Graph Similarity and Classification

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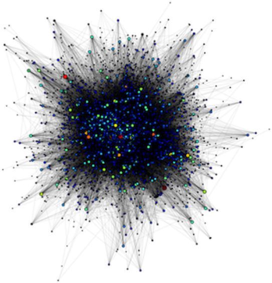
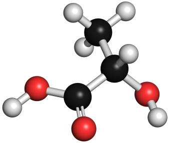
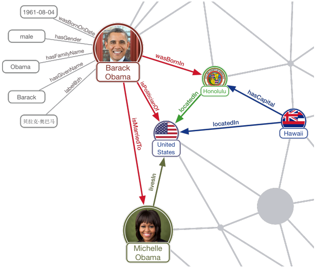
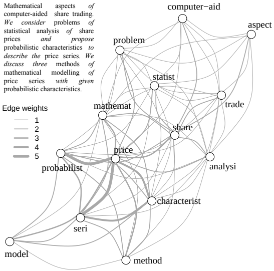
Graphs Are Everywhere









Mathematical aspects of computer-aided share trading. *We consider* problems *of* statistical analysis *of* share prices *and propose* probabilistic characteristics *to describe the* price series. *We discuss three* methods *of* mathematical modelling *of* price series *with given* probabilistic characteristics.

Why graphs?

Graph Comparison

Definition (Graph Comparison Problem)

Given two graphs G_1 and G_2 from the space of graphs $\mathcal{G}$, the problem of graph comparison is to find a mapping

$$s : \mathcal{G} \times \mathcal{G} \to \mathbb{R}$$

such that $s(G_1, G_2)$ quantifies the similarity of G_1 and G_2.

Graph comparison is a topic of high significance

- Data is often represented as graphs
- It is the central problem for all learning tasks on graphs such as clustering and classification
- Most machine learning algorithms make decisions based on the similarities or distances between pairs of instances (e.g. k-nn)

Not an Easy Problem

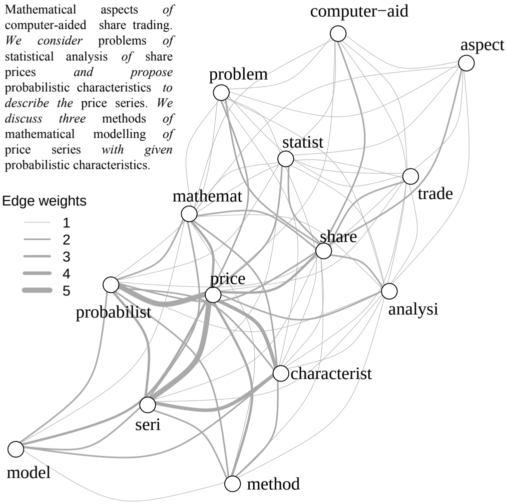
Although graph comparison seems a tractable problem, it is very complex

Many problems related to it are **NP-complete**

- subgraph isomorphism
- finding largest common subgraph

We are interested in algorithms capable of measuring the similarity between two graphs in **polynomial** time

Motivation - Text Categorization



Mathematical aspects *of* computer-aided share trading. *We consider* problems *of* statistical analysis *of* share prices *and propose* probabilistic characteristics *to describe the* price series. *We discuss three* methods *of* mathematical modelling *of* price series *with given* probabilistic characteristics.

Given a text, create a graph where

- vertices correpond to terms
- two terms are linked to each other if they co-occur within a fixed-size sliding window

Rousseau et al. “Text categorization as a graph classification problem.”. In ACL’15

Motivation - Text Categorization

Intuition: documents sharing same subgraphs belong to the same class

Given a set of documents and their graph representations:

Extract frequent subgraphs

- from the set of graphs

  or

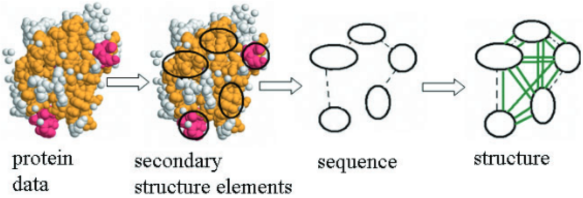
- from the set of the main cores of the graphs

Then, use frequent subgraphs as features for classification

Motivation - Protein Function Prediction

For each protein, create a graph that contains information about its

- structure
- sequence
- chemical properties



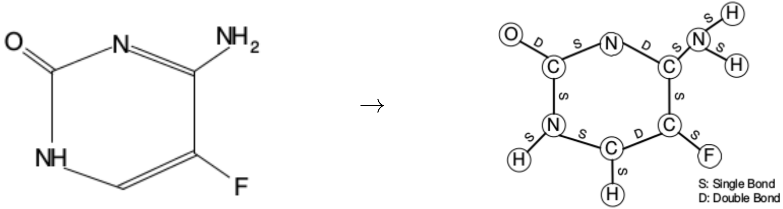
Use graph kernels to

- measure structural similarity between proteins
- predict the function of proteins

Borgwardt et al. "Protein function prediction via graph kernels". Bioinformatics 21

Motivation - Chemical Compound Classification

Represent each chemical compound as a graph



Use a frequent subgraph discovery algorithm to discover the substructures that occur above a certain support constraint

Perform feature selection

Use the remaining substructures as features for classification

Deshpande et al. “Frequent substructure-based approaches for classifying chemical compounds”. TKDE 17(8)

Motivation - Anomaly Detection for the Web Graph

Search engines create snapshots of the web → web graphs

These are necessary for

- monitoring the evolution of the web
- computing global properties such as PageRank

Identify anomalies in a single snapshot by comparing it with previous snapshots

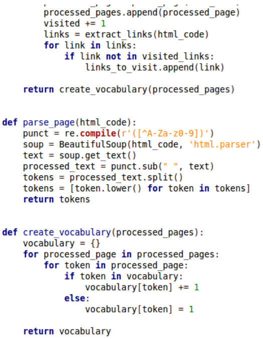
Employed similarity mesaures:

- vertex/edge overlap
- vertex ranking
- vertex/edge vector similarity
- etc

Papadimitriou et al. "Web graph similarity for anomaly detection". JISA 1(1)

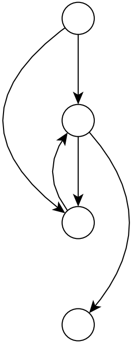
Motivation - Malware Detection

Given a computer program, create its control flow graph



```
        processed_pages.append(processed_page)
        visited += 1
        links = extract_links(html_code)
        for link in links:
            if link not in visited_links:
                links_to_visit.append(link)

    return create_vocabulary(processed_pages)


def parse_page(html_code):
    punct = re.compile(r'([^A-Za-z0-9])')
    soup = BeautifulSoup(html_code, 'html.parser')
    text = soup.get_text()
    processed_text = punct.sub(" ", text)
    tokens = processed_text.split()
    tokens = [token.lower() for token in tokens]
    return tokens


def create_vocabulary(processed_pages):
    vocabulary = {}
    for processed_page in processed_pages:
        for token in processed_page:
            if token in vocabulary:
                vocabulary[token] += 1
            else:
                vocabulary[token] = 1

    return vocabulary
```

→



Compare the control flow graph of the problem against the set of control flow graphs of known malware

If it contains a subgraph isomporphic to these graphs → malicious code inside the program

Gascon et al. "Structural detection of android malware using embedded call graphs". In AISec'13

Graph Isomorphism

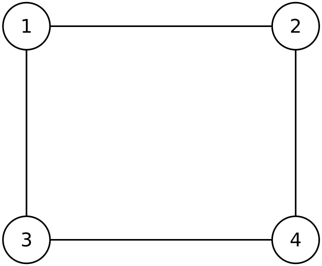
Definition (Graph Isomorphism (GI))

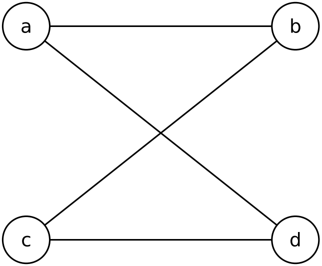
Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there is a bijective mapping $f : V_1 \to V_2$ such that $(v_i, v_j) \in E_1$ iff $(f(v_1), f(v_2)) \in E_2$. If the two graphs are isomorphic, we write $G_1 \cong G_2$

- Graph Isomorphism is an extreme case of the graph similarity problem
- It asks if two graphs are structurally equivalent to each other
- The problem became known during the 1960's as a method of comparing two chemical structures

Example

The following two graphs are isomorphic





The function f with

- $f(1) = a$
- $f(2) = b$
- $f(3) = d$
- $f(4) = c$

is a one-to-one correspondence between the vertices of the two graphs

Not a Trivial Problem

The following table lists the number of:

- all possible graphs with n vertices (# graphs)
- all non-isomorphic graphs with n vertices (# unique)

n	1	2	3	4	5	6	7	8
# graphs	1	2	8	64	1,024	32,768	2,097,152	268,435,456
# unique	1	2	4	11	34	156	1,044	12,346

Also, given two graphs with n vertices, not practical to solve the problem by brute force:

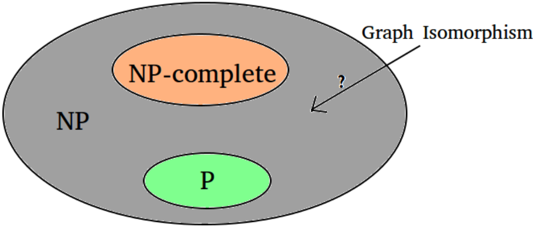
- there are n! bijections between the vertices of the graphs

Hence, the need for an efficient algorithm for the GI problem is of great significance

Complexity of GI

Unfortunately, even though GI has been extensively studied:

- no *polynomial-time* algorithm is known
- neither is it known to be *NP-complete*



Schoning showed that it is located in the low hierarchy of NP [Schöning, 1988]

GI has long been a favorite target of algorithm designers. Due to its intractable nature, it was already described as a "*disease*" in 1977 [Read and Corneil, 1977].

Algorithms for GI

- The best algorithms known for determining whether two graphs are isomorphic have exponential worst-case time complexity:
    - The best known algorithm for the problem is due to Babai and Luks and runs in $2^{\mathcal{O}(\sqrt{nlogn})}$ time [Babai and Luks, 1983].
- Recently, Babai presented an algorithm that runs in quasipolynomial time $2^{(\log n)^{\mathcal{O}(1)}}$ [Babai, 2016].
- There are also available algorithms with good time complexity in many practical cases:
    - `nauty`
    - `saucy`
    - `Traces`

  based on graph invariants - also very fast..

Graph Invariants

We saw that proving that two graphs are isomorphic is not a simple task

It is much simpler to show that two graphs are not isomorphic by finding a property that only one of the two graphs has. Such a property is called a *graph invariant*

Definition (Graph Invariant)

A graph invariant is a numerical property of graphs for which any two isomorphic graphs must have the same value

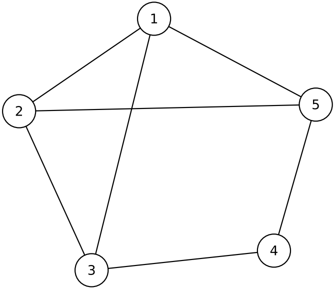
Some examples of graph invariants include:

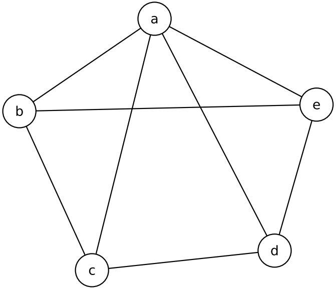
1. number of vertices
2. number of edges
3. number of spanning trees
4. degree sequence
5. spectrum

Example (1/2)

Two graphs with different graph invariants **cannot** be isomorphic

The following two graphs have different number of edges, hence we can say with confidence that they are not isomorphic



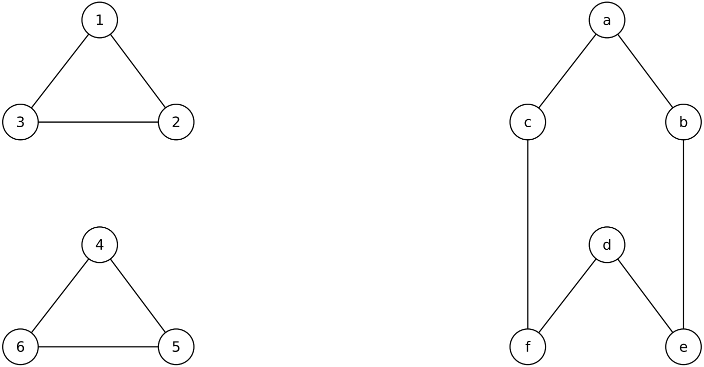


$$G_1 \qquad \ncong \qquad G_2$$

Example (2/2)

Two graphs with the same invariants may or may not be isomorphic

The following two graphs have the same degree sequence, but are **not** isomorphic



$$G_1 \qquad \ncong \qquad G_2$$

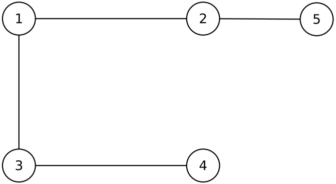
Subgraph Isomorphism

Definition (Subgraph Isomorphism (SI))

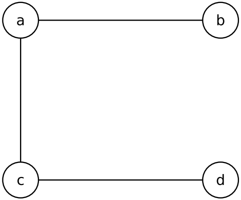
Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. A subgraph isomorphism from G_1 to G_2 is a function $f : V_1 \to V_2$ such that if $(v_i, v_j) \in E_1$, then $(f(v_1), f(v_2)) \in E_2$, and if $(v_i, v_j) \notin E_1$, then $(f(v_1), g(v_2)) \notin E_2$

- The Subgraph Isomorphism problem asks if a graph contains a subgraph that is topologically identical (isomorphic) to a second graph
- Subgraph isomorphism generalizes problems such as Clique and Hamiltonian Path, and is therefore NP-complete [Garey and Johnson, 1979]
    - Exponential runtime in worst case
    - Not practical for larger graphs with many nodes

Example



G_1



G_2

The subgraph of G_1 induced by vertices $\{1, 2, 3, 4\}$ is isomorphic to G_2 since

- $f(1) = a$
- $f(2) = b$
- $f(3) = c$
- $f(4) = d$

is a one-to-one correspondence between the vertices of the induced subgraph and G_2

Maximum Common Subgraph

Definition (Maximum Common Subgraph (MCS))

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. A common subgraph G of G_1 and G_2 is a graph such that there exist subgraph isomorphisms from G to G_1 and from G to G_2. Graph G is a maximum common subgraph of G_1 and G_2 if there exists no other common subgraph of of G_1 and G_2 that has more nodes than G

- Maximum Common Subgraph finds the largest subgraph of a graph that is isomorphic to a subgraph of a second graph

- It is known that the Maximum Common Subgraph problem is NP-complete [Garey and Johnson, 1979]
  - Same problems as in the case of Subgraph Isomorphism

Graph Edit Distance

The graph edit distance is a dissimilarity measure between graphs:

- takes as input two graphs
- outputs their distance

Computes the dissimilarity between two graphs by taking into account the *number* and the *strength* of the distortions that are needed to transform one graph to the other

Given two graphs, G_1 and G_2, a graph edit distance method transforms G_1 into G_2 using some edit operations

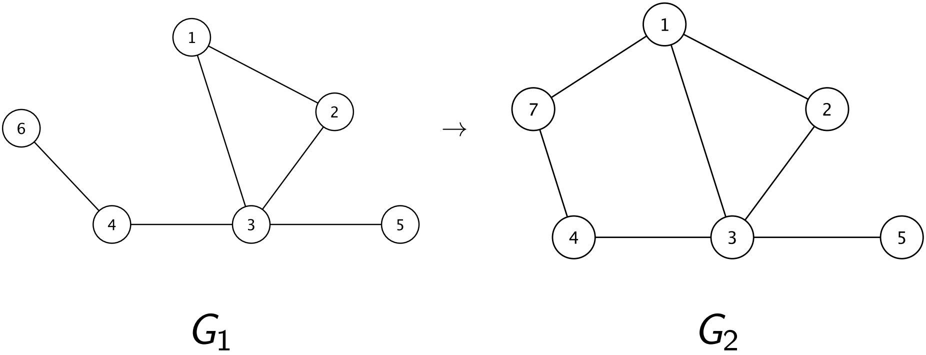
- insertions
- deletions
- substitutions

of both nodes and edges

It then computes their dissimilarity based on these operations

Gao et al. "A survey of graph edit distance". Pattern Analysis and applications 13(1)

Example



One of the edit operation sequences includes

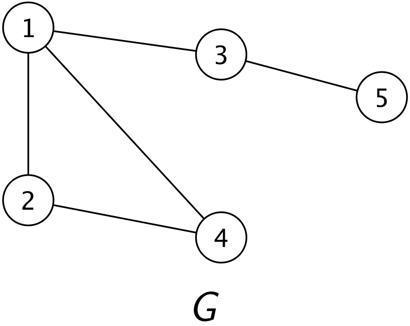
- insertion and edge insertion (vertex 7 and its relative edges)
- node deletion and edge deletion (vertex 6 and its relative edge)

A cost function is defined for each operation

Total cost of sequence → sum of costs for all operations in the sequence

Graph Preliminaries

Let $G = (V, E)$ be a simple unweighted, undirected graph where V is the set of vertices and E the set of edges

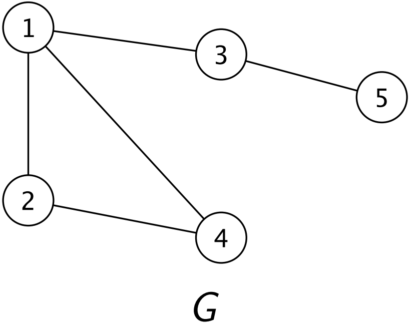


$V = \{1, 2, 3, 4, 5\}$

$E = \{(1, 2), (1, 3)(1, 4), (2, 4), (3, 5)\}$

Graph Preliminaries

The neighbourhood $\mathcal{N}(v)$ of vertex v is the set of all vertices adjacent to v, $\mathcal{N}(v) = \{u : (v, u) \in E\}$ where (v, u) is an edge between v and u

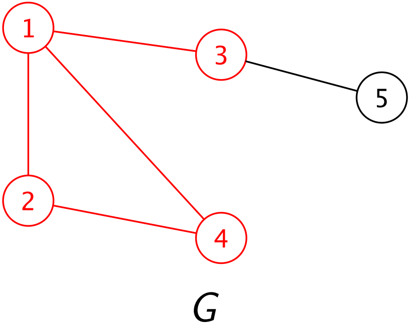


$\mathcal{N}(1) = \{2, 3, 4\}$

$\mathcal{N}(5) = \{3\}$

Graph Preliminaries

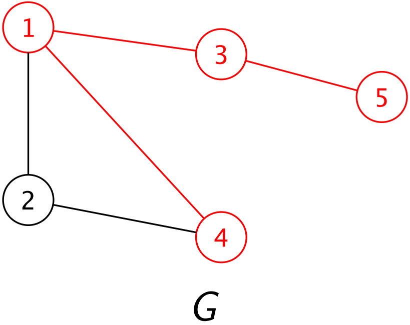
A walk in a graph G is a sequence of vertices $v_1, v_2, \ldots, v_{k+1}$ where $v_i \in V$ and $(v_i, v_{i+1}) \in E$ for $1 \leq i \leq k$



Walk: $1 \to 2 \to 4 \to 1 \to 3$

Graph Preliminaries

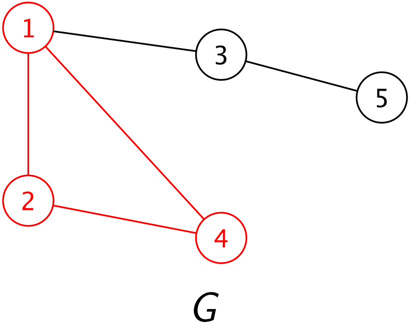
A walk in which $v_i \neq v_j \Leftrightarrow i \neq j$ is called a path



Path: $4 \rightarrow 1 \rightarrow 3 \rightarrow 5$

Graph Preliminaries

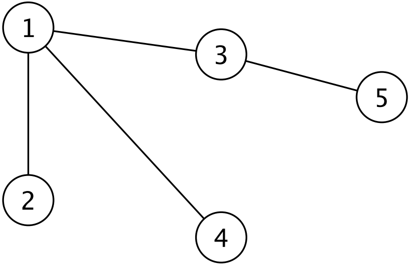
A cycle is a path with $(v_{k+1}, v_1) \in E$



Cycle: $1 \rightarrow 2 \rightarrow 4$

Graph Preliminaries

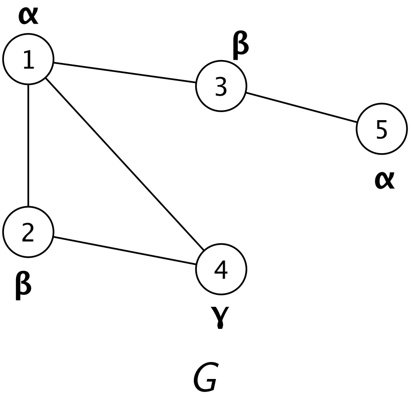
A subtree is an acyclic subgraph in which there is a path between any two vertices



G

Graph Preliminaries

A labeled graph is a graph with labels on vertices. Given a set of labels $\mathcal{L}$, $\ell : V \to \mathcal{L}$ is a function that assigns labels to the vertices of the graph

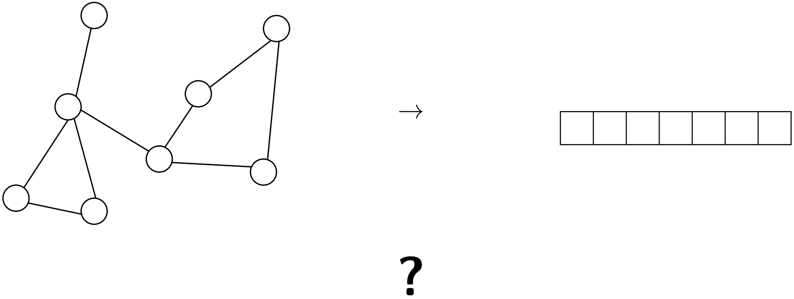


$\mathcal{L} = \{\alpha, \beta, \gamma\}$

$\ell(1) = \alpha \quad \ell(4) = \gamma$

Learning on Graphs

- Most machine learning algorithms require the input to be represented as a fixed-length feature vector
- Graphs cannot be naturally represented as vectors
- Typical vector-based classifiers (e. g., logistic regression) are not applicable



What is a Kernel?

Definition (Kernel Function)

The function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel if it is:

1. symetric: $k(x, y) = k(y, x)$
2. positive semi-definite: $\forall x_1, x_2, \dots, x_n \in \mathcal{X}$, the Gram Matrix $\mathbf{K}$ defined by $\mathbf{K}_{ij} = k(x_i, x_j)$ is positive semi-definite

- If a function satisfies the above two conditions on a set $\mathcal{X}$, it is known that there exists a map $\phi : \mathcal{X} \to \mathcal{H}$ into a Hilbert space $\mathcal{H}$, such that:

$$k(x, y) = \langle \phi(x), \phi(y) \rangle$$

for all $(x, y) \in \mathcal{X}^2$ where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathcal{H}$

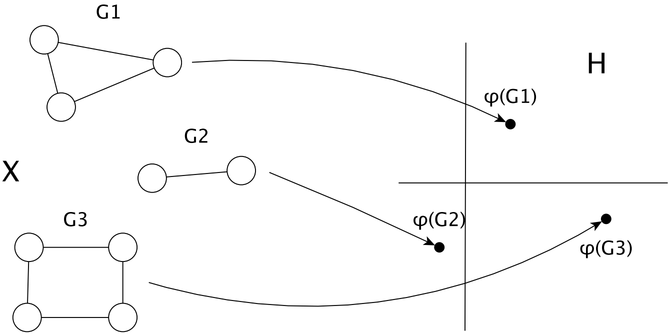
- Informally, $k(x, y)$ is a measure of similarity between x and y

Graph Kernels

Definition (Graph Kernel)

A graph kernel $k : \mathcal{G} \times \mathcal{G} \rightarrow \mathbb{R}$ is a kernel function over a set of graphs $\mathcal{G}$

- It is equivalent to an inner product of the embeddings $\phi : \mathcal{X} \rightarrow \mathcal{H}$ of a pair of graphs into a Hilbert space
- Makes the whole family of kernel methods applicable to graphs.



Kernel Trick

- Many machine learning algorithms can be expressed only in terms of inner products between vectors
- Let $\phi(G_1), \phi(G_2)$ be vector representations of graphs G_1, G_2 in a very high (possibly infinite) dimensional feature space
- Computing the explicit mappings $\phi(G_1), \phi(G_2)$ and their inner product $\langle \phi(x), \phi(y) \rangle$ for the pair of graphs can be computationally demanding
- The kernel trick avoids the explicit mapping by directly computing the inner product $\langle \phi(x), \phi(y) \rangle$ via the kernel function

Example

Let $\mathcal{X} = \mathbb{R}^2$ and $x = (x_1, x_2), y = (y_1, y_2) \in \mathcal{X}$

For any $x = (x_1, x_2)$ let ϕ be a map $\phi : \mathbb{R}^2 \to \mathbb{R}^3$ defined as:

$$\phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

Let also $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ a kernel defined as $k(x, y) = \langle x, y\rangle^2$. Then

$$\begin{aligned} k(x, y) &= \langle x, y\rangle^2 = (x_1y_1 + x_2y_2)^2 = x_1^2y_1^2 + 2x_1y_1x_2y_2 + x_2^2y_2^2 \\ &= \langle \phi(x), \phi(y)\rangle \end{aligned}$$

Hence, using the kernel we can compute the inner product $\langle \phi(x), \phi(y)\rangle$ without computing $\phi(x)$ and $\phi(y)$

Complete Graph Kernels

Definition (Complete Graph Kernel)

A graph kernel $k(G_1, G_2) = \langle \phi(G_1), \phi(G_2) \rangle$ is complete if ϕ is injective

Hence, for complete graph kernels, $\phi(G_1) = \phi(G_2)$ iff G_1 and G_2 are isomorphic

How **hard** is to compute a complete graph kernel?

Complete Graph Kernels

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Hence, for complete graph kernels, $\phi(G_1) = \phi(G_2)$ iff G_1 and G_2 are isomorphic

How **hard** is to compute a complete graph kernel?

Proposition (Gärtner et al., 2003)

Computing any complete graph kernel is at least as hard as the graph isomorphism problem

Expressiveness vs Efficiency

We are interested in kernels that can be computed in polynomial time (with small degree)

If the kernel is complete:

- Computation is at least as hard as the graph isomorphism problem
    - No polynomial algorithm for the graph isomorphism problem is known

If the kernel is not complete:

- It can be computed efficiently
- We can have $\phi(G_1) = \phi(G_2)$ even if $G_1 \ncong G_2$
    - The kernel is not expressive enough

Subgraph Kernel

Let $\mathcal{G}$ denote the set of all graphs

For any graph $G \in \mathcal{G}$, each feature of its subgraph space is defined as:

$$\forall H \in \mathcal{G}, \quad \phi_H(G) = |\{G' \text{ is a subgraph of } G : G' \cong H\}|$$

The subgraph kernel between two graphs G_1 and G_2 is defined as:

$$k(G_1, G_2) = \sum_{H \in \mathcal{G}} \lambda_H \phi_H(G_1) \phi_H(G_2)$$

where λ_H is a positive weight

How **hard** is to compute the subgraph kernel?

The subgraph kernel is a **complete** graph kernel

- it is at least as hard as solving the graph isomorphism problem

Subgraph Kernel

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where λ_H is a positive weight

How **hard** is to compute the subgraph kernel?

Proposition (Gärtner et al., 2003)

Computing the subgraph kernel is NP-hard

Substructures-based Kernels

A large number of graph kernels compare substructures of graphs that are computable in polynomial time:

- walks
- shortest paths
- cyclic patterns
- subtree patterns
- graphlets

$\vdots$

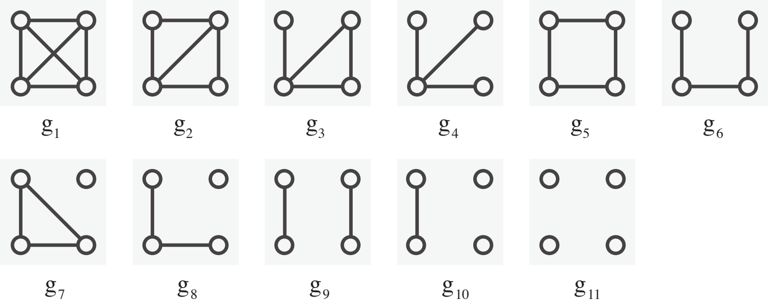
Graphlet Kernel

The graphlet kernel compares graphs by counting *graphlets*

A graphlet corresponds to a small subgraph

- typically of 3,4 or 5 vertices

Below is the set of graphlets of size 4



Shervashidze et al. “Efficient graphlet kernels for large graph comparison”. In AISTATS’09

Graphlet Kernel

Let $\mathcal{G} = \{graphlet_1, graphlet_2, \ldots, graphlet_r\}$ be the set of size-k graphlets

Let also $f_G \in \mathcal{N}^r$ be a vector such that its i-th entry is $f_{G,i} = \#(graphlet_i \sqsubseteq G)$

The graphlet kernel is defined as:

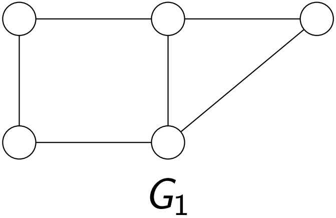
$$k(G_1, G_2) = f_{G_1}^\top f_{G_2}$$

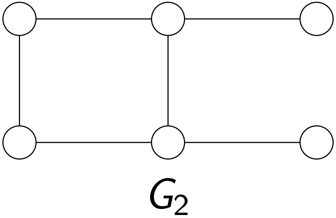
Problems:

- There are $\binom{n}{k}$ size-k subgraphs in a graph
- Exaustive enumeration of graphlets is very expensive

  Requires $O(n^k)$ time
- For labeled graphs, the number of graphlets increases further

Example





The vector representations of the graphs above according to the set of graphlets of size 4 is:

$$f_{G_1} = (0, 0, 2, 0, 1, 2, 0, 0, 0, 0, 0)^T$$
$$f_{G_2} = (0, 0, 0, 2, 1, 5, 0, 4, 0, 3, 0)^T$$

Hence, the value of the kernel is:

$$k(G_1, G_2) = f_{G_1}^{\top} f_{G_2} = 11$$

Subtree Kernel

Compares subtree patterns in two graphs

A subtree pattern is a subgraph of a graph which has

- a root vertex
- no cycles

The height of a subtree is the maximum distance between the root and any other node in the subtree

If there are cycles in the graph, a vertex can appear more than once in a subtree pattern

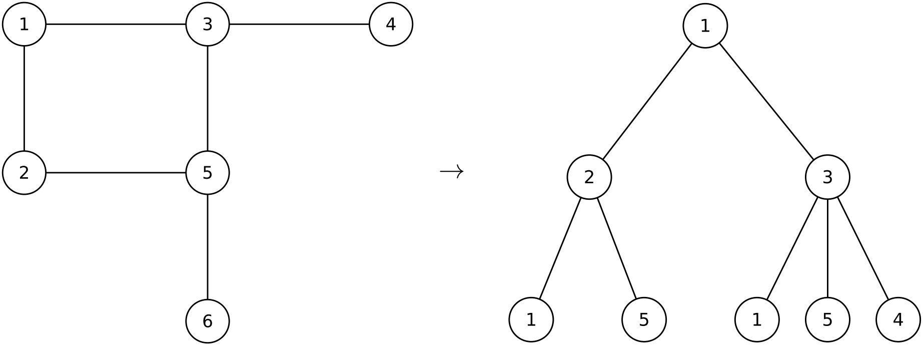
- it is treated as a distinct vertex such that the pattern is still a cycle-free tree

For all pairs of nodes v from G_1 and u from G_2:

- Create the subtree patterns of height h rooted at v, u
- Compare v and u via a kernel function
- Recursively compare all vertices of the subtree patterns of v and u via a kernel function

Ramon and Gärtner. "Expressivity versus efficiency of graph kernels". In MGTS'03

Example



Subtree of height 2
rooted at vertex 1

Subtree Kernel

Given a pair of graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, the subtree kernel of height h is defined as:

$$k(G_1, G_2) = \sum_{v_1 \in V_1} \sum_{v_2 \in V_2} k_h(v_1, v_2)$$

where

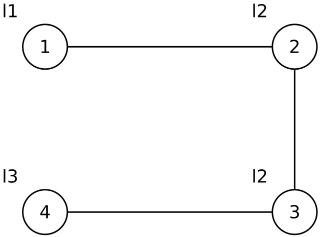
$$k_h(v_1, v_2) = \begin{cases} \delta(\ell(v_1) = \ell(v_2)) & \text{if } h = 0 \\ \lambda_{v_1} \lambda_{v_2} \delta(\ell(v_1) = \ell(v_2)) \displaystyle\sum_{R \in \mathcal{M}(v_1, v_2)} \prod_{(w_1, w_2) \in R} k_{h-1}(w_1, w_2) & \text{if } h > 0 \end{cases}$$

where $\delta(\cdot, \cdot)$ is the Kronecker delta function that equals 1 if its arguments are identical, 0 otherwise, λ_{v_1} and λ_{v_2} are weights associated with nodes v_1 and v_2, and

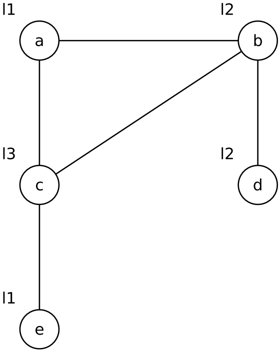
$$\begin{aligned} \mathcal{M}(v_1, v_2) = \Big\{ & R \subseteq \mathcal{N}(v_1) \times \mathcal{N}(v_2) | (\forall (u_1, u_2), (w_1, w_2) \in R : \\ & u_1 = w_1 \Leftrightarrow u_2 = w_2) \wedge (\forall (u_1, u_2) \in R : \ell(u_1) = \ell(u_2)) \Big\} \end{aligned}$$

Example

We are given the following graphs



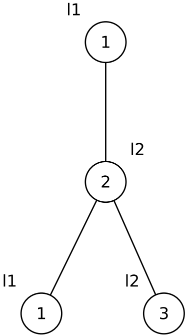
G_1

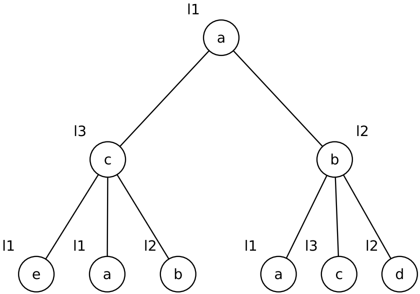


G_2

Example

Below are given the subtrees of G_1 and G_2 with height 2 rooted at 1 and a respectively





We will compute $k_2(1, a)$

Example

We set $\lambda_v = 1$ for all v and we have:

$$k_2(1,a) = \delta(\ell(1) = \ell(a)) \sum_{R \in \mathcal{M}(1,a)} \prod_{(v_1,v_2) \in R} k_1(v_1, v_2)$$

- $\delta(\ell(1) = \ell(a)) = 1$ since $\ell(1) = \ell(a) = l1$
- $\mathcal{M}(1,a) = \{(2,b)\}$ since $\ell(2) = \ell(b) = l2$

Hence, we have now to compute $k_1(2,b)$

$$k_1(2,b) = \delta(\ell(2) = \ell(b)) \sum_{R \in \mathcal{M}(2,b)} \prod_{(v_1,v_2) \in R} k_0(v_1, v_2)$$

- $\delta(\ell(2) = \ell(b)) = 1$ since $\ell(2) = \ell(b) = l2$
- $\mathcal{M}(2,b) = \{(1,a),(3,d)\}$ since $\ell(1) = \ell(a) = l1$ and $\ell(3) = \ell(d) = l2$

Example

At height 0, we have:

$$k_0(1, a) = k_0(3, d) = 1$$

Therefore,

$$k_1(2, b) = k_0(1, a)k_0(3, d) = 1$$

And finally,

$$k_2(1, a) = k_1(2, b) = 1$$

Subtree kernel

Pros: Richer representation of graph structure

Cons: Very high complexity

- $\mathcal{O}(n^2 h 4^d)$ where d is the maximum degree of the pair of graphs

Shortest Path Kernel

Compares the length of shortest-paths of two graphs

- and their endpoints in labeled graphs

Floyd-transformation

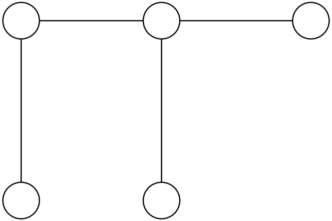
Transforms the original graphs into shortest-paths graphs

- Compute the shortest-paths between all pairs of vertices of the input graph G using some algorithm (i. e. Floyd-Warshall)
- Create a shortest-path graph S which contains the same set of nodes as the input graph G
- All nodes which are connected by a walk in G are linked with an edge in S
- Each edge in S is labeled by the shortest distance between its endpoints in G

Borgwardt and Kriegel. "Shortest-path kernels on graphs". In ICDM'05

Example

Floyd-transformation



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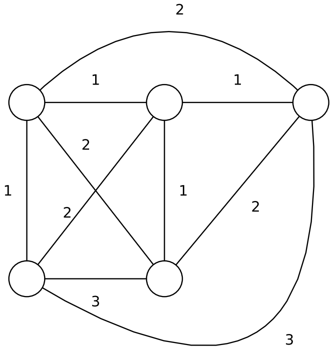


G

S

Shortest Path Kernel

Given the Floyd-transformed graphs $S_1 = (V_1, E_1)$ and $S_2 = (V_2, E_2)$ of G_1 and G_2, the shortest path kernel is defined as:

$$k(G_1, G_2) = \sum_{e_1 \in E_1} \sum_{e_2 \in E_2} k^{(1)}_{walk}(e_1, e_2)$$

where $k^{(1)}_{walk}$ is a kernel on edge walks of length 1

- For unlabeled graphs, it can be:

$$k^{(1)}_{walk}(e_1, e_2) = \delta(\ell(e_1), \ell(e_2)) = \begin{cases} 1 & \text{if } \ell(e_1) = \ell(e_2), \\ 0 & \text{otherwise} \end{cases}$$

  where $\ell(e)$ gives the label of edge e

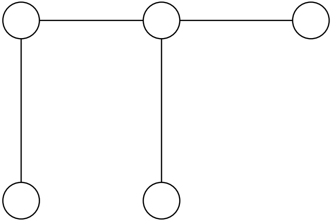
- For labeled graphs, it can be:

$$k^{(1)}_{walk}(e_1, e_2) = \begin{cases} 1 & \text{if } \ell(e_1) = \ell(e_2) \wedge \ell(e_1^1) = \ell(e_2^1) \wedge \ell(e_1^2) = \ell(e_2^2), \\ 0 & \text{otherwise} \end{cases}$$

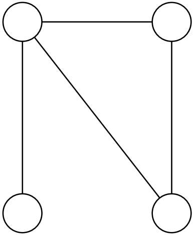
  where e^1, e^2 are the two endpoints of e

Example

Compute the shortest path kernel for the following pair of unlabeled graphs



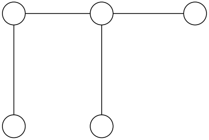
G_1



G_2

Example

Floyd-transformations



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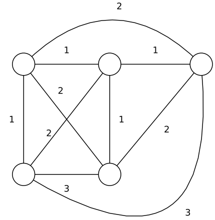
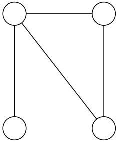


G_1

S_1



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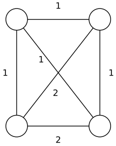


G_2

S_2

Example

In S_1 we have:

- 4 edges with label 1
- 4 edges with label 2
- 2 edges with label 3

In S_2 we have:

- 4 edges with label 1
- 2 edges with label 2

Hence, the value of the kernel is:

$$k(G_1, G_2) = \sum_{e_1 \in E_1} \sum_{e_2 \in E_2} k^{(1)}_{walk}(e_1, e_2) = 4 * 4 + 4 * 2 = 24$$

Shortest Path Kernel

Computing the shortest path kernel includes:

- Computing shortest paths for all pairs of vertices in the two graphs: $\mathcal{O}(n^3)$
- Comparing all pairs of shortest paths from the two graphs: $\mathcal{O}(n^4)$

Hence, runtime is $\mathcal{O}(n^4)$

Problems:

- Very high complexity for large graphs
- Shortest-path graphs may lead to memory problems on large graphs

Cyclic Pattern Kernel

Compares simple cycles and tree patterns in two graphs

- extracts the set of all simple cycles from the two graphs

Problems:

- Number of simple cycles is exponential in the number of vertices *n* in the worst case
- Computing the Cyclic pattern kernel on general graphs is NP-hard

Solution:

- Consider graphs whose number of simple cycles is bounded by a constant (graphs with up to *k* simple cycles)

However, can only be applied to the families of graphs where the number of simple cycles is polynomially bounded

- its practical use is limited

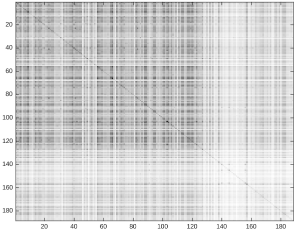
Horváth et al. "Cyclic pattern kernels for predictive graph mining". In KDD'04

A Structural Smoothing Framework

Diagonal dominance problem of kernels that compare specific substructures of graphs:

1. Very large feature space, hence, unlikely that two graphs will contain similar substructures
2. Kernel value between pairs of graphs $\ll$ kernel value between a graph and itself

This leads to the diagonal dominance problem



The resulting kernel matrix is close to the identity matrix

Yanardag and Vishwanathan. "A structural smoothing framework for robust graph comparison". In NIPS'15

A Structural Smoothing Framework

However, the substructures used to define a graph kernel are often **related** to each other (e. g., shortest path of length 10 more similar to shortest path of length 9 than to shortest path of length 3)

Solution: apply smoothing to alleviate the problem

First construct a Directed Acyclic Graph (DAG):

- each vertex corresponds to a substructure
- for each substructure s of size k determine all possible substructures of size $k-1$ that s can be reduced into
- these correspond to the parents of s
- draw a weighted directed edge from each parent to its children vertices

DAG provides a topological ordering of the vertices

- all descendants of a given substructure at depth $k-1$ are at depth k

A Structural Smoothing Framework

The structural smoothing for a substructure s at level k is defined as:

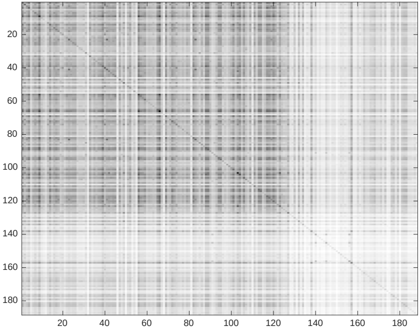
$$P_{SS}^{k}(s) = \frac{\max(c_s - d, 0)}{m} + \frac{m_d d}{m} \sum_{p \in \mathcal{P}_s} P_{SS}^{k-1}(p) \frac{w_{ps}}{\sum_{c \in \mathcal{C}_p} w_{pc}}$$

where

- c_a denotes the number of times substructure a appears in the graph
- $m = \sum_i c_i$ denotes the total number of substructures present in the graph
- $d > 0$ is a discount factor
- $m_d := |\{i : c_i > d\}|$ is the number of substructures whose counts are larger than d
- w_{ij} denotes the weight of the edge connecting vertex i to vertex j
- $\mathcal{P}_s$ denotes the parents of vertex s
- $\mathcal{C}_p$ the children of vertex p

Hence, even if the graph does not contain a substructure s ($c_s = 0$), its value in the feature vector can be greater than 0 ($P_{SS}(s) > 0$)

Example



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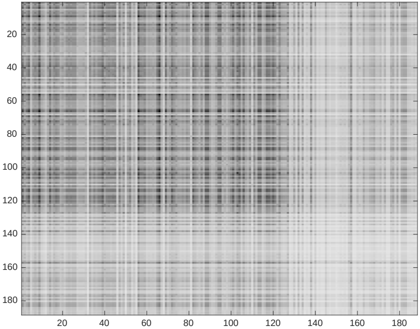


Kernel matrix before smoothing

Kernel matrix after smoothing

Random Walk Kernel

- Probably the most well-studied family of graph kernels
- Counts matching walks in two graphs

Product graph

Given two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, their direct product $G_\times$ is a graph with vertex set:

$$V_\times = \{(v_1, v_2) : v_1 \in V_1, v_2 \in V_2\} \text{ for unlabeled graphs}$$

or

$$V_\times = \{(v_1, v_2) : v_1 \in V_1, v_2 \in V_2, \ell(v1) = \ell(v2)\} \text{ for labeled graphs}$$

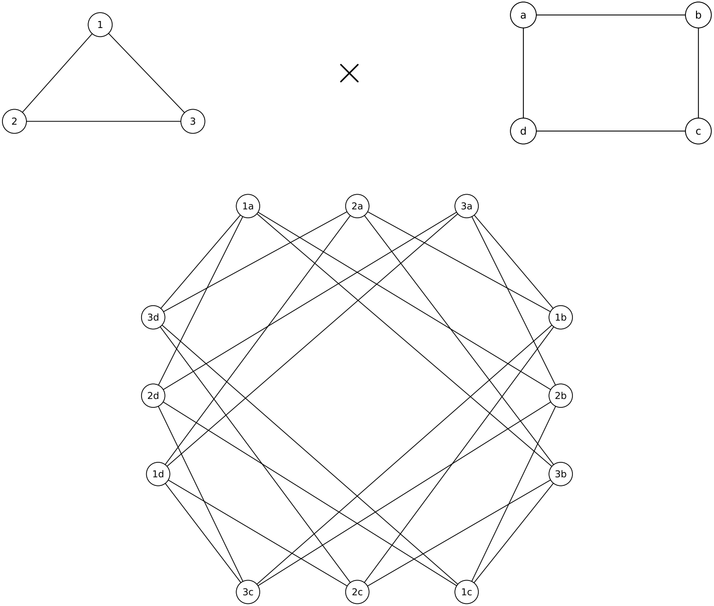
and edge set:

$$E_\times = \{((v_1, v_2), (u_1, u_2)) : (v_1, u_1) \in E_1, (v_2, u_2) \in E_2\}$$

- vertices: pairs of vertices from G_1 and G_2
- draw edge if corresponding vertices of G_1 and G_2 are adjacent in G_1 and G_2

Vishwanathan et al. "Graph kernels". JMLR 11(Apr)

Example



Random Walk Kernel

The k-th power of the adjacency matrix A of a graph G computes walks of length k

- $A^k_{ij} =$ number of walks of length k from vertex i to vertex j

Performing a random walk on $G_\times$ is equivalent to performing a simultaneous random walk on G_1 and G_2

- Common walks of length k can be computed using $A^k_\times$

For $k \in \mathbb{N}$, the k-step random walk kernel is defined as:

$$K^k_\times(G_1, G_2) = \sum_{i,j=1}^{|V_\times|} \Big[\sum_{l=0}^{k} \lambda_l A^l_\times \Big]_{ij}$$

where $\lambda_0, \lambda_1, \ldots, \lambda_k$ positive weights and $A^0_\times = I$, i. e. the identity matrix

Random Walk Kernel

For $k \to \infty$, we get the geometric random walk kernel $K_\times^\infty(G_1, G_2)$

If $\lambda_l = \lambda^l$, $K_\times^\infty(G_1, G_2)$ can be directly computed as follows:

$$K_\times^\infty(G_1, G_2) = \sum_{i,j=1}^{|V_\times|} \Big[\sum_{l=0}^{\infty} \lambda^l A_\times^l \Big]_{ij} = e^T (I - \lambda A_\times)^{-1} e$$

where I is the identity matrix and e the all-ones vector

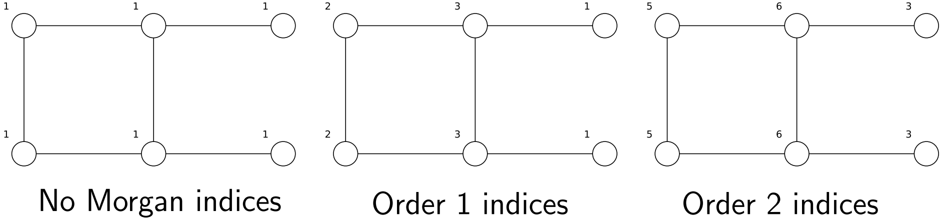
Problem: compitational complexity is $\mathcal{O}(n^6)$

Solution: Efficent computation using

- Sylvester equation
- Conjugate gradient solver
- Fixed-point iterations
- Spectral decompositions

Label Enrichment: Morgan Index

- Introduce new artificial node labels
- Initially all vertices are labeled with the number 1
- At each iteration, the label of a vertex is equal to the sum of the labels of its neighbors



Label enrichment:

- number of labels ↑
- size of product graph ↓
- number of common label paths between graphs ↓
- computation time ↓

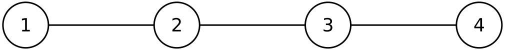
Mahé et al. "Extensions of marginalized graph kernels". In ICML'04

Random Walk Kernel

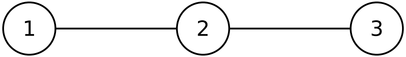
Random walk kernels suffer from **tottering**

A tottering walk is a walk $w = v_1 \ldots v_n$ where $v_i = v_{i+2}$ for some i

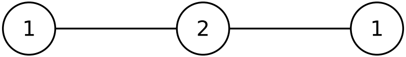
- after a move to a new vertex comes back to the original vertex
- results in redundant paths



Example graph



Non-tottering

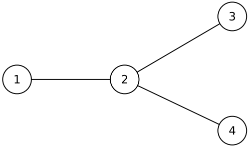


Tottering

Non-Tottering Random Walk Kernel

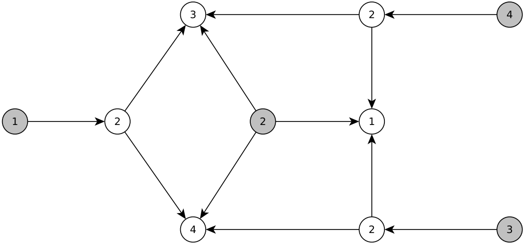
Second-order Markov random walk that forbids walks of the form $v \rightarrow u \rightarrow v$

Transform each graph G into a new directed graph G' and perform a normal random walk on G'



Original graph

→



Transformed graph

Mahé et al. "Extensions of marginalized graph kernels". In ICML'04

Weisfeiler-Lehman Framework

Uses the Weisfeiler-Lehman isomorphism test to improve the performance of existing kernels

- subtree kernel
- shortest path kernel

$\vdots$

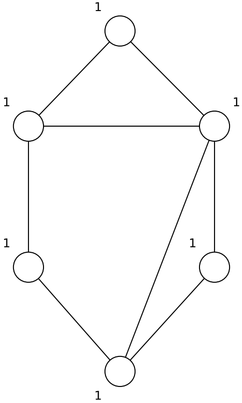
Weisfeiler-Lehman kernels achieve state-of-the-art results

Based on the Weisfeiler-Lehman algorithm: may answer if two graphs are not isomorphic

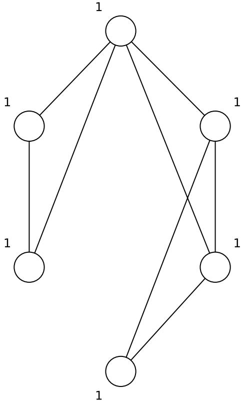
Shervashidze et al. "Weisfeiler-Lehman Graph Kernels". JMLR 12(Sep)

Example

Run the Weisfeiler-Lehman algorithm for the following pair of graphs



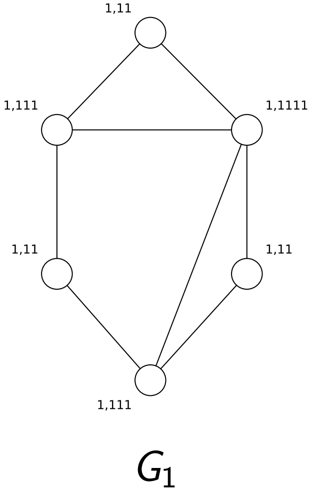
G_1

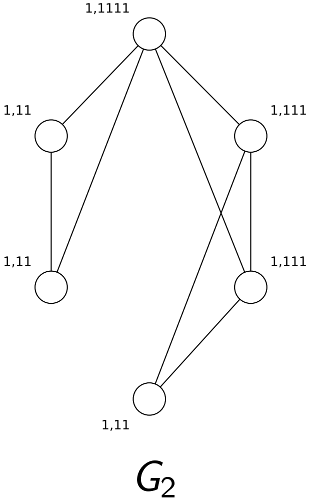


G_2

Iteration 1

First step: Augment the labels of the vertices by the sorted set of labels of neighbouring vertices

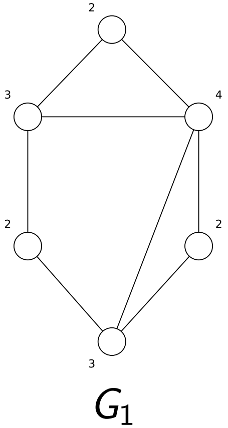


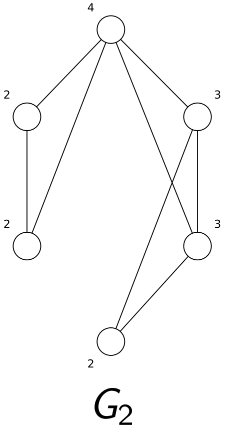


Iteration 1

Second step: Compress the augmented labels into new, short labels:

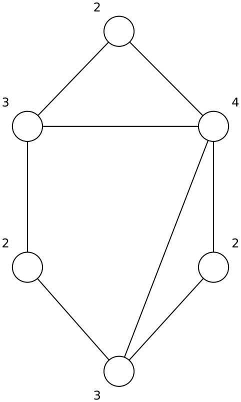
- $1, 11 \to 2$
- $1, 111 \to 3$
- $1, 1111 \to 4$



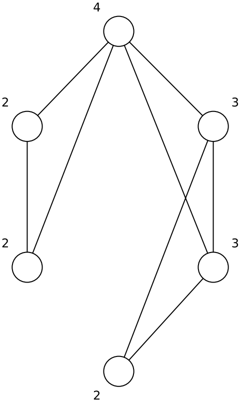


Iteration 1

Are the label sets of G_1 and G_2 identical?



G_1



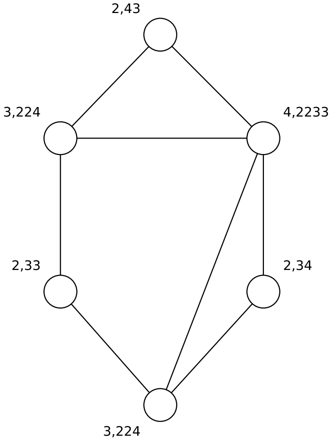
G_2

Yes!!!

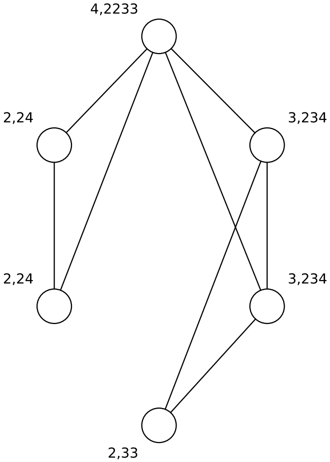
Continue to the next iteration

Iteration 2

First step: Augment the labels of the vertices by the sorted set of labels of neighbouring vertices



G_1

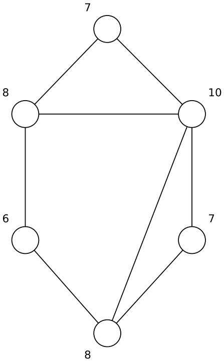


G_2

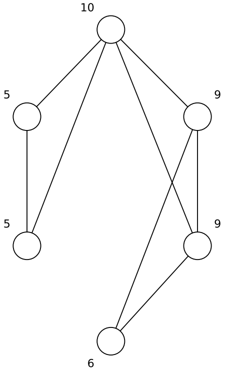
Iteration 2

Second step: Compress the augmented labels into new, short labels:

- $2, 24 \rightarrow 5$
- $2, 33 \rightarrow 6$
- $2, 34 \rightarrow 7$
- $3, 234 \rightarrow 9$
- $4, 2233 \rightarrow 10$



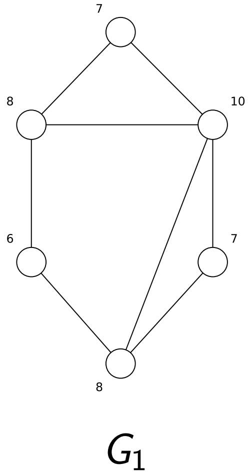
G_1

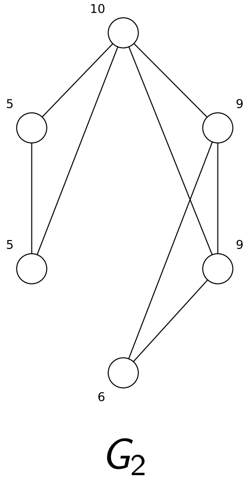


G_2

Iteration 2

Are the label sets of G_1 and G_2 identical?





No!!!

Graphs are not isomorphic

Weisfeiler-Lehman Framework

Let $G^1, G^2, \ldots, G^h$ be the graphs emerging from graph G at the iteration $1, 2, \ldots, h$ of the Weisfeiler-Lehman algorithm

Then, the Weisfeiler-Lehman kernel is defined as:

$$k_{WL}^h(G_1, G_2) = k(G_1, G_2) + k(G_1^1, G_2^1) + k(G_1^2, G_2^2) + \ldots + k(G_1^h, G_2^h)$$

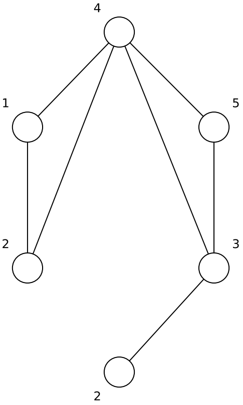
where $k(\cdot, \cdot)$ is a base kernel (e.g. subtree kernel, shortest path kernel, ...)

At each iteration of the Weisfeiler-Lehman algorithm:

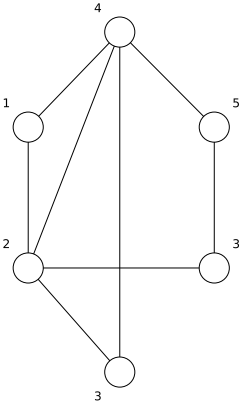
- runs a graph kernel for labeled graphs
- the new kernel values are added to the ones of the previous iteration

Weisfeiler-Lehman Subtree Kernel

Counts matching pairs of labels in two graphs after each iteration



G_1

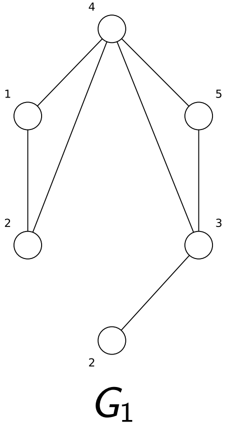


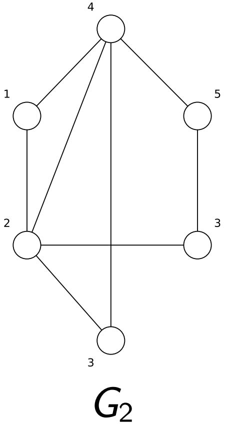
G_2

Initialization

Feature vector for a graph G:

$$\phi(G) = \{\#\text{nodes with label } 1, \#\text{nodes with label } 2, \ldots, \#\text{nodes with label } l\}$$



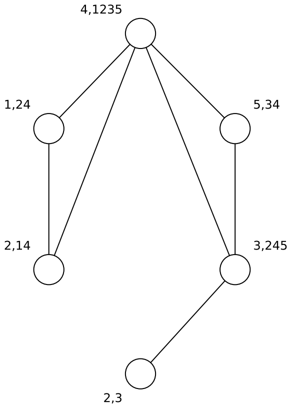


$$\phi(G_1) = \{1, 2, 1, 1, 1\}^\top \quad \phi(G_2) = \{1, 1, 2, 1, 1\}^\top$$

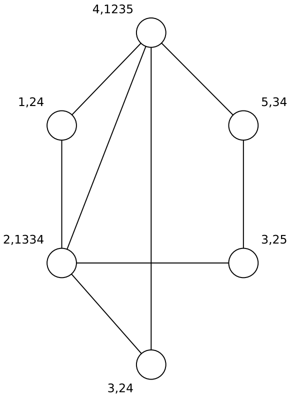
$$k(G_1, G_2) = \phi(G_1)^\top \phi(G_2) = 7$$

Iteration 1

First step: Augment the labels of the vertices by the sorted set of labels of neighbouring vertices



G_1

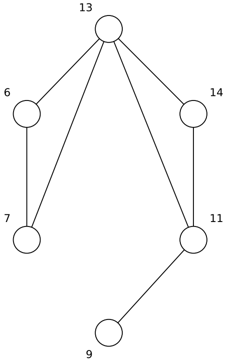


G_2

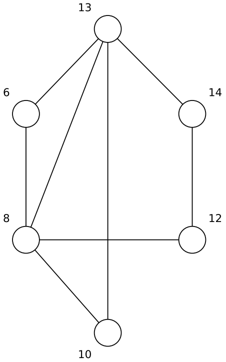
Iteration 1

Second step: Compress the augmented labels into new, short labels:

- $1, 24 \rightarrow 6$
- $2, 14 \rightarrow 7$
- $2, 1334 \rightarrow 8$
- $2, 3 \rightarrow 9$
- $3, 24 \rightarrow 10$
- $3, 245 \rightarrow 11$
- $3, 25 \rightarrow 12$
- $4, 1235 \rightarrow 13$
- $5, 34 \rightarrow 14$



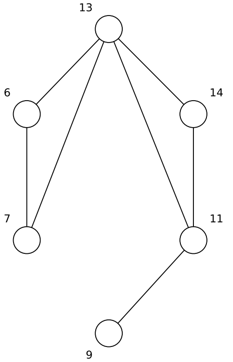
G_1



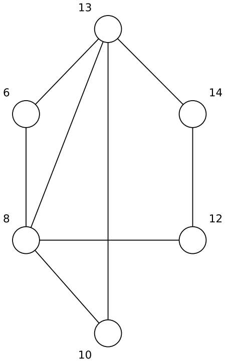
G_2

Iteration 1

Third step: Compute kernel value for iteration $h = 1$ and add it to previous kernel value



G_1



G_2

$$\phi(G_1^1) = \{1, 1, 0, 1, 0, 1, 0, 1, 1\}^\top \quad \phi(G_2^1) = \{1, 0, 1, 0, 1, 0, 1, 1, 1\}^\top$$

$$k(G_1^1, G_2^1) = \phi(G_1^1)^\top \phi(G_2^1) = 3$$

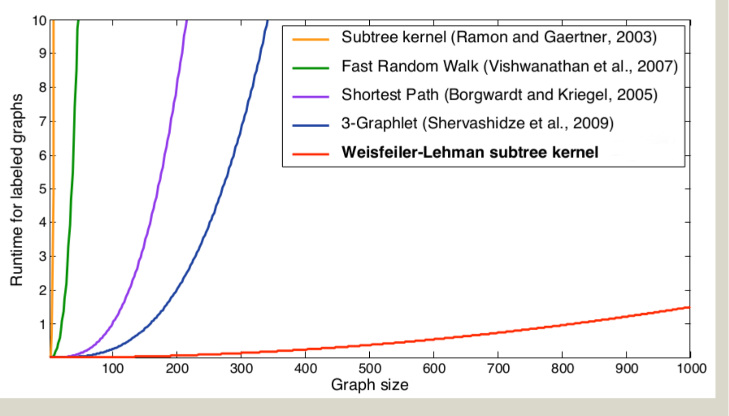
$$k_{WL}^1(G_1, G_2) = k(G_1, G_2) + k(G_1^1, G_2^1) = 10$$

Weisfeiler-Lehman Subtree Kernel

Computing the Weisfeiler-Lehman Subtree Kernel takes $\mathcal{O}(hm)$ time

- very **efficient**

Comparison to other well-known kernels



Local vs Global Graph Kernels

The previously presented graph kernels compare graphs in terms of features defined on small subgraphs:

- walks
- graphlets
- paths

Such kernels are inherently **local** since they

- operate only on a small set of vertices
- ignore the rest of the graph

However, several interesting properties are not captured in local substructures

- need graph kernels that capture **global** properties

Lovász ϑ kernel

Compares graphs based on the orthonormal representation associated with the Lovász number

- the orthonormal representation captures **global** graph properties

Orthonormal representation of a graph $G = (V, E)$:

- each vertex $i \in V$ is assigned a unit vector u_i, $||u_i|| = 1$
- let $U_G = \{u_1, u_2, \dots, u_n\}$ be the set of all vectors
- for $i, j \in V$, if $(i, j) \notin E$, then $u_i^\top u_j = 0$

An interesting orthonormal representation is associated with the Lovász number $\vartheta(G)$

Definition (Lovász number [Lovász, 1979])

For a graph $G = (V, E)$,

$$\vartheta(G) = \min_{c, U_G} \max_{i \in V} \frac{1}{(c^\top u_i)^2}$$

where the minimization is taken over all orthonormal representations U_G and all unit vectors c

Lovász ϑ kernel

Given a subset of vertices $S \subseteq V$, the Lovász value of the subgraph induced by S is:

$$\vartheta_S(G) = \min_{c} \max_{u_i \in U_{G|S}} \frac{1}{(c^\top u_i)^2}$$

where $U_{G|S} = \{u_i \in U_G : i \in S\}$ and U_G is the set of orthonormal representations of the vertices of G

The Lovász kernel is then defined as:

$$k_\vartheta(G_1, G_2) = \sum_{\substack{S_1 \subseteq V_1}} \sum_{\substack{S_2 \subseteq V_2 \\ |S_1| = |S_2|}} \frac{1}{Z} k(\vartheta_{S_1}(G_1), \vartheta_{S_2}(G_2))$$

where $Z = \binom{n_1}{d}\binom{n_2}{d}$, $d = |S_1| = |S_2|$ and $k(\cdot,\cdot)$ is a base kernel (e.g. linear, gaussian)

Kernel captures global properties since

- $\vartheta_{S_1}(G_1), \vartheta_{S_2}(G_2)$ utilize representations of U_{G_1} and U_{G_2} respectively
- U_{G_1} and U_{G_2} are sets of representations generated for the whole graphs

Lovász ϑ kernel

Computing the Lovász ϑ kernel for a pair of graphs G_1, G_2 is very expensive since it computes:

- the Lovász numbers of the two graphs
- the Lovász value for all subgraphs of the two graphs

Solution: sampling

- Evaluate the Lovász value for a smaller number of subgraphs of size d

Pyramid Match Graph Kernel

Embed all vertices in the d-dimensional vector space $\mathbb{R}^d$ as follows

- compute the eigendecomposition of the adjacency matrix
- use the eigenvectors of the d largest in magnitude eigenvalues

Such embeddings capture **global** properties of graphs
$\hookrightarrow$ **Example**: eigenvector corresponding to greatest eigenvalue contains eigenvector centrality scores of vertices → global property

After embedding: each vertex is a point in the d-dimensional unit hypercube

Then, use pyramid match kernel, a kernel function over unordered feature sets:

- Each feature set is mapped to a multiresolution histogram
- The histogram pyramids are then compared using a weighted histogram intersection computation

Nikolentzos et al. "Matching Node Embeddings for Graph Similarity". In AAAI'17

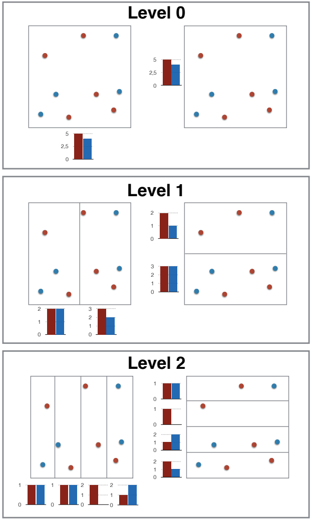
Pyramid Match Kernel

Given a sequence of levels from 0 to L, then at level l the d-dimensional unit hypercube has

- 2^l cells along each dimension
- $D = 2^{dl}$ cells in total

Given a pair of graphs G_1, G_2,

- $H^l_{G_1}$ and $H^l_{G_2}$ denote the histograms of the two graphs at level l
- $H^l_{G_1}(i)$, $H^l_{G_2}(i)$ denote the number of vertices of the two graphs that lie in the i^{th} cell



The number of points in two sets which match at level l is then computed using the histogram intersection function

$$\mathcal{I}(H^l_{G_1}, H^l_{G_2}) = \sum_{i=1}^{D} \min\left(H^l_{G_1}(i), H^l_{G_2}(i)\right)$$

The matches that occur at level l also occur at levels $l+1, \ldots, L$.

Pyramid Match Kernel

We are interested in the number of new matches found at each level

$$\mathcal{I}(H^l_{G_1}, H^l_{G_2}) - \mathcal{I}(H^{l+1}_{G_1}, H^{l+1}_{G_2}) \text{ for } l = 0, \ldots, L-1$$

- These matches are weighted according to the size of that level's cells
- Matches found within smaller cells are weighted less than those made in larger cells
- The weight for level l is set equal to $\frac{1}{2^{L-l}}$

The pyramid match kernel is then defined as follows:

$$k_\Delta(G_1, G_2) = \mathcal{I}(H^L_{G_1}, H^L_{G_2}) + \sum_{l=0}^{L-1} \frac{1}{2^{L-l}} \big(\mathcal{I}(H^l_{G_1}, H^l_{G_2}) - \mathcal{I}(H^{l+1}_{G_1}, H^{l+1}_{G_2})\big)$$

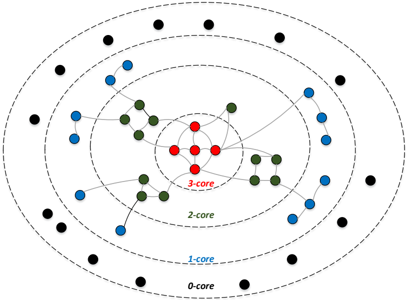
Degeneracy Framework for Graph Comparison

A framework that allows graph similarity algorithms to compare structure in graphs at multiple different scales

<u>k-core</u>

The *k*-core of a graph is defined as a maximal subgraph in which every vertex is connected to at least *k* other vertices within that subgraph

A *k-core decomposition* of a graph consists of finding the set of all *k*-cores



The set of all *k*-cores forms a nested sequence of subgraphs

The degeneracy $\delta^*(G)$ is defined as the maximum k for which graph G contains a non-empty k-core subgraph

Degeneracy Framework for Graph Comparison

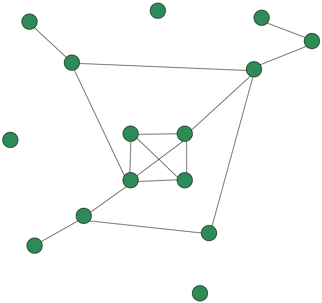
Uses the nested sequence of subgraphs generated by k-core decomposition to capture structure at multiple different scales

- Let $G = (V, E)$ and $G' = (V', E')$ be two graphs
- Let δ^*_{min} be the minimum of the degeneracies of G, G'
- Let $C_0, C_1, \ldots, C_{\delta^*_{min}}$ and $C'_0, C'_1, \ldots, C'_{\delta^*_{min}}$ be the 0-core, 1-core,. . ., δ^*_{min}-core subgraphs of G and G' respectively
- Let k be any kernel for graphs
- The **core variant** of the base kernel k is defined as:

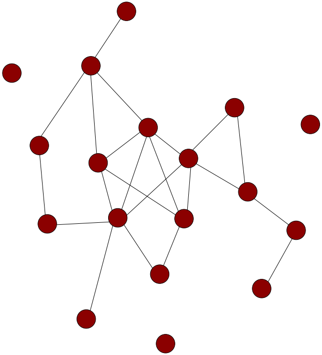
$$k_c(G, G') = k(C_0, C'_0) + k(C_1, C'_1) + \ldots + k(C_{\delta^*_{min}}, C'_{\delta^*_{min}})$$

Nikolentzos et al. "A Degeneracy Framework for Graph Comparison". In IJCAI'18

Example

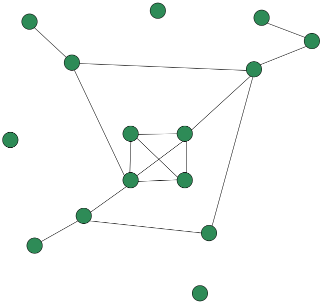


G

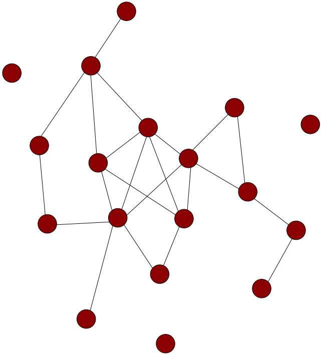


G'

Example



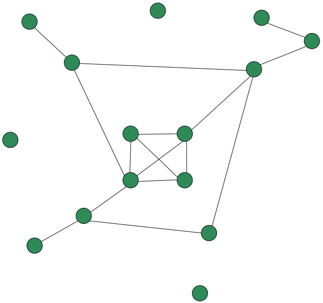
G



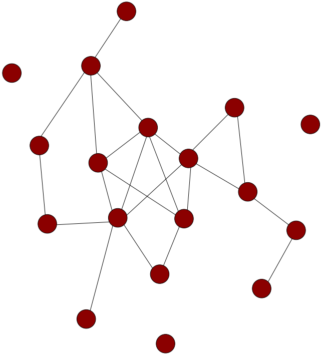
G'

k

Example



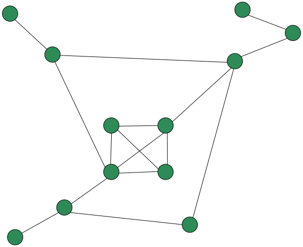
C_0



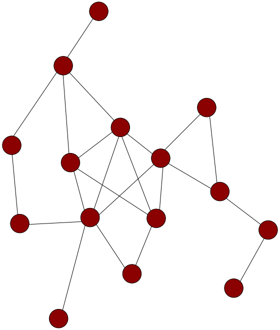
C_0'

$$k_c(G, G') = k(C_0, C_0')$$

Example



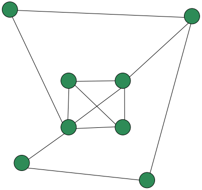
C_1



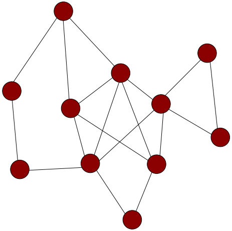
C_1'

$$k_c(G, G') = k(C_0, C_0') + k(C_1, C_1')$$

Example



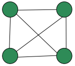
C_2



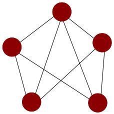
C_2'

$$k_c(G, G') = k(C_0, C_0') + k(C_1, C_1') + k(C_2, C_2')$$

Example



C_3



C'_3

$$k_c(G, G') = k(C_0, C'_0) + k(C_1, C'_1) + k(C_2, C'_2) + k(C_3, C'_3)$$

Dimensionality Reduction View

k-core decomposition can be seen as a method for performing dimensionality reduction on graphs

- each core can be considered as an approximation of the graph
- features of low importance are removed

Problem: For very large graphs, the running time of algorithms with high complexity (e.g. shortest path kernel) is prohibitive

Solution: Use high-order cores