Kernels on structures

Similarity between structured data

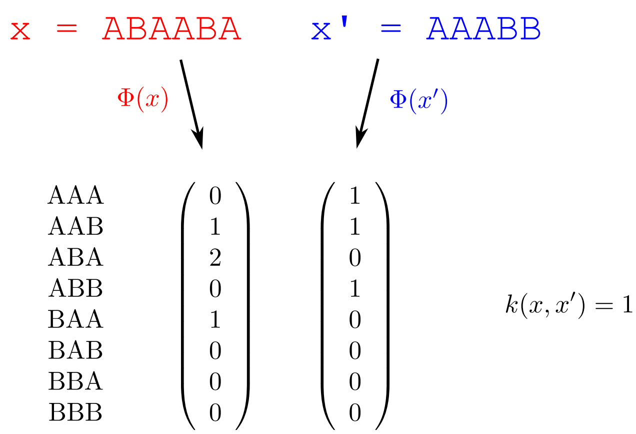
- Kernels allow to generalize notion of dot product (i.e. similarity) to arbitrary (non-vector) spaces
- Decomposition kernels suggest a constructive way to build kernels considering *parts* of objects
- Kernels have been developed for the most general structural representations: sequences, trees, graphs.

Kernels on sequences

Sequences for data representation

- Variable length objects where order of elements matters
- Biological sequences (DNA, RNA)
- Text documents as sequences of words
- Sequences of sensor readings for human activity

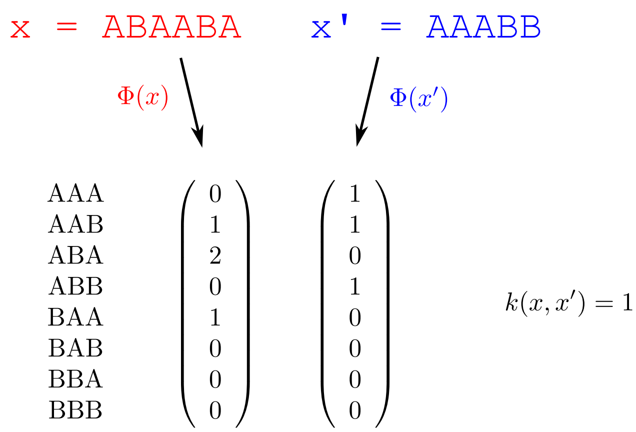
Kernels on sequences



Spectrum kernel

- Feature space is space of all possible k-grams (subsequences)
- An efficient procedure based on suffix trees allows to compute kernel without explicitly building feature maps

Kernels on sequences



Spectrum kernel: problem

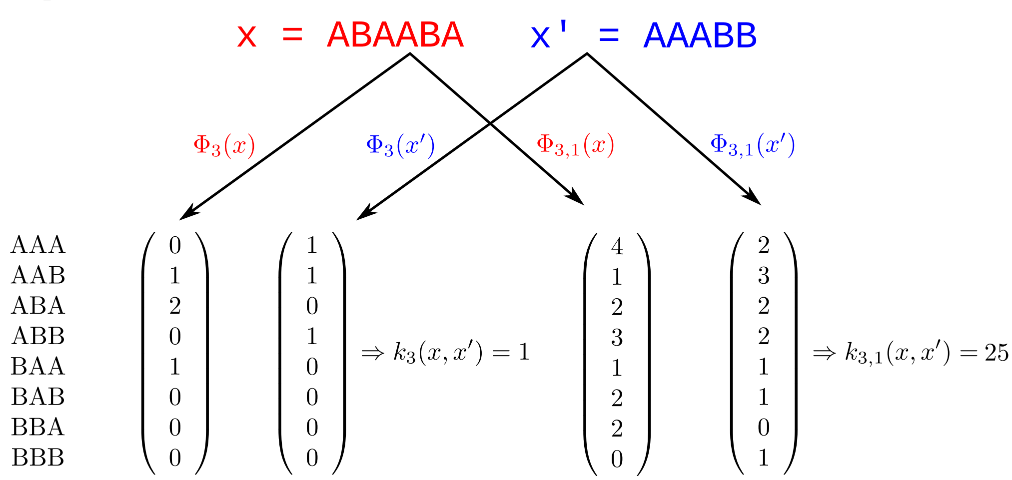
- Feature space representation can be very sparse (many zero features, especially for high k)
- Sparse feature maps tend to produce orthogonal examples (an example is only similar to itself)

Kernels on sequences

Mismatch string kernel

- Allows for approximate matches between k-grams
- Defines a $(k\text{-}m)$-neighbourhood of a k-gram as all k-grams with at most m mismatches to it
- Each k-gram counts as a feature for its entire $(k\text{-}m)$-neighbourhood
- The kernel can be efficiently computed using a $(k\text{-}m)$-mismatch tree (similar to suffix tree)

Kernels on sequences



Mismatch string kernel

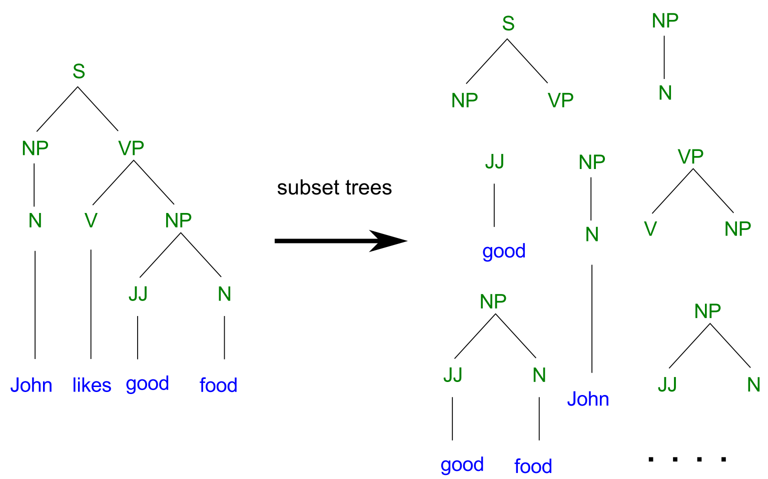
- The feature map is denser than that of the spectrum kernel

Kernels on trees

Trees for data representation

- Objects having hierarchical internal representation
- Taxonomies of concepts in a domain
- E.g. phylogenetic trees representing evolution of organisms
- Parse trees representing syntactic structure of sentences

Kernels on trees



Subset tree kernel

- A subset tree is a subtree having either all or no children of a node (and is not a single node)
- A subset tree kernel corresponds to a feature map of all subset trees
- It is a special type of tree-fragment kernel (many other exist), justified by grammatical considerations (do not break a grammar rule)

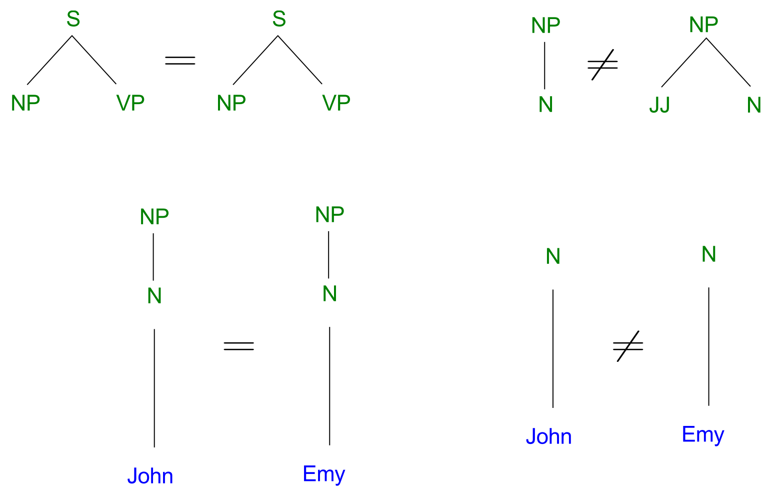
Kernels on trees

Subset tree kernel

$$k(t,t') = \sum_{i=1}^{M} \phi_i(t)\phi_i(t') = \sum_{n_i \in t} \sum_{n'_j \in t'} C(n_i, n'_j)$$

- The subset tree kernel is the product of the subset tree mapping $\Phi(\cdot)$ of the two trees t and t'.
- It can be computed summing the number of common subtrees $C(n_i, n'_j)$ rooted at nodes n_i, n'_j, for all n_i and n'_j

Kernels on trees



Subset tree: node matching

- Two nodes n_i,n'_j *match* if:

  1. they have the same label
  2. they have the same number of children
  3. each child of n_i has the same label of the corresponding child of n'_j

Kernels on trees

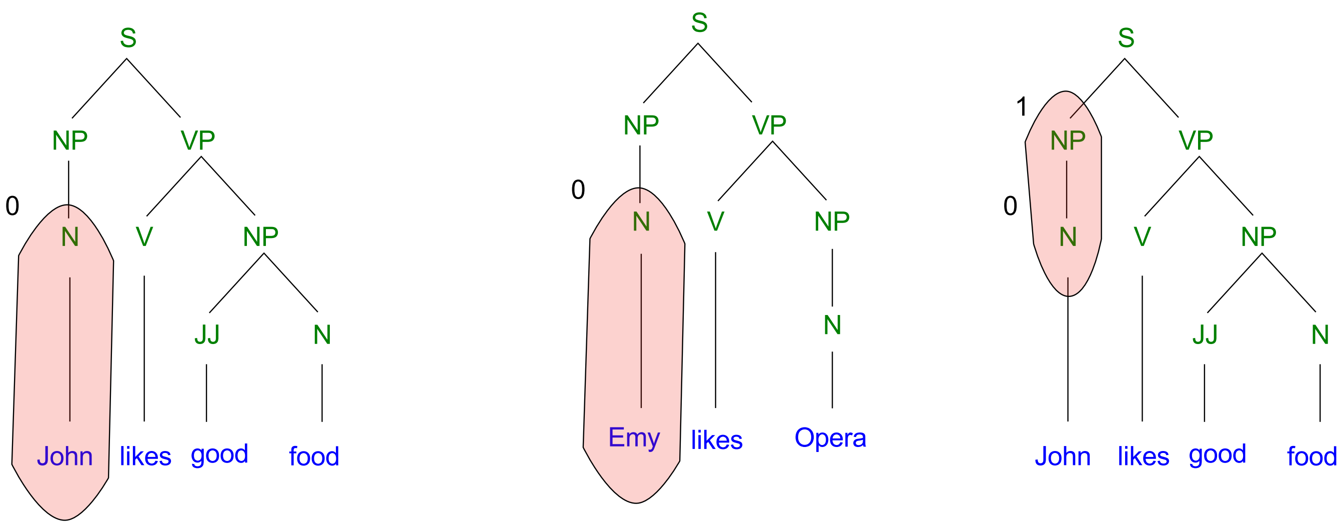
Recursive procedure for $C(n_i, n'_j)$

- If n_i and n'_j don't match $C(n_i, n'_j) = 0$.
- if n_i and n'_j match, and they are both pre-terminals (parents of leaves) $C(n_i, n'_j) = 1$.
- Else

$$C(n_i, n'_j) = \prod_{j=1}^{nc(n_i)} (1 + C(ch(n_i, j), ch(n'_j, j)))$$

  where $nc(n_i)$ is the number of children of n_i (equal to that of n'_j for the definition of match) and $ch(n_i, j)$ is the j^{th} child of n_i.

Kernels on trees



Kernels on trees

Dominant diagonal

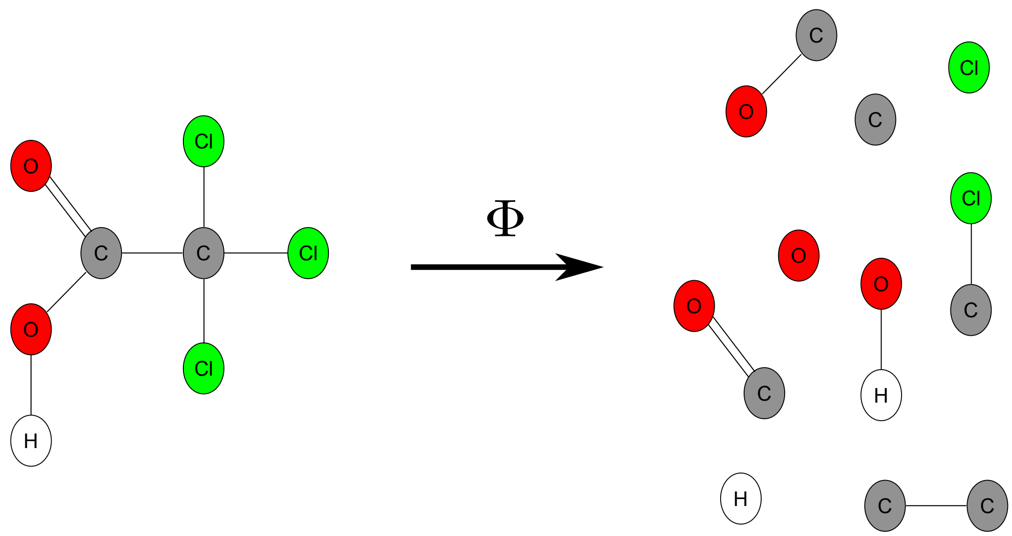
- The kernel value strongly depends on the size of the tree (normalize!!)
- It is difficult that very large portion of trees are identical in different examples
- Similary of example to itself tend to be orders of magnitude higher than to any other example (*dominant diagonal* problem)
- One solution consists of downweighting larger subtrees:
  - simply replace 1 by $0 \leq \lambda \leq 1$ in previous procedure

Kernels on graphs

Graphs for data representation

- graphs are a powerful formalism allowing to represent data with arbitrary structures
- Chemical molecules are commonly represented as graphs made of atoms and bonds
- Networked data (e.g. a web site, the Internet) can be naturally encoded as graphs

Kernels on graphs



Bag of subgraphs

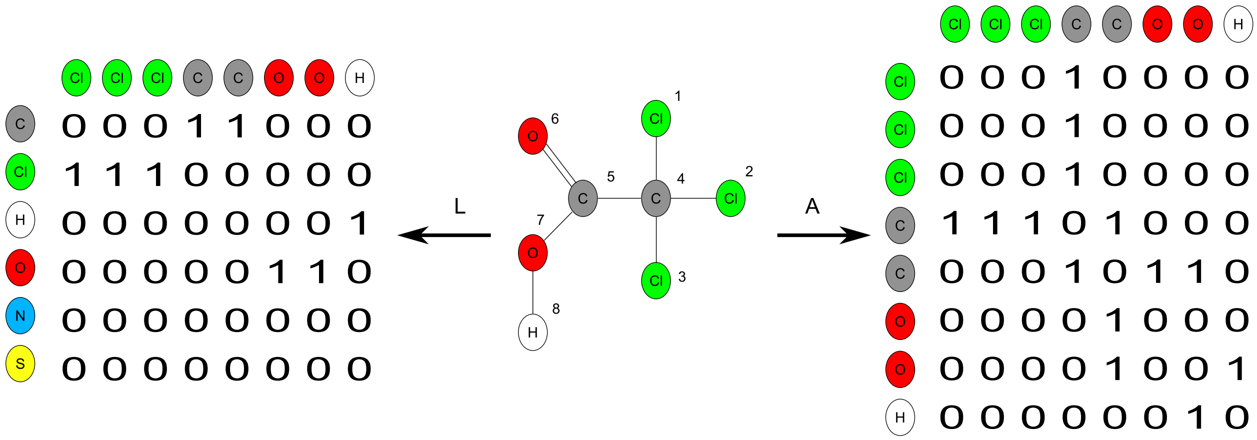
- One feature for all possible subgraphs up to a certain size (2 in figure)
- Feature value is frequency of occurrence of subgraph
- PB of graph isomorphisms (ok for small subgraphs)

Kernels on graphs

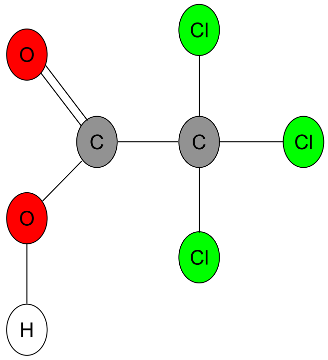
Main definitions

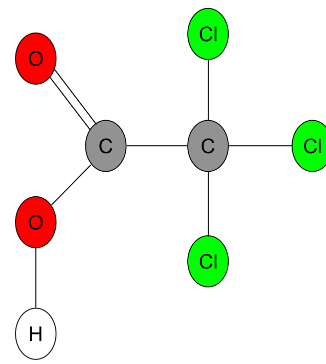
- A graph $G = (\mathcal{V}, \mathcal{E})$ is a finite set of vertices (or nodes) $\mathcal{V}$ and edges $\mathcal{E} \in \mathcal{V} \times \mathcal{V}$
- A (node)labelled graph is a graph whose nodes are labelled with symbols $l(v_j) = \ell_i$ from $\mathcal{L}$.
- A (node)labelled graph can be also encoded with:
  - A square *adjacency* matrix A such that $A_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$ and 0 otherwise
  - A (node)label matrix L such that $L_{ij} = 1$ if $l(v_j) = \ell_i$ and zero otherwise

Kernels on graphs: definitions



Kernels on graphs





Walk kernels

- A *walk* in a graph is a sequence of nodes $\{v_1, \ldots, v_{n+1}\}$ such that $(v_i, v_{i+1}) \in \mathcal{E}$ for all i
- The length of a walk is the number of its edges
- The set of all walks of length n is written as $W_n(G)$

Kernels on graphs

Walk kernels

- A possible walk kernels compares graphs considering the set of walks starting and ending with the same labels ℓ_{start},ℓ_{end}.

- This corresponds to having a feature for all possible label pairs ℓ_i, ℓ_j with value:

$$\begin{aligned}\phi_{\ell_i,\ell_j}(G) &= \sum_{n=1}^{\infty} \lambda_n |\{(v_1,\ldots,v_{n+1}) \in W_n(G) \\ &\qquad : l(v_1) = \ell_i \wedge l(v_{n+1}) = \ell_j\}|\end{aligned}$$

- i.e. a weighted (by $\lambda_n \geq 0$ for all n) sum of the number of walks starting with label ℓ_i and ending with label ℓ_j

Kernels on graphs

Walk kernels

- The n^{th} power of the adjacency matrix, A^n, computes the number of walks of length n between any two nodes.
- I.e. $(A^n)_{ij}$ is the number of walks of length n between v_i and v_j
- This can be used to efficiently compute the overall feature map as:

$$\phi_{\ell_i,\ell_j}(G) = \left(\sum_{n=1}^{\infty} \lambda_n L A^n L^T\right)_{\ell_i,\ell_j}$$

Kernels on graphs
Walk kernels

- The corresponding kernel is:

$$k(G,G') = \langle L\left(\sum_{i=1}^{\infty} \lambda_i A^i\right) L^T, L'\left(\sum_{j=1}^{\infty} \lambda_j A'^j\right) L'^T\rangle$$

  where the dot product between two matrices M, M' is defined as:

$$\langle M, M'\rangle = \sum_{i,j} M_{ij} M'_{ij}.$$

Exponential graph kernel

- An example of walk kernel is:

$$k_{exp}(G,G') = \langle L e^{\beta A} L^T, L' e^{\beta A'} L'^T\rangle$$

  where $\beta \in \mathbb{R}$ is a parameter

Kernels on graphs

Weistfeiler-Lehman graph kernel

- Efficient graph kernel for large graphs
- Relies on (approximation of) Weistfeiler-Lehman test of graph isomorphism
- Defines a family of graph kernels

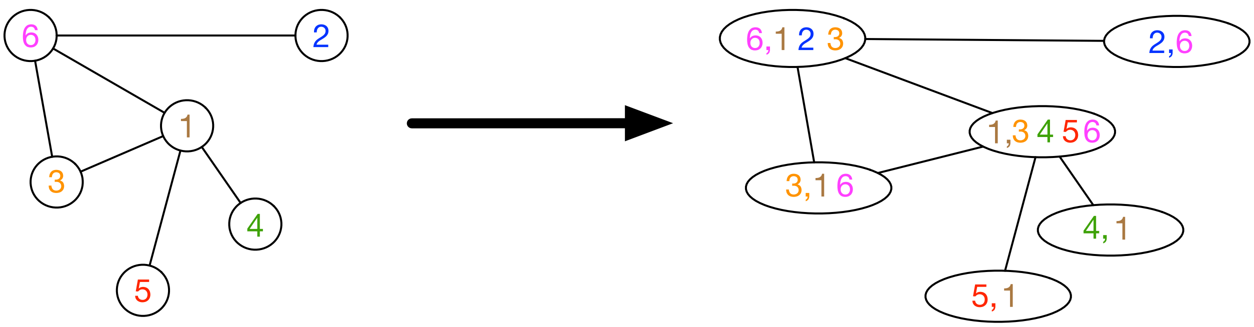
Kernels on graphs

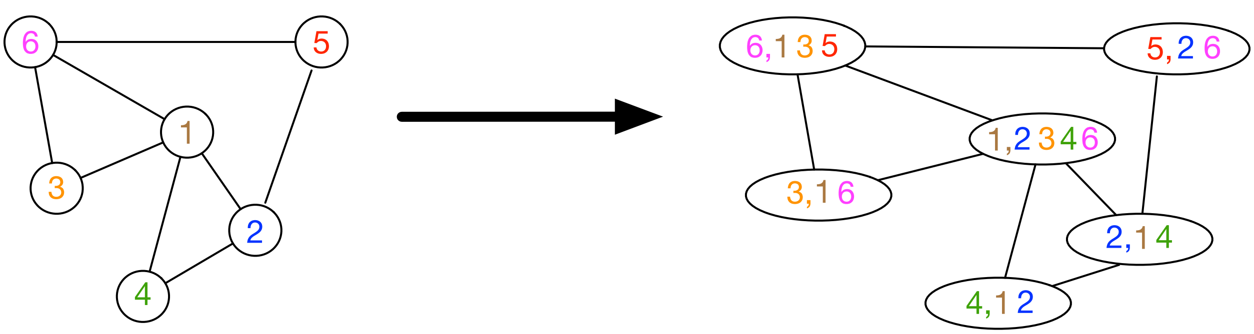
Weistfeiler-Lehman (WL) isomorphism test

Given $G = (\mathcal{V}, \mathcal{E})$ and $G' = (\mathcal{V}', \mathcal{E}')$, with $n = |\mathcal{V}| = |\mathcal{V}'|$. Let $L(G) = \{l(v)|v \in \mathcal{V}\}$ be the set of labels in G, and let $L(G) == L(G')$. Let $label(s)$ be a function assigning a unique label to a string.

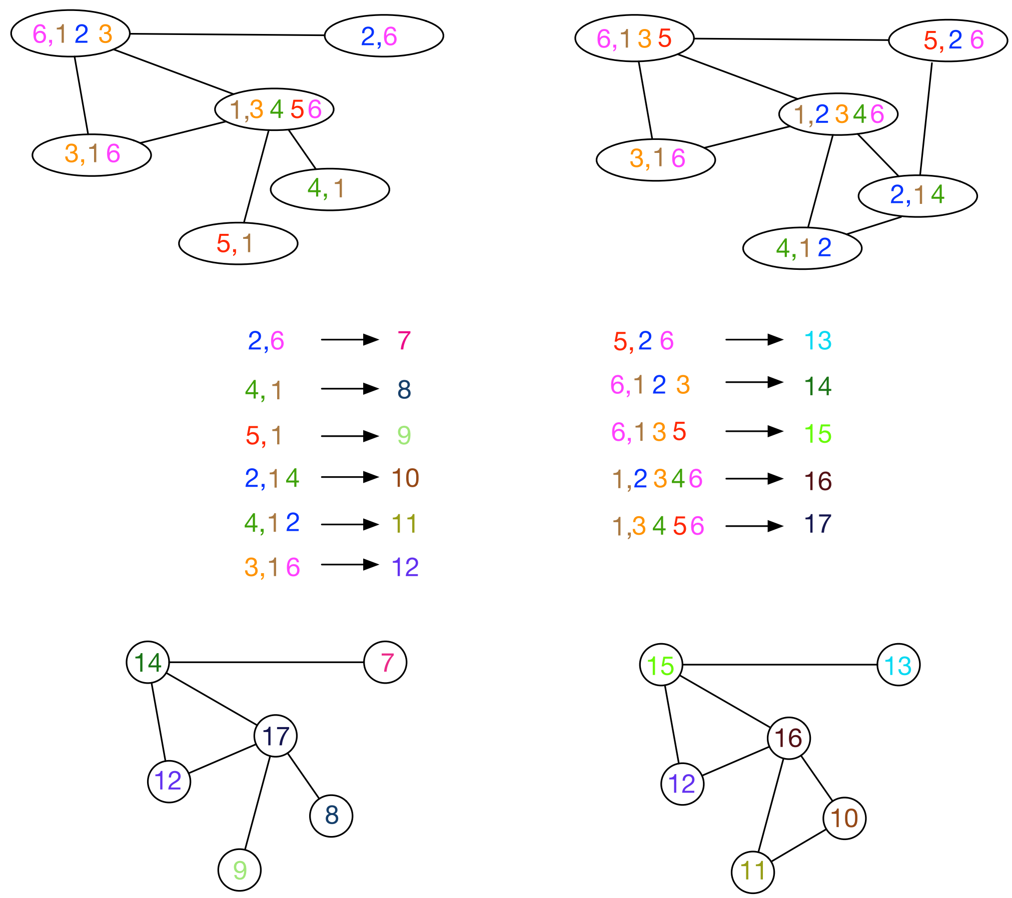
- Set $l_0(v) = l(v)$ for all v.
- For $i \in [1, n-1]$
  1. For each node v in G and G'
  2. Let $M_i(v) = \{l_{i-1}(u)|u \in neigh(v)\}$
  3. Concatenate the sorted labels of $M_i(v)$ into $s_i(v)$
  4. Let $l_i(v) = label(l_{i-1}(v) \circ s_i(v))$ ($\circ$ is concatenation)
  5. If $L_i(G) \neq L_i(G')$
  6. Return **Fail**
- Return **Pass**

WL isomorphism test: string determination





WL isomorphism test: relabeling



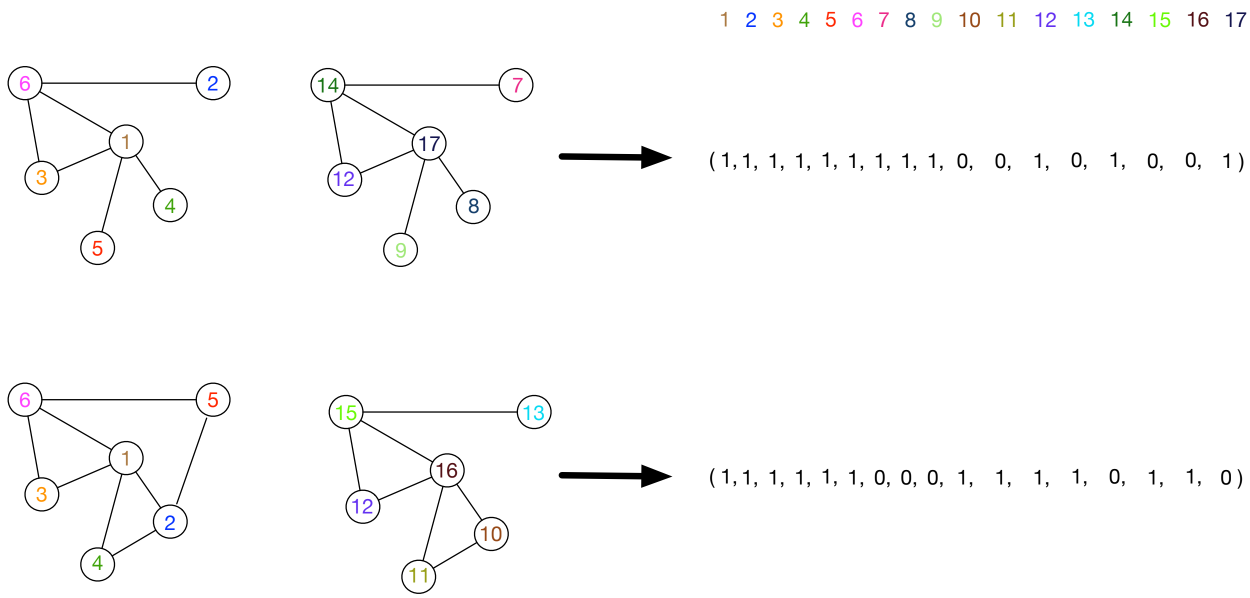
Kernels on graphs

Weistfeiler-Lehman graph kernel

- Let $\{G_0, G_1, \ldots, G_h\} = \{(\mathcal{V}, \mathcal{E}, l_0), (\mathcal{V}, \mathcal{E}, l_1), \ldots, (\mathcal{V}, \mathcal{E}, l_h)\}$ be a sequence of graphs made from G, where l_i is the node labeling of the i-th WL iteration.
- Let $k : G \times G' \to \mathbb{R}$ be any kernel on graphs.
- The Weistfeiler-Lehman graph kernel is defined as:

$$k^h_{WL}(G, G') = \sum_{i=0}^{h} k(G_i, G'_i)$$

Example: WL subtree kernel



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