CLIQUE POOLING FOR GRAPH CLASSIFICATION

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ABSTRACT

We propose a novel graph pooling operation using cliques as the unit pool. As this approach is purely topological, rather than featural, it is more readily interpretable, a better analogue to image coarsening than filtering or pruning techniques, and entirely nonparametric. The operation is implemented within graph convolution network (GCN) and GraphSAGE architectures and tested against standard graph classification benchmarks. In addition, we explore the backwards compatibility of the pooling to regular graphs, demonstrating competitive performance when replacing two-by-two pooling in standard convolutional neural networks (CNNs) with our mechanism.

1 INTRODUCTION & RELATED WORK

The ongoing deep learning renaissance has proved remarkably fruitful and long lived, with state-of-the-art performance in tasks spanning the breadth of machine learning. The dominance of CNNs in the domain of image classification is of particular note, with superhuman performance becoming almost pedestrian. Images can be thought of as highly regular, Euclidean graphs, where pixels are nodes connected to the eight neighbouring pixels by edges. Graphs of different structures are used to represent problems from the biological, social and physical (Kipf et al., 2018; Gilmer et al., 2017) sciences as well as more abstract problems such as knowledge representation. Generalising the advances made for CNNs for use on irregular graphs has thus become an important direction for the application of deep learning, under the umbrella term geometric deep learning (Bronstein et al., 2017).

The key operations in CNNs are the convolution and pooling. Convolutions extract features, with adaptations for the exploitation of locality and translational invariance. Pooling literally reduces the spatial dimensionality, aiding in the expansion of the receptive field and building consensus and saliency through coarsening. The convolution has been well adapted to non-Euclidean graphs (Kipf & Welling, 2016; Defferrard et al., 2016; Veličković et al., 2017; Gilmer et al., 2017) with many variations as a result of a strong interest from the research community. Pooling has not received the same treatment, unsurprisingly given its CNN and not PNN, and prior to recent developments the standard method was to pool globally[1] and then feed this into a multilayer perceptron (MLP) (Duvenaud et al., 2015). The current state-of-the-art methods implement gradual coarsening in hierarchies of representations (Gao & Ji, 2018; Cangea et al., 2018; Ying et al., 2018) but require hyperparameterisation, in the form of a preset allowed number of clusters or number of nodes to prune, and are not purely topologically derived. This means they are poor analogues of pooling in CNNs. If the aim of the community is to produce robust, transferable algorithms able to be used with many graphs then the inapplicability of these methods to regular graphs should be viewed as a serious deficiency.

In this work we introduce an operation that is purely topological, static, nonparametric and, has a natural correspondence in regular graphs and when substituted into GNN or traditional CNN for image classification, achieves performance competitive with the state-of-the-art parametric alternatives and

[1] Equal contribution
[1] Take all node features and form a single set of features through some aggregation, typically element-wise max or averaging.
improves on the performance of other nonparametric approaches. Being nonparametric renders the
approach far more interpretable as there are no learned parameters to pick apart – we can state quite
clearly what our approach does, it puts nodes into groups where every member is connected to every
other member. In addition to these properties the operation is biased towards producing a dendritic
pooling hierarchy which, in combination with being static and precomputable, permits concurrent
processing of the graph without loss of accuracy.

![Figure 1: Clique Pooling for an irregular graph. The colored borders represent the maximal cliques
(also labeled with numbers or letters next to them), dotted arrows indicate the cliques to which the
nodes are assigned. Notice that although some of the nodes belong to more than one clique they
do not necessarily contribute to the respective node in the coarsened graph. This is the case for the
node belonging to the red (1) and blue (2) maximal clique. Since the blue clique is bigger (in terms
of nodes), the node is assigned to the blue (2) cluster only. In the case of the node intersecting the
blue (2) and purple (3) maximal cliques, the node is assigned to both cliques since the cliques have
the same size. Hence, it contributes to the features of both of the respective nodes in the coarsened
graph. The grey maximal clique (6) is not represented in the new coarsened graph since the nodes
in that clique have already been assigned to larger cliques: the green (5) and blue (2) cliques. The
nodes in the coarsened graph are connected if any two nodes in the respective cliques are connected.

2 PROPOSED METHOD

2.1 PRELIMINARIES

We use the standard representation of graphs in graph classification tasks. The graph $G$ with $N$
nodes is represented as a pair $(A, X)$ where the adjacency matrix $A \in \mathbb{R}^{N \times N}$ and the node feature
matrix, with $F$ features per node, $X \in \mathbb{R}^{N \times F}$. Additionally, our method assumes undirected graphs.

**Graph Convolution** In principle, our method does not require a convolution operator however, a
CNN-like architecture requires one. The graph convolution needs to be inductive. In our experiments we use GraphSAGE and GCN as particular implementations of the message-passing scheme.

**Readout Function** The readout function is needed in two different cases in our architecture: to
get a representation of each layer and to combine the nodes in a pool into one to produce the coars-
ened graph. For the former, we use the concatenation of mean and max pooling operator. For the
latter, we use the mean pooling operator. The final representation of the graph is the concatenated
representation of each layer which is then fed to the MLP.

2.2 PROPOSED OPERATION

Our approach is to coarsen the graph by aggregating maximal cliques. We attempt to limit the
dispersal of nodes by assigning each to a single clique-pool, ranked by size, where possible. Only
in the case of equally large options is the node assigned to multiple pools.
To accomplish this, the maximal cliques are found using the Bron-Kerbosch algorithm (Bron & Kerbosch, 1973) with modifications shown to improve performance on large real-world graphs (Eppstein et al., 2010; Eppstein & Strash, 2011). Nodes are assigned to pools greedily starting with the largest. When a node has been assigned it is removed from the remaining smaller pools and does not count towards that pool’s size for the assignment of other nodes. Edges are inherited from the clique members such that if a node in one clique shares an edge with a node in another, the cliques will share an edge in the coarsened graph. The resulting graph shares some features with the clique-graph though with fewer nodes and more edges in all but the simplest cases. The assigned cliques are then pooled using whichever pooling function is desired, average- and max-pooling in the experiments presented here.

**Lemma (Convergence).** Given a connected and finite graph, the clique-pooling operator converges to a single node after finitely many steps.

The proof for the above can be found in Appendix C. This guarantees that in any graph we can have a CNN-like architecture. As the approach is based only on the topology of the original graph it is both nonparametric and static. This means that the pools can be precomputed and opens the door to greater parallelization for dealing with very large graphs. Having found the entire pooling structure it is trivial to generate the dependency diagram, allowing graph partitions to be loaded and operated on separately, which will be key to dealing with very-large graphs, as discussed in Zhang et al. 2005 for the case of systems biology.

### 2.3 Application to Images as Regular Graphs

Images can be thought of as highly regular graphs. Indeed, this is the primary motivation for most work in the field of graph neural networks (Kipf & Welling, 2016; Defferrard et al., 2016) and often image recognition techniques are straightforwardly adapted to graphs with great success (Veličković et al., 2017; Cangea et al., 2018). Our method goes against the grain in this sense as, whilst it is based on concepts native to irregular graphs, we are able to apply it to images without issue.

To do this we must first define the graph structure for images. We argue that the use of 3-by-3 convolutions implies the graph structure as shown in figure 2 that is, pixels are connected to their eight immediate neighbours. As the figure shows, the first pool will be 2-by-2 with a stride of 1. The second pool will then be 3-by-3 with a stride of 1. We can analyse how this progresses by considering the 1-dimensional case, without loss of generality, as the 2D case is no more complicated than the same thing happening in two directions at the once.

**Lemma (Length Reduction).** Applying clique-pool n-times on a 1-dimensional grid (a chain) reduces the length of the grid by $r_n = 2^n - 1$.

In a typical CNN, the architecture will be such that the pools reduce the input to a single pixel in the spatial dimension by the final layer, using $(2 \times 2)$ pooling to do so. The length can be expressed in terms of the number of pools, n, as $L = 2^n$ and therefore, conveniently,

$$L - r_n = L - 2^n + 1 = 1$$

so the same number of clique-pooling operations will reduce the input to a single spatial dimension. As such the clique pool operation can be substituted into existing CNN architectures directly, replacing pools without any additional changes.

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3The graph formed by maximal cliques where edges occur where cliques intersect.
4And the same can be said for an N-dimensional grid.
4See Appendix C for proof and illustration.
3 Experimental Setup & Results

We test the approach extensively on irregular graph classification problems and also demonstrate how the pooling works being substituted into a standard CNN architecture of the VGG-form.

| Model          | Enzymes | DD   | PROTEINS | COLLAB |
|----------------|---------|------|----------|--------|
| GRAPHLET       | 41.03   | 74.85| 64.66    | 72.91  |
| SHORTEST-PATH  | 42.32   | 78.86| 59.10    | 76.43  |
| 1-WL           | 53.43   | 74.02| 78.61    | 73.76  |
| WL-QA          | 60.13   | 79.04| 80.74    | 75.26  |
| PATCHYSAN      | -       | 76.27| 72.60    | 75.00  |
| GRAPHSAGE      | 54.25   | 75.42| 68.25    | 70.48  |
| ECC            | 53.50   | 74.10| 67.79    | 72.65  |
| SET2SET        | 60.15   | 78.12| 71.75    | 74.29  |
| SORTPOOL       | 57.12   | 79.37| 73.76    | 75.54  |
| DIFFPOOL-DET   | 58.33   | 75.47| 82.13    | 75.62  |
| DIFFPOOL-NoLP  | 61.95   | 79.98| 76.22    | 75.58  |
| DIFFPOOL       | 62.53   | 80.64| 82.13    | 75.48  |
| SPARSE HC, CANGEA ET AL. (2018) | 64.17 | 78.59| 74.54    | 75.46  |
| CLIQUEPOOL (OURS) | 60.71   | 77.33| 72.59    | 74.50  |

Table 1: Classification accuracy percentages.

| POOL            | PARAMETERS |
|-----------------|------------|
| DIFFPOOL        | 27,776     |
| GRAPH U-NET     | 192        |
| CLIQUE POOL     | 0          |

Table 2: Total number of parameters for three pooling layers in the DD dataset.

Our experiments show that our non-parametric approach is competitive with the parametric approaches, as detailed in table 3. The method outperforms the GraphSAGE baseline and most of the kernel-based and GNN approaches. Moreover, because we do not introduce any additional parameters our method is fast to train and does not suffer the instabilities associated with DIFFPOOL. It also outperforms the DIFFPOOL with deterministic clustering on two datasets. The image investigation found a small, but sig-

\footnote{Full specification is given in appendix A}
significant \((p = 0.02)\), reduction of in mean accuracy over
the 2-BY-2 pool baseline in a 10-fold cross-validation comparison, presented in table 3.

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A NETWORK ARCHITECTURES

In the interests of clarity and reproducibility we present here the network architectures used in our investigations. We believe the following to be a complete description though the authors would gladly welcome any correspondence requesting further specification, clarification or suggestions relating to improving these descriptions.

For compactness, we’ve used abbreviations. Conv.* is a block consisting of a convolutional layer with a $3 \times 3$ kernel, batch-normalization \cite{Ioffe2015} with numerical stabilisation ($\epsilon = 1 \times 10^{-5}$) and momentum of 0.1 for the affine transform parameters $(\gamma, \beta)$, with a ReLU activation. ‘× N’ refers to how many times this block is repeated, which could also be inferred from the numbering in the Layer column. Flatten returns the layer input with dimensions of size 1 removed, sometimes called squeezing. Linear layers are fully-connected and followed by a ReLU activation except in the final layer where a softmax is used. For pooling layers the size is given as $(\Delta x \times \Delta y)$, stride.

| Layer | Type    | Size/Features | Shape   |
|-------|---------|---------------|---------|
| Input | -       | -             | (32,32,3) |
| 1,2   | Conv.*x2| 64            | (32,32,64) |
| -     | Maxpool | $(2 \times 2)$, 2 | (16,16,64) |
| 3,4   | Conv.*x2| 128           | (16,16,128) |
| -     | Maxpool | $(2 \times 2)$, 2 | (8,8,128) |
| 5,6,7 | Conv.*x3| 256           | (8,8,256) |
| -     | Maxpool | $(2 \times 2)$, 2 | (4,4,256) |
| 8,9,10| Conv.*x3| 512           | (4,4,512) |
| -     | Maxpool | $(2 \times 2)$, 2 | (2,2,512) |
| 11,12,13| Conv.*x3| 512          | (2,2,512) |
| -     | Maxpool | $(2 \times 2)$, 2 | (1,1,512) |
| -     | Flatten | -             | (512) |
| 14    | Linear  | 512           | (512) |
| -     | Dropout | $p = 0.3$     | (512) |
| 15    | Linear  | 10            | (10) |

**Table 4: Baseline VGG-like architecture.**

| Layer | Type    | Size/Features | Shape   |
|-------|---------|---------------|---------|
| Input | -       | -             | (32,32,3) |
| 1,2   | Conv.*x2| 64            | (32,32,64) |
| -     | Maxpool | $(2 \times 2)$, 1 | (31,31,64) |
| 3,4   | Conv.*x2| 128           | (31,31,128) |
| -     | Maxpool | $(3 \times 3)$, 1 | (29,29,128) |
| 5,6,7 | Conv.*x3| 256           | (29,29,256) |
| -     | Maxpool | $(5 \times 5)$, 1 | (25,25,256) |
| 8,9,10| Conv.*x3| 512           | (25,25,512) |
| -     | Maxpool | $(9 \times 9)$, 1 | (17,17,512) |
| 11,12,13| Conv.*x3| 512        | (17,17,512) |
| -     | Maxpool | $(17 \times 17)$, 1 | (1,1,512) |
| -     | Flatten | -             | (512) |
| 14    | Linear  | 512           | (512) |
| -     | Dropout | $p = 0.3$     | (512) |
| 15    | Linear  | 10            | (10) |

**Table 5: Clique-pooled VGG-like architecture.**

B MAXIMAL CLIQUES

The enumeration of maximal cliques has been a core component in gene expression networks analysis, cis regulatory motif finding, and the study of quantitative trait loci for high-throughput molecular phenotypes \cite{Zhang2005}. As such, significant effort has gone to developing efficient methods.
of enumerating all the maximal cliques in a graph. The upper bound of the number of cliques is $3^{n/3}$. The algorithm for finding maximal cliques presented by Bron & Kerbosch (1973) was adapted by Tomita et al. (2006) to find the maximal cliques in an iterative way without having to store previous cliques or many candidates in memory. Zhang et al. (2005) showed a way of enumerating the cliques, sorted by size, in a parallelized way. While their primary focus is parallelizing this method in shared-memory machines, they show that it is possible to do the same in distributed machines. They also demonstrate that it is possible to load-balance the sub-tasks efficiently, showing a near ideal relative speedup (defined as the ratio between $2p$ processors and $p$ processors run times). Finally, several modifications have been made showing improved performance on large real-world graphs (including social graphs) Eppstein et al. (2010); Eppstein & Strash (2011); Conte et al.

C PROOFS

C.1 CONVERGENCE

Lemma (Convergence). Given a connected and finite graph, the clique-pooling operator converges to a single node after finitely many steps.

Proof. Consider the shortest-path between two nodes, $d(u, v)$, and the corresponding distance in the new graph, $d(u', v')$ where $u'$ and $v'$ are the most distant cliques containing $u$ and $v$, respectively. For each assigned maximal clique that the path between $u$ and $v$ traverses, $d(u', v')$ is reduced from $d(u, v)$ by 1. If the path does not traverse any pooled cliques then the distance remains constant as the path will be unchanged. As there is always a largest clique, the distance between some nodes is always reduced in the newly formed graph. Therefore the sum of the distances between all pairs of original nodes must decrease in each pooling. As the graph is finite and connected the sum of the distances between nodes must also be finite and so will reduce to 0, a single node, within a finite number of pooling operations.

However, it is possible to construct graphs that will initially grow in the number of nodes through pooling, the most straightforward example being a bipartite graph. In this case every pair of nodes sharing an edge forms a maximal clique, all of size 2 and thus all equally large. The pooled-graph then has as many nodes as the original graph had edges. In the worst possible case, the number of nodes in the pooled graph will balloon to the maximal clique limit, $O(3^{n/3})$ (Moon & Moser, 1965), although this will be fully-connected and collapse immediately.

C.2 RECEPTIVE FIELD

Lemma (Length Reduction). Applying clique-pool $n$-times on a 1-dimensional grid (a chain) reduces the length of the grid by $r_n = 2^n - 1$.

![Figure 3](image)

Figure 3: In this diagram we consider the pooling operation applied to a 1D chain. The 2D case, that of images, only differs in that the process occurs in both directions in parallel – the pools remain the same size. Nodes and edges are shown in black, blue indicates how the nodes are pooled into the cliques with the next chain being the result of the pooling operation. In this way we can illustrate four iterations of the pooling operation. In the first the cliques are of size two and the chain reduces in length by one – half from each end. In the second the cliques are of size three, due to the greater reach of the inherited edge connections, and the chain has reduced by two more, one from each end, for a total of three. This process continues with the reach becoming greater, the size of the pools increasing and the chain reducing more rapidly, as indicated on the left.
Proof. Figure 3 illustrates how the pools grow over successive iterations. The trend appears to be $2^n - 1$ and we can show that this is indeed the case. Consider the size of the cliques at a particular iteration, $c_i$, and the distance along the chain each node is connected, $d_i$. By inspection, each node is connected to every neighbour up to $d_i$ and so this group forms a clique of size

$$c_i = d_i + 1$$

with the additional 1 accounting for the node itself. Tracing the inheritance of connections into the next layer gives the connected distance of the pooled nodes as

$$d_{i+1} = \frac{1}{2}(c_i - 1) + d_i + \frac{1}{2}(c_i - 1)$$

$$= c_i - 1 + d_i = 2d_i.$$

Where we first go up one side of the clique, along the connected distance and then back down the side of another clique. So the distance does double each time with the cliques, and pools, being one more. The pooling routine as applied to images then, is to use pools of increasing size, with no padding, and a unit stride. Specifically, given the initial degree of 1 implied by the convolutions, $(2 \times 2), (3 \times 3), (5 \times 5), (9 \times 9) \ldots (2^{n-1} + 1 \times 2^{n-1} + 1)$

In addition to the simplicity of the operation, if we observe the reduction in the length a second benefit is made apparent. On the left we reduce by the left half of the pool, on the right by the right half, but not by the middle on either. So the length is reduced by $c_i - 1 = d_i$. As $d_i$ doubles each time, starting from 1, the reduction after $n-$pools is

$$r_i = \sum_{i=1}^{n} 2^{n-1} = 2^n - 1.$$