 However the goal of this paper is not to write a one more survey, rather a historical excursion  
26 of the use of graphs in pattern recognition. And even more than a historical excursion, to point out

27 some method that was a pillar in this topic.

28 The intention here is to propose a generic view of the different possibilities of the use of graphs  
29 in Pattern Recognition, possibly for a non-expert audience (which might differentiate it from other  
30 surveys). By presenting the best successes, and also what did not succeed, the reader can already  
31 get an idea of where to start when beginning research in this field. The reader will then be able  
32 to realize where graphs can be used effectively, and possibly jump into the fray to propose new  
33 solutions to open problems.

34 The rest of the paper is organized as follows: in the Section 2 we present some of the main  
35 methods that have had successful results in the use of graphs in pattern recognition; graph-based  
36 representation presents some drawbacks that we illustrate in the Section 3; we cannot pass over  
37 in silence, of course, a discussion of recent propositions of graph neural networks (GNN) which  
38 we do in the Section 4; in the Section 5 we describe the main applications and benchmarks used  
39 for graph problems in pattern recognition; and we discuss of main open problem in the Section 6;  
40 finally we draw some conclusions in the Section 7.

## 41 **2 Some successes on the use of graphs in pattern recognition**

### 42 *2.1 Graph Matching*

43 Graph matching is the problem of finding an optimal correspondence between the vertices and  
44 edges of two graphs. The Graph Matching problem can be divided into two general categories:  
45 exact matching and inexact matching. Exact matching aims to find a strict correspondence, or  
46 at least among their substructures. In the inexact matching, this constraint is relaxed to find the  
47 bijection between the vertex that optimizes a certain affinity or distortion criterion.

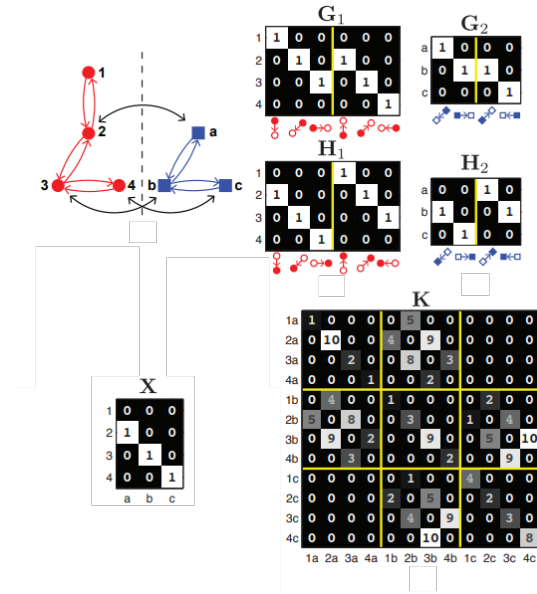
48 Graph Matching is a fundamental problem in computer science and relates to many areas such  
 49 as combinatorics, pattern recognition, multimedia and computer vision.

50 Referring back to other surveys for details, we would like to highlight here some of the most  
 51 effective methods of graph matching.

52 Graph Matching can be formulated as quadratic assignment problem (QAP) that is known to  
 53 be NP-hard. One of the most successfully proposal for finding a solution in a reasonable time  
 54 is the one proposed by Zhou et al.<sup>12</sup> Following<sup>12</sup> graph with  $n$  nodes and  $m$  directed edges are  
 55 represented by a 4-tuple  $G = \{\mathbf{P}, \mathbf{Q}, \mathbf{G}, \mathbf{H}\}$ , where  $\mathbf{P}^{dp \times n}$  contains features for nodes and  $\mathbf{Q}^{dq \times m}$   
 56 features for edges ( $dp$  and  $dq$  are the dimensions of the features space). The topology of the graph  
 57 is encoded by two node-edge incidence matrices  $\mathbf{G}, \mathbf{H}$  where  $g_{ic} = h_{jc} = 1$  if the  $c^{th}$  edge starts  
 58 from the  $i^{th}$  node and ends at the  $j^{th}$  node. Given a pair of graphs,  $G_1$  and  $G_2$ , an affinity matrix  
 59  $\mathbf{K} \in \mathbb{R}^{n_1 n_2 \times n_1 n_2}$  is defined encoding the node and edge affinities, to measure the similarity of each  
 60 node and edge pair respectively. Therefore, the problem of Graph Mathing consists in finding the  
 61 optimal correspondence  $\mathbf{X}$  between nodes, such that the sum of the node and edge compatibility is  
 62 maximized. Using  $K$ , Graph Mathing can be formulated as the QAP of Eq. 1. Given  $\mathbf{X}$ , which is a  
 63 matrix in which each element  $(i, j)$  is one if node  $i$  of graph  $G_1$  is to be associated with node  $j$  of  
 64 graph  $G_2$  and zero otherwise, the formula expresses the fact that, among all possible combinations  
 65 of values for the matrix  $X$ , the algorithm provides as a solution the one that maximizes the affinities  
 66 between the nodes.

$$\max_{\mathbf{X} \in \Pi} \text{vec}(\mathbf{X})^T \mathbf{K} \text{vec}(\mathbf{X}) \quad (1)$$

67 where  $\mathbf{X}$  is constrained to be a one-to-one mapping, and  $\Pi$  is the set of partial permutation



**Fig 1** Example of Graph Matching definition as defined in<sup>12</sup> (Figure modified from the paper). Note that the assignment of  $X$  corresponds to the node associations for which in the  $K$  matrix the affinities have the highest values.

68 matrices. In Fig. 1 there is an illustrative example of these definitions.

69 The main idea of this paper is to propose a new factorization of the pairwise affinity matrix  
70  $K$ . This factorization provides a light-weight representation for Graph Matching problems, allows  
71 a unification of Graph Matching methods (subgraph isomorphism, graph edit distance, etc.), and  
72 it allow a good performance in terms of time. For details on this factorization please refer to.<sup>12</sup>  
73 Results are very competitive in terms of time and quality of assignment, with respect many of  
74 state-of-the-art methods.<sup>13-15</sup>

75 A particular Graph Matching (GM) problem which has been addressed by many researchers is  
76 the so-called Graph Edit Distance (GED). The latter can be stated as follows: given two graphs, and  
77 some edit operations with an edit cost, graph edit distance is the problem of finding the minimum  
78 sum of edit cost to transform a graph into the other; Graph Edit Distance provides also a node-to-  
79 node correspondence between the nodes of the two graphs. Actually in 2021, Raveaux<sup>16</sup> shows  
80 that the GED problem can be equivalent to the GM problem under certain permissive conditions.

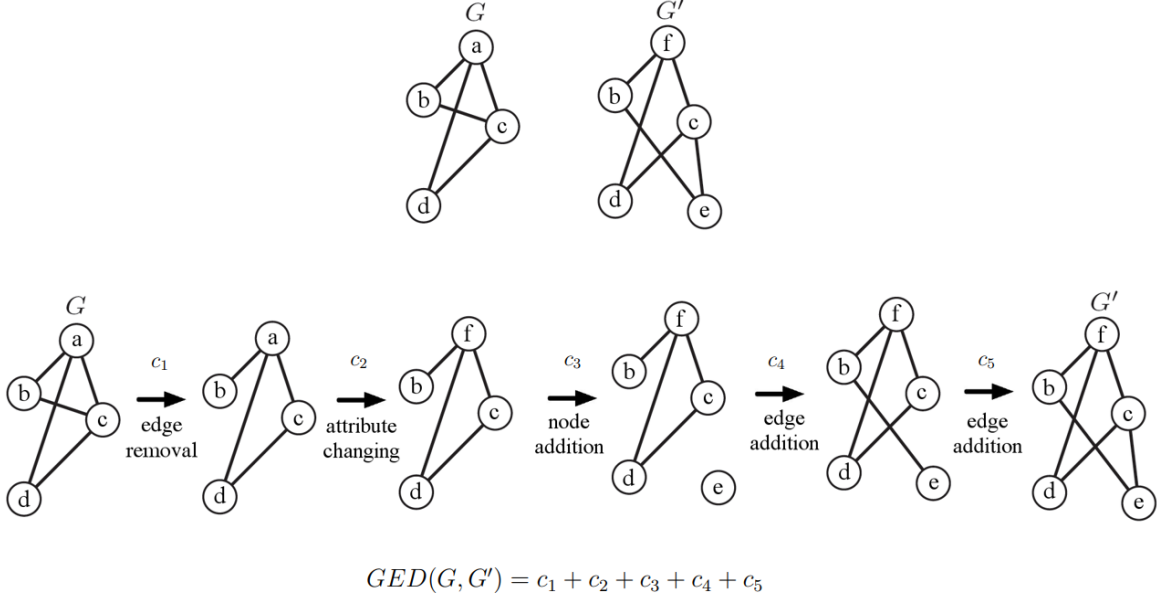
81 Nevertheless, as GED was widely addressed in literature we propose here some of key papers on  
 82 this specific problem.

83 We have seen a quadratic formulation of Graph Matching problem, and therefore equivalently  
 84 there are some quadratic formulation of GED. But as quadratic formulation is NP-hard, many  
 85 papers proposed a linear formulation of the GED problem, at the expense of a less precise but  
 86 still acceptable final solution. However some researcher have tried to find techniques for solving  
 87 the linear formulation that are both fast and accurate. Darwiche et al.<sup>17</sup> propose the use of some  
 88 research operational methods, in particular here is the Local Branching technique, to solve efficacy  
 89 the GED problem. Here we present the general principle of this proposal.

90 First an attributed graph is defined as a 4-tuple  $G = (V, E, \mu, \xi)$  where,  $V$  is the set of vertices,  
 91  $E$  is the set of edges, such that  $E \subseteq V \times V$ ,  $\mu : V \rightarrow L_V$  (resp.  $\xi : E \rightarrow L_E$ ) is the function  
 92 that assigns attributes to a vertex (resp. an edge), and  $L_V$  (resp.  $L_E$ ) is the label spaces for vertices  
 93 (resp. edges). Next, given two graphs  $G = (V, E, \mu, \xi)$  and  $G' = (V', E', \mu', \xi')$ , GED is the task  
 94 of transforming one graph source into another graph target. To accomplish this, GED introduces  
 95 the vertices and edges edit operations:  $(u \rightarrow v)$  is the substitution of two nodes,  $(u \rightarrow \epsilon)$  is the  
 96 deletion of a node, and  $(\epsilon \rightarrow v)$  is the insertion of a node, with  $u \in V, v \in V'$  and  $\epsilon$  refers to the  
 97 empty node. The same logic goes for the edges. In mathematical formula the Graph Edit Distance  
 98 between two graphs  $G$  and  $G'$  is defined by:

$$d_{\lambda_{min}}(G, G') = \min_{\lambda \in \Gamma(G, G')} \sum_{e_i \in \lambda} c(e_i) \quad (2)$$

99 where  $\Gamma(G, G')$  is the set of all complete edit paths,  $\lambda_{min}$  represents the set of operations with  
 100 the minimal cost, and  $c$  is the cost function that assigns the costs to elementary edit operations. See



**Fig 2** An intuitive explanation of the GED: Given two graphs  $G$  and  $G'$ , the figure shows the edit operations to transform  $G$  in  $G'$ , each operation having a cost  $c_i$ . The sum of the costs is the GED measure between the two graphs.

101 at the Fig. 2 for an intuitive explanation of the GED.

102 The main idea in the linear formulation of GED consists in determining the permutation matrix  
 103 minimizing the  $L_1$  norm of the difference between adjacency matrix of the input graph and the  
 104 permuted adjacency matrix of the target one. The model is as follows:

$$\min_{P, S, T \in \{0,1\}^{N \times N}} \sum_{i=1}^N \sum_{j=1}^N c(\mu(u_i), \mu'(v_j)) P^{ij} + \left( \frac{1}{2} \times const \times (S + T)^{ij} \right) \quad (3)$$

105 such that

$$(AP - PA' + S - T)^{ij} = 0 \quad \forall i, j \in \{1, N\} \quad (4)$$

106

$$\sum_{i=1}^N P^{ik} = \sum_{j=1}^N P^{kj} = 1 \quad \forall k \in \{1, N\} \quad (5)$$

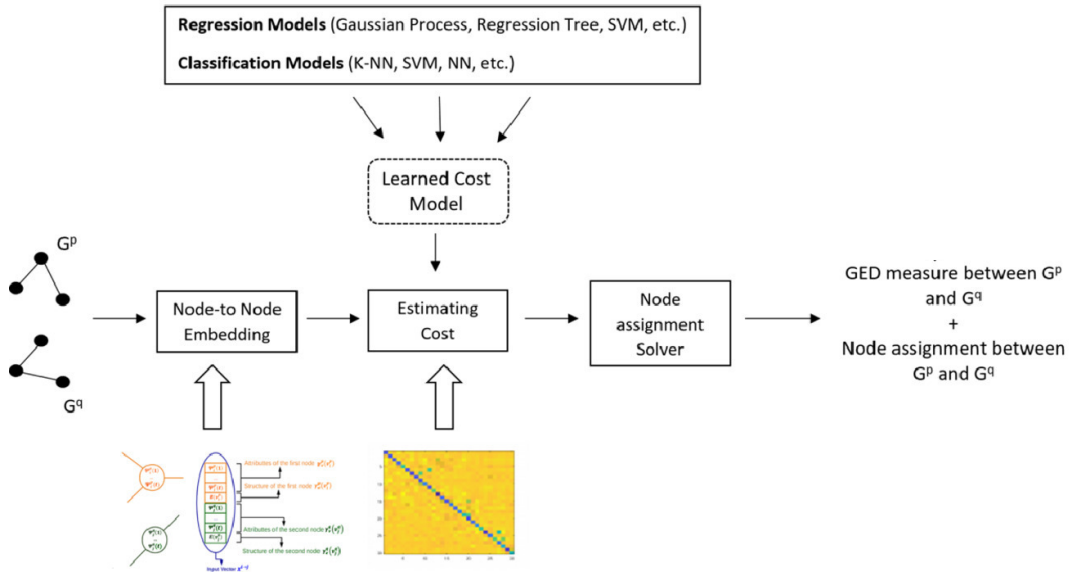
107 where  $A$  and  $A'$  are the adjacency matrices of graphs  $G$  and  $G'$  respectively,  $c : (\mu(u_i), \mu'(v_j)) \rightarrow$

108  $\mathbb{R}^+$  is the cost function that measures the distance between two vertices attributes. As for  $P, S$

109 and  $T$ , they are the permutation matrices of size  $N \times N$ , and of type boolean.  $P$  represents the  
110 vertices matching e.g.  $P^{ij} = 1$  means a vertex  $i \in V \cup \{v_\phi\}$  is matched with vertex  $j \in V' \cup \{v_\phi\}$ .  
111 While  $S$  and  $T$  are for edges matching. Local Branching heuristic is a local search approach, that  
112 makes use of MILP solver to explore the neighborhood of solutions through a branching scheme.  
113 In addition, it involves mechanisms such as intensification and diversification. In<sup>17</sup> they adapt the  
114 branching scheme and intensification and diversification phases in the case of Graph Matching. We  
115 refer to the paper for details. Authors show that for classical benchmarks for GED (see Section 5  
116 for details on benchmarks) the method is in average more accurate than others by one or two orders  
117 of magnitude while remaining competitive in terms of execution time.

118 The difficulty of solving the GED and the quality of the result also depends on the definition of  
119 the edit cost. For this reason, some researchers, instead of focusing on the search for new resolution  
120 techniques, propose to learn which are the best edit costs, based on the problem at hand, and in  
121 some precise application contexts where it is possible to know some instances of correspondence  
122 between graphs from which to learn. Some examples of this technique can be found in.<sup>18-21</sup> More  
123 recently there some deep learning technique to learn edit costs for GED, we will discuss about that  
124 in Secion 4. In Fig. 3 we illustrate the basic principle of edit cost learning: some ground truth  
125 data are available that indicate the true correspondences between a set of graph couples; theses  
126 correspondences are used in some learning schema (neural networks or other regression schema)  
127 to learn the best edit cost that give the true correspondence between graphs as solution of GED  
128 problem; then these cost are used in an application context. In<sup>19</sup> authors show that, learning costs,  
129 given a fixed dataset in which some graph correspondences are known, provide better results than  
130 using some fixed edit costs.



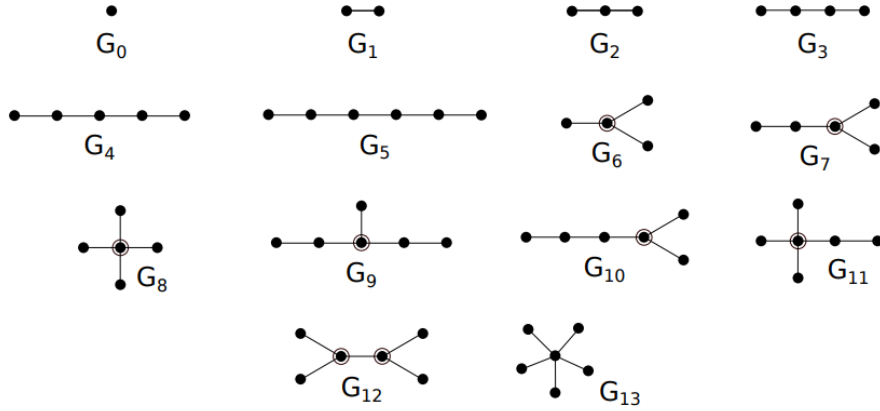


**Fig 3** A general framework for edit cost learning (Figure modified from the paper<sup>19</sup>).

## 131 2.2 Graph Embedding

132 In some contexts, particularly in classification and regression applications, the node-to-node cor-  
 133 respondence between graphs is not necessary, and what is useful is to be able to compare graphs  
 134 with each other in order to have a measure of distance for use with machine learning tools for re-  
 135 gression and classification. In these cases graph embedding has emerged as a promising solution.  
 136 Graph embedding methods map either explicitly or implicitly graphs into high dimensional spaces  
 137 hence allowing to perform the basic mathematical computations required by various statistical pat-  
 138 tern recognition techniques. Graph embedding methods appear thus as an interesting solution to  
 139 address graph clustering and classification problems.

140 The implicit graph embedding methods are based on graph kernels. A graph kernel is a function  
 141 that can be thought of as a dot product in some implicitly existing vector space. Explicit graph  
 142 embedding methods explicitly embed an input graph into a feature vector and thus enable the use  
 143 of all the methodologies and techniques devised for vector spaces.



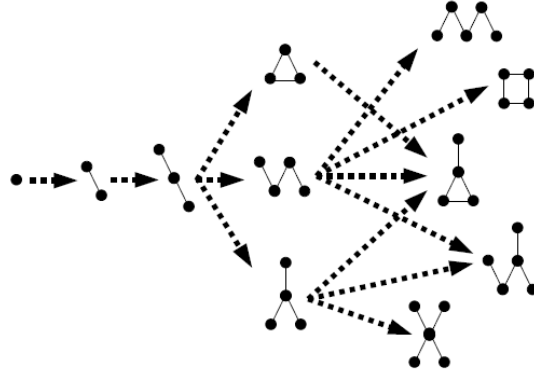
**Fig 4** The set of treelets having a size lower than or equals to 6 nodes (taken from<sup>22</sup>).

144 Among the proposals that have been made in recent years, we choose two in particular that  
 145 have proven particularly effective in classification contexts.

146 Treelet kernel<sup>22</sup> is a graph kernel based on a bag of non linear patterns which computes an  
 147 explicit distribution of each pattern within a graph. This method explicitly enumerates the set of  
 148 treelets included within a graph. The set of treelets, denoted  $\mathcal{T}$ , is defined as the 14 trees having  
 149 a size lower than or equals to 6 nodes (Fig. 4, taken from the paper, shows the set of treelets).  
 150 Thanks to the limited number of different patterns encoding treelets, an efficient enumeration of  
 151 the number of occurrences of each labeled pattern within a graph can be computed by algorithm  
 152 defined in the paper.<sup>22</sup> Treelet kernel between graphs is defined as a sum of sub kernels between  
 153 common treelets of both graphs (Eq. 6)

$$K_{\mathcal{T}}(G, G') = \sum_{t \in \mathcal{T}(G) \cap \mathcal{T}(G')} k(f_t(G), f_t(G')) \quad (6)$$

154 where  $\mathcal{T}(G)$  encodes the set of treelets included within  $G$ ,  $f_t(G)$  encodes the number of occur-  
 155 rences of each treelet  $t \in \mathcal{T}$  and  $k(., .)$  defines any positive definite kernel between real numbers



**Fig 5** The non-isomorphic graph network used to embed the topology.<sup>4</sup>

156 such as linear, Gaussian or polynomial kernel. Each sub kernel  $k(\cdot, \cdot)$  encodes the similarity of the  
 157 number of occurrences for each treelet  $t$  common to both graphs to be compared.

158 The topological embedding method proposed in<sup>23</sup> uses a generic lexicon of topological struc-  
 159 tures that could be enumerated in graphs during the computation of the vectorial signature of the  
 160 graphs. This lexicon must be comprehensive enough to ensure discrimination from a graph to  
 161 another. They have therefore decided to take as a baseline the non-isomorphic graphs network  
 162 presented in.<sup>24</sup> The network presents all graphs composed of  $n$  edges up to  $N$  (where  $N$  is the  
 163 maximum number of edges) (see Fig. 5 for an example). The vectorial representation of a graph  
 164 topology will be built by counting the occurrences of each pattern of the lexicon: each element of  
 165 the vector is the frequency of apparition of a pattern, which represents a descriptor of a part of the  
 166 graph. This vectorial representation needs now to be enriched by encapsulating the information  
 167 provided by attributes that can be associated to the edges and vertices, or by discretizing numerical  
 168 attributes or by performing a clustering in the label space using attributes as feature vectors. More  
 169 details about this topological embedding method can be found in.<sup>23</sup>

170 Just to get an idea of the efficiency of these methods, we present in Table 1 an extract of the  
 171 results of both methods, presented in,<sup>4</sup> on known graph bases for classification.

**Table 1** Classification results for different graph embedding methods and datasets (extracted from<sup>4</sup>).

	AIDS	MAO
Treelet kernel <sup>22</sup>	99.1	91.2
Topological Embedding <sup>23</sup>	99.4	91.2

### 172 2.3 Graph Topology

173 Graph representation is particularly useful when the data encodes information in which topology  
174 is important, notably image processing. Many classical image processing have been efficiently  
175 handled by a graph-based representation: image segmentation,<sup>25</sup> LBP coding,<sup>26</sup> Connected Com-  
176 ponents Labeling.<sup>27</sup>

177 Graph representation is particularly efficient when we want to represent an image at different  
178 resolution in a multi-level representation of an image called pyramid.<sup>28</sup> This hierarchy may be  
179 encoded using Irregular Pyramids.<sup>29,30</sup> These data structures encode each image as a graph whose  
180 nodes and edges respectively correspond to regions and region’s adjacencies. Irregular pyramids  
181 are a stack of successively reduced graphs where each graph is constructed from the graph below  
182 by selecting a specific subset of vertices and edges. For generation of irregular pyramids, two  
183 basic operations on graphs are needed: edge contraction and edge removal. The former merge  
184 two connected nodes in one, removing the edge connecting them. All edges that were incident  
185 to the joined vertices will be incident to the resulting vertex after the operation. Edge removal  
186 removes an edge from the graph, without changing the number of vertices or affecting the incidence  
187 relationships of other edges. In each level of the pyramid, the vertices and edges disappearing in  
188 level above are called *non-surviving* and those appearing in the upper level *surviving* ones.

189 There are different structures to build the irregular pyramid such as simple graphs,<sup>31</sup> dual  
190 graphs<sup>32</sup> and combinatorial maps.<sup>33</sup> Combinatorial Maps are most efficient data structure to built  
191 and represent irregular pyramid.<sup>25</sup> within the combinatorial maps the dual graphs may be implicitly

192 encoded and thus updated, this property allows to decrease both the memory and computational  
193 time requirements; combinatorial maps preserve the local orientation of edges around vertices and  
194 faces; combinatorial map formalism may be easily extended to higher dimensions.

### 195 **3 Drawbacks of graph-based representation**

196 The main drawback in the use of graph data structures is the processing times. In all the problems  
197 described above, the execution time remains a challenge to solve. The GED and GM problems  
198 have been proven to be NP-hard.<sup>34,35</sup> So, solving the problem to optimality cannot be done in  
199 polynomial time with respect to the size of the input graphs. On the other hand, heuristics are  
200 used when the demand for low computational time dominates the need to obtain optimal solutions.  
201 Graph embedding is also a costly operation. For example, treelet kernel requires to enumerate  
202 all labeled treelets from a graph with an overall complexity required equals to  $O(nd^5)$  where  $n$   
203 is the number of nodes and  $d$  is the maximum degree of the graph.<sup>22</sup> Construction of Irregular  
204 Pyramid requires also many operations,<sup>36</sup> and for this reason some parallel algorithms are proposed  
205 to overcome this problem.<sup>6</sup>

206 Another drawback of using graph-based representation, is that in several application context  
207 this kind of representation is not unique and the way in which the graphs are defined to represent  
208 the data strongly influences the results. If, for example, a graph-based representation of chemical  
209 data, or social networks, is quite straightforward, in domains such as image processing or computer  
210 vision, there are many possible alternatives of graph-based representations. Attributes on nodes  
211 and edge contribute to the variety of possible data representations. Data should be represented as  
212 nodes, or attributes on it, as edges or edges attributes. For example, when you deal with spatio-  
213 temporal data, you should choose to represent temporal data by a sequence of nodes at the different

214 time instances, or you can choose to represent a time series data as an attribute of a node. This  
215 variety of representations makes it difficult to generalise the algorithms to all application domains.  
216 Even more, in the contexts of learning, the solutions proposed are very specific to the domain under  
217 consideration.

#### 218 **4 The revival of graphs: Graph Neural Networks (GNN) and other machine learning tools** 219 **for graphs**

220 For the reasons mentioned in the previous section 3, research in the domain of graphs has always  
221 remained a somewhat niche research, without crossing the boundaries of a more or less restricted  
222 community. This is not the case nowadays: with the advent of Deep Learning, many researchers  
223 have proposed graph-based neuron network solutions. The positive and surprising thing is that  
224 these solutions have provided excellent results in many application contexts, particularly in the  
225 domain of image processing and computer vision, in which graphs had not been very successful  
226 until now (apart from a few happy exceptions). Today, however, there is great interest in graph-  
227 based neural networks and the major conferences in the field of pattern recognition, computer  
228 vision, and machine learning always contain many papers on this topic.

229 In this section, we give a brief overview of the principles behind these techniques and a brief  
230 excursion of the possible proposals in the domain of GNNs, referring to the numerous papers in  
231 the scientific literature to explore the subject further. We are inspired here mainly by the work of  
232 Wu et al.<sup>8</sup> which is a good survey to introduce the topic.

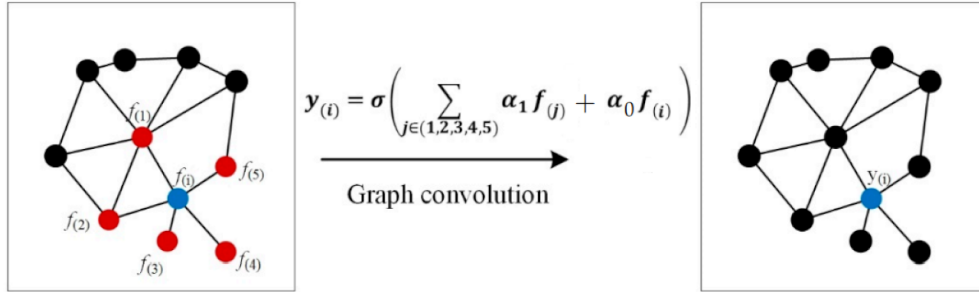
233 *4.1 Basics on Graph Neural Networks*

234 The basic principle of a Graph Neural Network is to update node features, in the different level of  
 235 the network, based on an information diffusion mechanism, i.e. by exchanging node neighborhood  
 236 information. This exchange is made by means of convolution operators defined on graph nodes.  
 237 Convolution operators fall into two categories, spectral-based and spatial-based. Spectral based  
 238 approaches define graph convolutions by introducing filters from the perspective of graph signal  
 239 processing.<sup>37</sup> Spatial-based approaches defines graph convolutions by information propagation.  
 240 Since GCN<sup>38</sup> bridged the gap between spectral-based approaches and spatial-based approaches,  
 241 spatial-based methods have developed rapidly recently due to its attractive efficiency, flexibility,  
 242 and generality.<sup>8</sup>

243 The basic convolution operator expressed in mathematical formulas is as follows. For this  
 244 purpose we define here a graph as  $G = (V, E)$  where  $V$  is the set of vertices and  $E$  is the set of  
 245 edges. The neighborhood of a node  $i$  is defined as  $N(i) = \{j \in V | (i, j) \in E\}$ .  $\mathbf{A}$  is the adjacency  
 246 matrix of  $G$  ( $A_{ij} = 1$  if  $e_{ij} \in E$ , 0 otherwise) and  $\mathbf{F} \in \mathbf{R}^{n \times d}$  is node feature matrix where  $f_i \in \mathbf{R}^d$   
 247 represents the feature vector of a node  $i$ . Analogously graph may have an edge attributes matrix  
 248  $\mathbf{F}^e \in \mathbf{R}^{m \times e}$ . So a generic convolution operator for a node  $i$  in a layer  $k$  is defined by Eq. 7, where  
 249  $a(\cdot)$  is an activation function and  $\mathbf{h}^{(0)} = 0$ .  $\mathbf{W}$  and  $\Theta$  are learnable model parameters that are  
 250 learned with classical tools of Deep Learning.

$$\mathbf{y}_i^{(k)} = a(\mathbf{W}^{(k)} \mathbf{f}_i + \sum_{j \in \mathbf{N}(i)} \Theta^{(k)} \mathbf{h}^{(k-1)}) \quad (7)$$

251 The main intuition behind the formula is that, at each convolution level, the new features of a  
 252 node results from the features of the node itself, plus the weighted average of all neighbors' node



**Fig 6** An illustration of graph convolution on a graph node: here  $f(i)$  is the input features vector of the node  $i$ ,  $f(j)$  are the features vectors of the neighboring nodes  $j$  of  $i$ ,  $\alpha_0, \dots, \alpha_5$  are learnable parameters, and  $y(i)$  is the output feature vector (figure adapted from<sup>39</sup>).

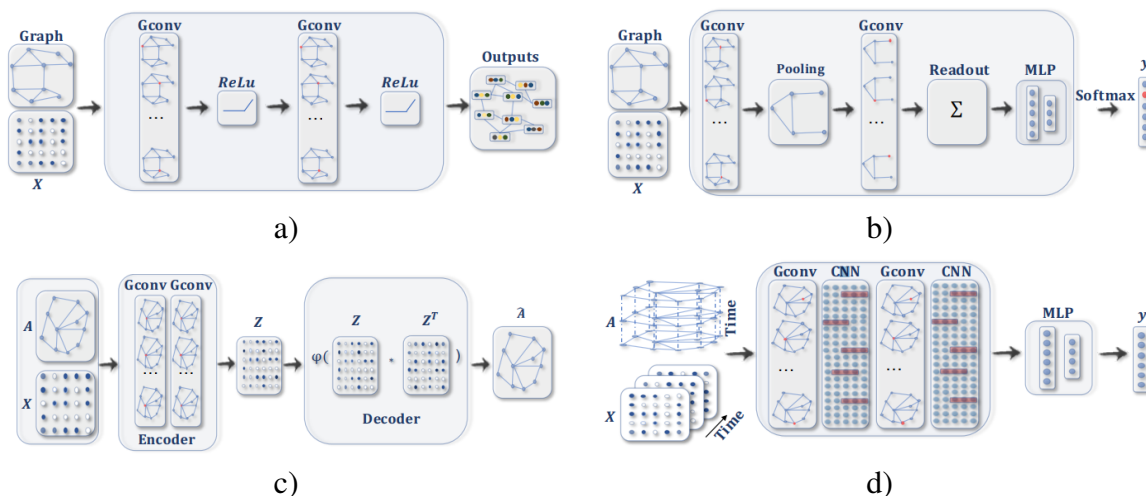
253 features. In the Fig. 6 this principle is visually explained for a node of an example graph.

#### 254 4.2 A brief survey on GNN models

255 The general formula presented above, declines in various versions in the various propositions of  
 256 GNN models. Diffusion Graph Convolution (DGC)<sup>40</sup> add a transition probability matrix in the  
 257 convolution to measure the contribution of each neighbors to a central node. As the number of  
 258 neighbors of a node can vary from one to a thousand or even more, it is inefficient to take the full  
 259 size of a node's neighborhood. GraphSage<sup>41</sup> adopts sampling to obtain a fixed number of neighbors  
 260 for each node. Graph Attention Network (GAT)<sup>42</sup> adopts attention mechanisms to learn the relative  
 261 weights between connected nodes. Mixture Model Network (MoNet)<sup>43</sup> introduces node pseudo-  
 262 coordinates to determine the relative position between a node and its neighbor. In such a way,  
 263 the parameters of a graph filter can be shared across different locations. PATCHY-SAN<sup>44</sup> orders  
 264 neighbors of each node according to their graph labelings and selects the top  $q$  neighbors. As each  
 265 node now has a fixed number of ordered neighbors, graph-structured data can be converted into  
 266 grid-structured data.

267 Based on the convolution operator, many Neural Networks architectures have been developed  
 268 for different tasks: Convolutional graph neural networks for node or graph classification, graph





**Fig 7** Figure extracted from paper of Wu et al.<sup>8</sup> different models of GNN: a) a Convolutional GNN for node classification, b) a Convolutional GNN for graph classification, c) a Graph Auto Encoder and d) a Spatio-Temporal GNN.

269 autoencoders, spatio-temporal graph neural networks.

## 270 5 Applications and Datasets

271 Many application domains have exploited graph-based representation. We present here some of the  
 272 main domains in which graph was successfully used. In these contexts we also present the typical  
 273 benchmarks used for evaluating algorithms based on graph representation.

### 274 5.1 Chemistry

275 Graph theory provides a very natural representation of a 2D chemical structure, with the nodes  
 276 and edges of a graph denoting the atoms and bonds of a molecule, and enables the exploitation  
 277 of previously developed algorithms for the manipulation of graphs.<sup>45</sup> There are many properties  
 278 of chemical compounds that are dependent on the structure of the components; problems related  
 279 to these properties (searching for molecules that have similar properties, or searching for chem-  
 280 ical components that have a particular action such as carcinogenicity, etc.) are therefore solved

281 through graph matching<sup>46-48</sup> or even graph embedding techniques.<sup>4</sup> Some of classical datasets in  
282 this domain are briefly described below.

- 283 • **AIDS:**<sup>49</sup> This dataset consists of two classes (active, inactive) of 2000 graphs representing  
284 molecules with activity against HIV or not.
- 285 • **Mutagenicity:**<sup>49</sup> This dataset is divided in two classes regarding the mutagenicity (one of  
286 the numerous adverse properties of a compound that hampers its potential to become a mar-  
287 ketable drug) of 4337 molecules.
- 288 • **Predictive Toxicology Challenge (PTC):**<sup>50</sup> This dataset deals with the predicting of the  
289 outcome of biological tests for the carcinogenicity of chemicals using information related  
290 to chemical structure only (positive or negative) on four categories of animals : female rats  
291 (FR), male rats (MR), female mice (FM), male mice (MM) with about 240 graphs per set.
- 292 • **Monoamine oxidase dataset (MAO):**<sup>22</sup> This problem is defined on a set of 68 molecules  
293 divided into two classes: the molecules that inhibit the monoamine oxidase (antidepressant  
294 drugs) and those that do not.

295 With respect to these datasets we would like to emphasize here one very important thing. While  
296 from the application point of view the use of these databases still makes sense to solve some prob-  
297 lems in chemo informatics, using these benchmarks to test algorithms on graphs (graph matching,  
298 etc.) does not make much sense nowadays. It has proved that these data have known defects for  
299 benchmarking graph matching algorithms: for example the dataset Mutagenicity is known<sup>51</sup> to  
300 have an error, all vertices of graphs with more than 99 vertices are isolated, so it is not appro-  
301 priate to evaluate graph matching problems; Solnon<sup>52</sup> shows also that graph size is not the only

302 parameter to take into consideration for evaluating graph matching problem, in fact there are still  
303 small but hard instances which cannot be solved within a reasonable amount of time by any of  
304 state-of-the-art methods.

305 In conclusion, our opinion is that the above described datasets are somehow out to date and it  
306 is important to evaluate solvers on other hard instances and more recent benchmarks.

### 307 *5.2 Social Networks*

308 Another application domain in which is immediate to represent the data in terms of graphs is social  
309 or web network analysis. In this context nodes of graphs can represent people, web pages, papers,  
310 etc. and edges represent interactions between people, or citation between papers, hyperlinks.

311 In this context there are many problems dealt with graph-based algorithms: Community detec-  
312 tion<sup>53</sup> or interaction,<sup>54</sup> recommendation systems.<sup>55</sup>

313 A good collection of benchmarks in this context can be found on the website of Stanford Large  
314 Network Dataset Collection<sup>56</sup> (**SNAP**).

### 315 *5.3 Image Processing*

316 The representation of images by graphs is less immediate than in other areas. Nevertheless several  
317 image processing problems were addressed through graph-based representations. We have seen  
318 (Section 2) that irregular pyramids have been successfully used for representing images at differ-  
319 ents resolution levels and for dealing with some classical problem: image segmentation, connected  
320 component labeling, and so on.

321 Thus, in this field we can mention the following databases: the **YACCLAB**,<sup>57</sup> a dataset for

322 comparing Connected Components Labeling Algorithms; the dataset for evaluating image seg-  
323 mentation problem proposed by **Martin et al.**<sup>58</sup>

324 In the context of image processing, several databases exist also as benchmark for graph match-  
325 ing problems. The **CMU house/hotel** image sequence<sup>59</sup> was commonly used to test the perfor-  
326 mance of graph matching algorithms. This dataset consists of 111 frames of a house, each of  
327 which has been manually labeled with 30 landmarks. The **car and motorbike image dataset** was  
328 also created in.<sup>59</sup> This dataset consists of 30 pairs of car images and 20 pairs of motorbike im-  
329 ages taken from the PASCAL challenges. The **UCF shape** dataset<sup>60</sup> has also been widely used for  
330 comparing graph matching algorithms.

#### 331 *5.4 Computer Vision*

332 Deep Learning with graph-based representation has been widely used in the field of Computer  
333 Vision. The notably graph representations are based on the extraction of features points from  
334 object of interest in videos, that will represent the node of graphs, and connecting them by edge  
335 based on some rules (e.g. the proximity of points). In this category are widely used the following  
336 datasets for skeleton-based action recognition. The **Kinetics** dataset<sup>61</sup> is a large-scale, high-quality  
337 dataset for human action recognition in videos. The dataset consists of around 500,000 video  
338 clips covering 600 human action classes with at least 600 video clips for each action class. The  
339 **Human3.6M**<sup>62</sup> dataset is one of the largest motion capture datasets, which consists of 3.6 million  
340 human poses and corresponding images captured by a high-speed motion capture system. **NTU**  
341 **RGB+D**<sup>63</sup> is a large-scale dataset for RGB-D human action recognition. It involves 56,880 samples  
342 of 60 action classes collected from 40 subjects.

343 But some other graph-based representation was proposed for addressing computer vision prob-

344 lem. Thus, the very famous image datasets **ImageNet**,<sup>64</sup> **Coco**,<sup>65</sup> **Pascal VOC**,<sup>66</sup> used for object  
345 detection and recognition, are also used by graph-based Deep Learning techniques.

## 346 **6 To go further: open problems**

347 As we have seen, graph-based techniques have evolved greatly in recent years, with many effective  
348 proposals. However, some open problems remain, and can be addressed in the coming years.

349 The first main problem, which we described earlier but which still remains unresolved, is that of  
350 **execution time**. Graph-based algorithms still spend a lot of resources, in terms of time, compared  
351 to equivalent algorithms that are based on a statistical representation of data. Many efforts have  
352 been made in this direction, but there is still room for improvement.

353 We also talked about a second, still open, problem which we want to call the **representation**  
354 **gap** here. In itself this is not a problem, but it is inherent in graph-based representation: data  
355 can be represented as graphs by many different ways. This means that algorithms cannot always  
356 be generalized to all application contexts because performance depends very much on how the  
357 data has been represented. This fact actually, rather than a problem, may also prove to be a good  
358 opportunity to propose new graph-based representations that provide surprising results in various  
359 application domains, such as image processing and computer vision.

## 360 **7 Conclusions**

361 In this paper we wanted to discuss pattern recognition techniques that make use of graphs. De-  
362 ferring a full presentation to other survey papers, our proposed objective was rather to show the  
363 successes of using graphs in pattern recognition in some applications and the drawbacks yet to be  
364 overcome.

365 The research domain of graph-based pattern recognition is increasingly in vogue with the ad-  
366 vent of deep learning, and there is much room to research and propose increasingly effective solu-  
367 tions.

368 We hope that this paper will fuel the desire of researchers to delve into this wonderful world of  
369 graphs.

### 370 *References*

- 371 1 D. Conte, P. Foggia, C. Sansone, *et al.*, “Thirty years of graph matching in pattern recogni-  
372 tion,” *International journal of pattern recognition and artificial intelligence* **18**(03), 265–298  
373 (2004).
- 374 2 J. Yan, X.-C. Yin, W. Lin, *et al.*, “A short survey of recent advances in graph matching,” in  
375 *Proceedings of the 2016 ACM on International Conference on Multimedia Retrieval*, 167–  
376 174 (2016).
- 377 3 H. Cai, V. W. Zheng, and K. C.-C. Chang, “A comprehensive survey of graph embedding:  
378 Problems, techniques, and applications,” *IEEE Transactions on Knowledge and Data Engi-  
379 neering* **30**(9), 1616–1637 (2018).
- 380 4 D. Conte, J.-Y. Ramel, N. Sidère, *et al.*, “A comparison of explicit and implicit graph embed-  
381 ding methods for pattern recognition,” in *International Workshop on Graph-Based Represen-  
382 tations in Pattern Recognition*, 81–90, Springer (2013).
- 383 5 N. M. Kriege, F. D. Johansson, and C. Morris, “A survey on graph kernels,” *Applied Network  
384 Science* **5**(1), 1–42 (2020).
- 385 6 L. Brun and W. Kropatsch, “Contains and inside relationships within combinatorial pyra-  
386 mids,” *Pattern Recognition* **39**(4), 515–526 (2006).

- 387 7 D. Batavia, R. Gonzalez-Diaz, and W. G. Kropatsch, “Image= structure+ few colors,” in  
388 *Joint IAPR International Workshops on Statistical Techniques in Pattern Recognition (SPR)*  
389 *and Structural and Syntactic Pattern Recognition (SSPR)*, 365–375, Springer (2021).
- 390 8 Z. Wu, S. Pan, F. Chen, *et al.*, “A comprehensive survey on graph neural networks,” *IEEE*  
391 *transactions on neural networks and learning systems* **32**(1), 4–24 (2020).
- 392 9 J. Zhou, G. Cui, S. Hu, *et al.*, “Graph neural networks: A review of methods and applica-  
393 tions,” *AI Open* **1**, 57–81 (2020).
- 394 10 L. Brun, P. Foggia, and M. Vento, “Trends in graph-based representations for pattern recog-  
395 nition,” *Pattern Recognition Letters* **134**, 3–9 (2020).
- 396 11 A. H. Osman and O. M. Barukub, “Graph-based text representation and matching: A review  
397 of the state of the art and future challenges,” *IEEE Access* **8**, 87562–87583 (2020).
- 398 12 F. Zhou and F. De la Torre, “Factorized graph matching,” *IEEE transactions on pattern anal-*  
399 *ysis and machine intelligence* **38**(9), 1774–1789 (2015).
- 400 13 M. Leordeanu and M. Hebert, “A spectral technique for correspondence problems using pair-  
401 wise constraints,” (2005).
- 402 14 M. Leordeanu, M. Hebert, and R. Sukthankar, “An integer projected fixed point method for  
403 graph matching and map inference,” *Advances in neural information processing systems* **22**  
404 (2009).
- 405 15 S. Gold and A. Rangarajan, “A graduated assignment algorithm for graph matching,” *IEEE*  
406 *Transactions on pattern analysis and machine intelligence* **18**(4), 377–388 (1996).
- 407 16 R. Raveaux, “On the unification of the graph edit distance and graph matching problems,”  
408 *Pattern Recognition Letters* **145**, 240–246 (2021).

- 409 17 M. Darwiche, D. Conte, R. Raveaux, *et al.*, “A local branching heuristic for solving a graph  
410 edit distance problem,” *Computers & Operations Research* **106**, 225–235 (2019).
- 411 18 M. Neuhaus and H. Bunke, “Automatic learning of cost functions for graph edit distance,”  
412 *Information Sciences* **177**(1), 239–247 (2007).
- 413 19 X. Cortés, D. Conte, and H. Cardot, “Learning edit cost estimation models for graph edit  
414 distance,” *Pattern Recognition Letters* **125**, 256–263 (2019).
- 415 20 M. Neuhaus and H. Bunke, “A probabilistic approach to learning costs for graph edit dis-  
416 tance,” in *Proceedings of the 17th International Conference on Pattern Recognition, 2004.*  
417 *ICPR 2004.*, **3**, 389–393, IEEE (2004).
- 418 21 A. Solé-Ribalta, F. Serratos, and A. Sanfeliu, “On the graph edit distance cost: properties  
419 and applications,” *International Journal of Pattern Recognition and Artificial Intelligence*  
420 **26**(05), 1260004 (2012).
- 421 22 B. Gaüzère, L. Brun, and D. Villemin, “Two new graphs kernels in chemoinformatics,” *Pat-*  
422 *tern Recognition Letters* **33**(15), 2038 – 2047 (2012).
- 423 23 N. Sidere, P. Héroux, and J.-Y. Ramel, “Vector representation of graphs: Application to the  
424 classification of symbols and letters,” in *2009 10th International Conference on Document*  
425 *Analysis and Recognition*, 681–685, IEEE (2009).
- 426 24 J. Jaromczyk and G. Toussaint, “Relative neighborhood graphs and their relatives,” *In Pro-*  
427 *ceedings of the IEEE* (1992).
- 428 25 L. Brun, M. Mokhtari, and F. Meyer, “Hierarchical watersheds within the combinatorial pyra-  
429 mid framework,” in *International Conference on Discrete Geometry for Computer Imagery*,  
430 34–44, Springer (2005).



- 431 26 M. Cerman, R. Gonzalez-Diaz, and W. Kropatsch, “Lbp and irregular graph pyramids,” in  
432 *International Conference on Computer Analysis of Images and Patterns*, 687–699, Springer  
433 (2015).
- 434 27 M. Banaeyan and W. G. Kropatsch, “Parallel computation of the adjacency of connected  
435 components,” in *International Conference on Pattern Recognition and Artificial Intelligence*,  
436 102–113, Springer (2022).
- 437 28 S. L. Horowitz and T. Pavlidis, “Picture segmentation by a tree traversal algorithm,” *Journal*  
438 *of the ACM (JACM)* **23**(2), 368–388 (1976).
- 439 29 A. Montanvert, P. Meer, and A. Rosenfeld, “Hierarchical image analysis using irregular tes-  
440 sellations,” in *European Conference on Computer Vision*, 28–32, Springer (1990).
- 441 30 L. Brun and W. Kropatsch, “Introduction to combinatorial pyramids,” in *Digital and image*  
442 *geometry*, 108–128, Springer (2001).
- 443 31 L. Brun and W. Kropatsch, “Hierarchical graph encodings,” *Image processing and analysis*  
444 *with graphs: theory and practice* (2012).
- 445 32 W. G. Kropatsch, “Building irregular pyramids by dual-graph contraction,” *IEE Proceedings-*  
446 *Vision, Image and Signal Processing* **142**(6), 366–374 (1995).
- 447 33 L. Brun and W. Kropatsch, “Combinatorial pyramids,” in *Proceedings 2003 International*  
448 *Conference on Image Processing (Cat. No. 03CH37429)*, **2**, II–33, IEEE (2003).
- 449 34 Z. Zeng, A. K. Tung, J. Wang, *et al.*, “Comparing stars: On approximating graph edit dis-  
450 tance,” *Proceedings of the VLDB Endowment* **2**(1), 25–36 (2009).
- 451 35 J. Hartmanis, “Computers and intractability: a guide to the theory of np-completeness  
452 (michael r. garey and david s. johnson),” *Siam Review* **24**(1), 90 (1982).

- 453 36 K. S. Camilus and V. Govindan, “A review on graph based segmentation,” *International Jour-*  
454 *nal of Image, Graphics and Signal Processing* **4**(5), 1 (2012).
- 455 37 D. I. Shuman, S. K. Narang, P. Frossard, *et al.*, “The emerging field of signal processing on  
456 graphs: Extending high-dimensional data analysis to networks and other irregular domains,”  
457 *IEEE signal processing magazine* **30**(3), 83–98 (2013).
- 458 38 T. N. Kipf and M. Welling, “Semi-supervised classification with graph convolutional net-  
459 works,” *arXiv preprint arXiv:1609.02907* (2016).
- 460 39 Y. Han, S. Wang, Y. Ren, *et al.*, “Predicting station-level short-term passenger flow in a  
461 citywide metro network using spatiotemporal graph convolutional neural networks,” *ISPRS*  
462 *International Journal of Geo-Information* **8**(6), 243 (2019).
- 463 40 Y. Li, R. Yu, C. Shahabi, *et al.*, “Diffusion convolutional recurrent neural network: Data-  
464 driven traffic forecasting,” *arXiv preprint arXiv:1707.01926* (2017).
- 465 41 W. Hamilton, Z. Ying, and J. Leskovec, “Inductive representation learning on large graphs,”  
466 *Advances in neural information processing systems* **30** (2017).
- 467 42 P. Veličković, G. Cucurull, A. Casanova, *et al.*, “Graph attention networks,” *arXiv preprint*  
468 *arXiv:1710.10903* (2017).
- 469 43 F. Monti, D. Boscaini, J. Masci, *et al.*, “Geometric deep learning on graphs and manifolds  
470 using mixture model cnns,” in *Proceedings of the IEEE conference on computer vision and*  
471 *pattern recognition*, 5115–5124 (2017).
- 472 44 M. Niepert, M. Ahmed, and K. Kutzkov, “Learning convolutional neural networks for  
473 graphs,” in *International conference on machine learning*, 2014–2023, PMLR (2016).

- 474 45 P. Willett, “Chemoinformatics: a history,” *Wiley Interdisciplinary Reviews: Computational*  
475 *Molecular Science* **1**(1), 46–56 (2011).
- 476 46 M. Fuchs and K. Riesen, “Matching of matching-graphs-a novel approach for graph classifi-  
477 cation,” in *2020 25th International Conference on Pattern Recognition (ICPR)*, 6570–6576,  
478 IEEE (2021).
- 479 47 Z. Abu-Aisheh, B. Gaüzere, S. Bougleux, *et al.*, “Graph edit distance contest: Results and  
480 future challenges,” *Pattern Recognition Letters* **100**, 96–103 (2017).
- 481 48 M. Martineau, R. Raveaux, D. Conte, *et al.*, “Graph matching as a graph convolution operator  
482 for graph neural networks,” *Pattern Recognition Letters* **149**, 59–66 (2021).
- 483 49 K. Riesen and H. Bunke, “Iam graph database repository for graph based pattern recognition  
484 and machine learning,” in *Joint IAPR International Workshops on Statistical Techniques in*  
485 *Pattern Recognition (SPR) and Structural and Syntactic Pattern Recognition (SSPR)*, 287–  
486 297, Springer (2008).
- 487 50 H. Toivonen, A. Srinivasan, R. D. King, *et al.*, “Statistical evaluation of the predictive toxic-  
488 ology challenge 2000–2001,” *Bioinformatics* **19**(10), 1183–1193 (2003).
- 489 51 D. B. Blumenthal, “New techniques for graph edit distance computation,” *arXiv preprint*  
490 *arXiv:1908.00265* (2019).
- 491 52 C. Solnon, “Experimental evaluation of subgraph isomorphism solvers,” in *International*  
492 *Workshop on Graph-Based Representations in Pattern Recognition*, 1–13, Springer (2019).
- 493 53 K. S. Phyu and M. M. Min, “Graph-based community detection in social network,” in *2019*  
494 *IEEE/ACIS 18th International Conference on Computer and Information Science (ICIS)*, 12–  
495 17, IEEE (2019).

- 496 54 S. Kumar, W. L. Hamilton, J. Leskovec, *et al.*, “Community interaction and conflict on the  
497 web,” in *Proceedings of the 2018 world wide web conference*, 933–943 (2018).
- 498 55 Z. Wang, Y. Tan, and M. Zhang, “Graph-based recommendation on social networks,” in *2010*  
499 *12th International Asia-Pacific Web Conference*, 116–122, IEEE (2010).
- 500 56 J. Leskovec and A. Krevl, “SNAP Datasets: Stanford large network dataset collection.”  
501 <http://snap.stanford.edu/data> (2014).
- 502 57 C. Grana, F. Bolelli, L. Baraldi, *et al.*, “Yacclab-yet another connected components labeling  
503 benchmark,” in *2016 23rd International Conference on Pattern Recognition (ICPR)*, 3109–  
504 3114, IEEE (2016).
- 505 58 D. Martin, C. Fowlkes, D. Tal, *et al.*, “A database of human segmented natural images and  
506 its application to evaluating segmentation algorithms and measuring ecological statistics,”  
507 in *Proceedings Eighth IEEE International Conference on Computer Vision. ICCV 2001*, **2**,  
508 416–423, IEEE (2001).
- 509 59 T. S. Caetano, J. J. McAuley, L. Cheng, *et al.*, “Learning graph matching,” *IEEE transactions*  
510 *on pattern analysis and machine intelligence* **31**(6), 1048–1058 (2009).
- 511 60 H. Chui and A. Rangarajan, “A new point matching algorithm for non-rigid registration,”  
512 *Computer Vision and Image Understanding* **89**(2-3), 114–141 (2003).
- 513 61 J. Carreira, E. Noland, C. Hillier, *et al.*, “A short note on the kinetics-700 human action  
514 dataset,” *arXiv preprint arXiv:1907.06987* (2019).
- 515 62 C. Ionescu, D. Papava, V. Olaru, *et al.*, “Human3.6m: Large scale datasets and predictive  
516 methods for 3d human sensing in natural environments,” *IEEE Transactions on Pattern Anal-*  
517 *ysis and Machine Intelligence* **36**, 1325–1339 (2014).

- 518 63 A. Shahroudy, J. Liu, T.-T. Ng, *et al.*, “Ntu rgb+d: A large scale dataset for 3d human activity  
519 analysis,” in *Proceedings of the IEEE conference on computer vision and pattern recognition*,  
520 1010–1019 (2016).
- 521 64 J. Deng, W. Dong, R. Socher, *et al.*, “Imagenet: A large-scale hierarchical image database,”  
522 in *2009 IEEE conference on computer vision and pattern recognition*, 248–255, Ieee (2009).
- 523 65 T.-Y. Lin, M. Maire, S. Belongie, *et al.*, “Microsoft coco: Common objects in context,” in  
524 *European conference on computer vision*, 740–755, Springer (2014).
- 525 66 M. Everingham, S. M. A. Eslami, L. Van Gool, *et al.*, “The pascal visual object classes  
526 challenge: A retrospective,” *International Journal of Computer Vision* **111**, 98–136 (2015).

527 **Donatello Conte** received his Ph.D. degree in 2006 by a joint supervision between LIRIS labo-  
528 ratory of the INSA of Lyon (France) and MIVIA laboratory of the University of Salerno (Italy).  
529 He is Associate Professor at the Computer Science Laboratory of the University of Tours. He is  
530 currently head of the Computer Science Department at Polytech Tours School of Engineering. His  
531 main research fields are: structural pattern recognition (graph matching, graph kernels, combinato-  
532 rial maps), video analysis (objects detection and tracking, trajectories analysis, behavioral analysis,  
533 etc.), and affective computing (emotion recognition, multimodality analysis for affective analysis,  
534 physiological measures by video analysis, etc.). He is the author of more than 70 publications and  
535 reviewers in the main journals in his research field (PAMI, PR, CVIU, TIP, etc.). He is member  
536 of the Editorial Board of the Elsevier Journal Internet of Things, MDPI Journal of Imaging and  
537 he is Guest Editor for the Pattern Recognition Letters journal and IEEE Transactions on Emerging  
538 Topics in Computing journal. He has been co-chair of the International Workshop on Graph-based  
539 Representation in Pattern Recognition (GbR2019) and he is the chairman of the International IAPR

540 Technical Committee 15 dedicated to the promotion of graphs in the Pattern Recognition.

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## 558 **List of Tables**

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