Graphlet Kernels

Karsten Borgwardt and Nino Shervashidze

joint work with SVN Vishwanathan, Tobias Petri, and Kurt Mehlhorn

Interdepartmental Bioinformatics Group
MPI for Biological Cybernetics
MPI for Developmental Biology

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String kernels

Recall the \textit{k-mer kernel} on strings

- Basic idea: count the number of common contiguous substrings of length \( k \)

This is equivalent to:

- count the number of occurrences of all \( k \)-mers in strings \( s_1 \) and \( s_2 \) separately,
- compute the inner product between these counts.

\[
\begin{align*}
\text{ACCTTGTA} & \quad \text{TGTCCTG} \\
\text{ACC} & \quad \text{TGT}
\end{align*}
\]

\[
\begin{align*}
f(s_1) &= (...,1, ..., 1, ..., 0, ..., 1, ..., 0, ..., 1, ..., 1, ..., ) \\
f(s_2) &= (...,0, ..., 1, ..., 1, ..., 0, ..., 0, ..., 1, ..., 1, ..., 0, ...) \\
K(s_1,s_2) &= f(s_1)f(s_2)'
\end{align*}
\]
Graph comparison

Mutagenetic

Not Mutagenetic
Graph kernels have traditionally been based on different ideas:

- Random walk kernel: $O(n^3)$
- Shortest path kernel: $O(n^4)$
- Subtree kernel: NP-hard
- Cycle kernel: NP-hard
- All possible subgraphs kernel: NP-hard
We call graphlets subgraphs of size \{3, 4, 5\}.

Let \( \mathcal{G} = \{\text{graphlet}(1), \ldots, \text{graphlet}(N_k)\} \) be the set of size-\( k \) graphlets and \( G \) be a graph of size \( n \).

Define a vector \( f_G \) of length \( N_k \) such that

\[
f_{G_i} = \#(\text{graphlet}(i) \sqsubseteq G).
\]

We call \( f_G \) the \( k \)-spectrum of \( G \).

In this figure \( n = 5, k = 3, f_G = (1, 3, 6, 0) \).
Given two graphs $G$ and $G'$ of size $n \geq k$, the graphlet kernel $k_g$ is defined as

$$k_g(G, G') := f_G^\top f_{G'}.$$

**Problem:** if $G$ and $G'$ have different sizes, this will greatly skew the counts $f_G$

**Solution:** normalize the counts to frequency vectors:

$$D_G = \frac{1}{\# \text{all graphlets in } G} f_G$$

and work with the normalized variant of $k_g$

$$k_g(G, G') = D_G^\top D_{G'}.$$
Isomorphism of graphs $\rightarrow$ equality of their $k$-spectra.

Equality of their $k$-spectra $\rightarrow$ isomorphism?

Yes, when $n = k + 1$ and $n \leq 11$...

**Graph reconstruction conjecture**

- Let $G_v$ denote a subgraph of $G$, obtained by deleting node $v$ and all the edges incident to it.
- Let $G$ and $G'$ be graphs of size greater than 2 and $g : V \rightarrow V'$ be an isomorphism function such that $G_v$ is isomorphic to $G'_g(v)$ for all $v \in V$. Then $G$ is isomorphic to $G'$.
Recursive definition of the graphlet kernel

Given two graphs $G$ and $G'$ of size $n \geq k$, let $\mathcal{M}$ and $\mathcal{M}'$ denote the set of size-$n$-1 subgraphs of $G$ and $G'$ respectively.

The recursive graph kernel based on these subgraphs is defined as

$$k_n(G, G') = \begin{cases} 
\frac{1}{(n-k)^2} \sum_{S \in \mathcal{M}, S' \in \mathcal{M}'} k_{n-1}(S, S') & \text{if } n > k, \\
\delta(G \cong G') & \text{if } n = k
\end{cases}$$

where $\delta(G \cong G')$ is 1 if $G$ and $G'$ are isomorphic, 0 otherwise.

The graphlet kernel is defined as $k_g(G, G') := k_n(G, G')$. 
How to reduce runtime?

The kernel is defined, but how to compute graphlet distributions? Counting size-$k$ graphlets by exhaustive enumeration takes $O(n^k)$. This is too expensive.

We propose 2 schemes to speed up the computation. We show that

- **sampling** a fixed number of graphlets suffices to bound the $l_1$ deviation of the empirical estimates of the graphlet distribution from the true distribution.

- for **graphs of degree bounded by $d$**, the exact number of all graphlets of size $k$ can be determined in time $O(nd^{k-1})$. Large real world graphs are often sparse with $d \ll n$. 

Given a multiset $X := \{X_j\}_{j=1}^m$ of independent identically distributed (iid) random variables $X_j \sim D$, the empirical estimate of $D$ is defined as

$$\hat{D}^m(i) = \frac{1}{m} \sum_{j=1}^m \delta(X_j = i),$$

where $i \in \mathcal{A}$, and $\delta$ is an indicator function.

Let $D$ be a probability distribution on the finite set $\mathcal{A} = \{1, \ldots, a\}$. Let $X := \{X_j\}_{j=1}^m$, with $X_j \sim D$. For a given $\epsilon > 0$ and $\delta > 0$,

$$m = \left\lceil \frac{2 \left( \log 2 \cdot a + \log \left( \frac{1}{\delta} \right) \right)}{\epsilon^2} \right\rceil$$

samples suffice to ensure that $P \left\{ \|D - \hat{D}^m\|_1 \geq \epsilon \right\} \leq \delta$. 

Karsten Borgwardt and Nino Shervashidze: Biological Network Analysis, Page 10
Example

- Consider size-5 graphlets with $\epsilon = 0.05$, $\delta = 0.05$
- $a = 34$, as there are 34 pairwise non-isomorphic graphlets of size 5

We obtain $m = 21251$ independent from the size of graphs we want to compare

$21251 \ll n^5, \forall n > 9$. 
Bounded degree graphs

There is a large fraction of graphs on which complete counting of graphlets can be performed efficiently: graphs of bounded degree \( d \).

We present 2 algorithms which exploit the low degree:

- one for enumerating all connected graphlets,
- one for counting all graphlets.

Both have \( O(nd^{k-1}) \) runtime complexity, but the first one is faster in practice.
Count connected graphlets of size $k$, $k \in \{3, 4, 5\}$

Notice that most connected graphlets contain size-$k$ simple paths

Provided this, the idea is simple:

- enumerate simple paths of $k$ nodes ($O(nd^{k-1})$)
- for each path, look up adjacencies among these $k$ nodes to decide which graphlet we obtain ($O(1)$ provided that we have a data structure allowing for this)
- each graphlet will be counted as many times, as the number of $k$-node paths it contains $\rightarrow$ divide counts by these numbers
Count connected graphlets of size \( k, k \in \{3, 4, 5\} \) (continued)

**Problem:** while for size-3 graphlets all connected graphlets contain simple paths of \( k \) nodes, this is no more the case for size-4 and 5 graphlets.

**Solution:**

- To count I, we look up the \( \binom{d_i}{3} \) neighbor triplets of each \( v_i \), and check if they induce the graphlet we are interested in \( (O(nd^3)) \)
- II, III and IV contain I. So we first enumerate all occurrences of I, and then check the neighbors of each node in I to see if they induce the graphlets in question \( (O(nd^4)) \)
Count all graphlets of size $k$, $k \in \{3, 4, 5\}$

The basic idea:

- enumerate all connected graphlets
- obtain counts of disconnected graphlets by subtracting previously obtained quantities from precomputed quantities
Count all graphlets of size $k$, $k \in \{3, 4, 5\}$ (continued)

**Example: 3-node graphlets**

There are 4 types of 3-node graphlets: denote them $F_i$, $i \in \{0, 1, 2, 3\}$, $F_i$ contains $i$ edges

First count graphlets containing at least one edge

\[
|F_1| = |F_2| = |F_3| = 0
\]

For all edges do \((0(\text{nd}))\)

\[
|F_3| = |F_3| + \#(\text{red nodes})
|F_2| = |F_2| + \#(\text{green nodes})
|F_1| = |F_1| + (n-2-\#(\text{red and green nodes}))
\]

\[
|F_3| = |F_3|/6, \quad |F_2| = |F_2|/4, \quad |F_1| = |F_1|/2
|F_0| = \binom{n}{3} - (|F_1|+|F_2|+|F_3|)
\]
Experiments

Statistics on datasets

<table>
<thead>
<tr>
<th>dataset</th>
<th>size</th>
<th>classes</th>
<th># nodes</th>
<th># edges</th>
<th>d</th>
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<tbody>
<tr>
<td>MUTAG</td>
<td>188</td>
<td>2 (125 vs. 63)</td>
<td>17.7</td>
<td>38.9</td>
<td>4</td>
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<tr>
<td>PTC</td>
<td>344</td>
<td>2 (192 vs. 152)</td>
<td>26.7</td>
<td>50.7</td>
<td>4</td>
</tr>
<tr>
<td>Enzyme</td>
<td>600</td>
<td>6 (100 each)</td>
<td>32.6</td>
<td>124.3</td>
<td>9</td>
</tr>
<tr>
<td>D &amp; D</td>
<td>1178</td>
<td>2 (691 vs. 587)</td>
<td>284.4</td>
<td>1921.6</td>
<td>52</td>
</tr>
</tbody>
</table>

MUTAG, PTC - chemicals

Enzyme, D & D - biological datasets

We did not consider node labels
Experiments

Classification accuracy for $k = 4$

![Classification accuracy graph for different datasets and methods.](image-url)
## Experiments

### Runtime

<table>
<thead>
<tr>
<th>Kernel</th>
<th>MUTAG</th>
<th>PTC</th>
<th>Enzymes</th>
<th>D &amp; D</th>
</tr>
</thead>
<tbody>
<tr>
<td>RW</td>
<td>42.3&quot;</td>
<td>2’ 39”</td>
<td>10’ 45”</td>
<td>&gt; 1 day</td>
</tr>
<tr>
<td>SP</td>
<td>23.2&quot;</td>
<td>2’ 35”</td>
<td>5’ 1”</td>
<td>&gt; 1 day</td>
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<tr>
<td>GK A3 1016</td>
<td>21.5”</td>
<td>29.7”</td>
<td>39”</td>
<td>2’ 9”</td>
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<tr>
<td>GK A3 1154</td>
<td>23.1”</td>
<td>42.6”</td>
<td>48.7”</td>
<td>2’ 19”</td>
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<tr>
<td>GK A3 4061</td>
<td>1’ 18”</td>
<td>2’ 39”</td>
<td>1’ 51”</td>
<td>6’ 35”</td>
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<tr>
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<td>1’ 38”</td>
<td>3’ 1”</td>
<td>2’ 51”</td>
<td>5’ 58”</td>
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<tr>
<td>GK A3 all</td>
<td>0.35”</td>
<td>0.9”</td>
<td>3.34”</td>
<td>2’ 34”</td>
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<tr>
<td>GK C3</td>
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<td>0.36”</td>
<td>1.3”</td>
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<tr>
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<td>4’ 36”</td>
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<tr>
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<td>12’ 3”</td>
<td>16’ 35”</td>
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<tr>
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<td>10.8”</td>
<td>49.3”</td>
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<td>0.9”</td>
<td>4.1”</td>
<td>35’ 22”</td>
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<td>8’ 1”</td>
<td>16’ 57”</td>
<td>1h 29’ 54”</td>
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<td>8’ 6”</td>
<td>17’ 3”</td>
<td>1h 1’ 54”</td>
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<td>42’ 2”</td>
<td>1h 30’ 18”</td>
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<td>18’ 4”</td>
<td>27”</td>
<td>2h 6’ 45”</td>
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<tr>
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<td>7’ 17”</td>
<td>16h 2’ 16”</td>
<td>20h 26’ 8”</td>
<td>&gt; 1 day</td>
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<td>0.79”</td>
<td>2.1”</td>
<td>40.7”</td>
<td>&gt; 1 day</td>
</tr>
</tbody>
</table>
We have proposed efficient graph kernels based on counting or sampling limited size subgraphs in a graph.

Our methods for efficient counting of graph features are not limited to being used in graph kernels.

Future research: take node labels into account.