An Introduction to Graph Kernels

Karsten Borgwardt and Oliver Stegle

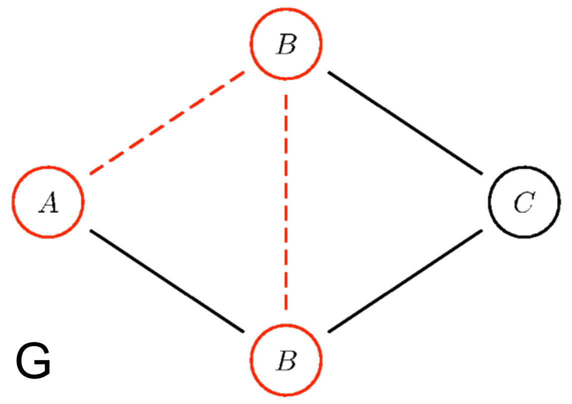
Machine Learning and
Computational Biology Research Group,
Max Planck Institute for Biological Cybernetics and
Max Planck Institute for Developmental Biology, Tübingen

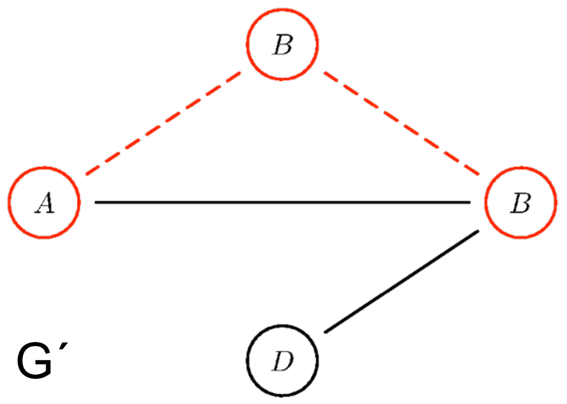
Graph Comparison

Definition 1 (Graph Comparison Problem) *Given two graphs G and G' 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 $s(G, G')$ quantifies the similarity (or dissimilarity) of G und G'.





Applications of Graph Comparison

- Function prediction of chemical compounds
- Structural comparison and function prediction of protein structures
- Comparison of social networks
- Analysis of semantic structures in Natural Language Processing
- Comparison of UML diagrams

Graph Isomorphism

Graph isomorphism

- Find a mapping f of the vertices of G_1 to the vertices of G_2 such that G_1 and G_2 are identical; i.e. (x,y) is an edge of G_1 iff (f(x),f(y)) is an edge of G_2. Then f is an isomorphism, and G_1 and G_2 are called isomorphic
- No polynomial-time algorithm is known for graph isomorphism
- Neither is it known to be NP-complete

Subgraph isomorphism

- Subgraph isomorphism asks if there is a subset of edges and vertices of G_1 that is isomorphic to a smaller graph G_2
- Subgraph isomorphism is NP-complete

Subgraph Isomorphism

NP-completeness

- A decision problem C is NP-complete iff
- C is in NP
- C is NP-hard, i.e. every other problem in NP is reducible to it.

Problems for the practitioner

- Excessive runtime in worst case
- Runtime may grow exponentially with the number of nodes
- For larger graphs with many nodes and for large datasets of graphs, this is an enormous problem

Graph Edit Distances

Principle

- Count operations that are necessary to transform G_1 into G_2
- Assign costs to different types of operations (edge/node insertion/deletion, modification of labels)

Advantages

- Captures partial similarities between graphs
- Allows for noise in the nodes, edges and their labels
- Flexible way of assigning costs to different operations

Disadvantages

- Contains subgraph isomorphism check as one intermediate step
- Choosing cost function for different operations is difficult

Topological Descriptors

Principle

- Map each graph to a feature vector
- Use distances and metrics on vectors for learning on graphs

Advantages

- Reuses known and efficient tools for feature vectors

Disadvantages

- Efficiency comes at a price: feature vector transformation leads to loss of topological information (or includes subgraph isomorphism as one step)

Polynomial Alternatives

Wanted

- Polynomial-time similarity measure for graphs

Graph kernels

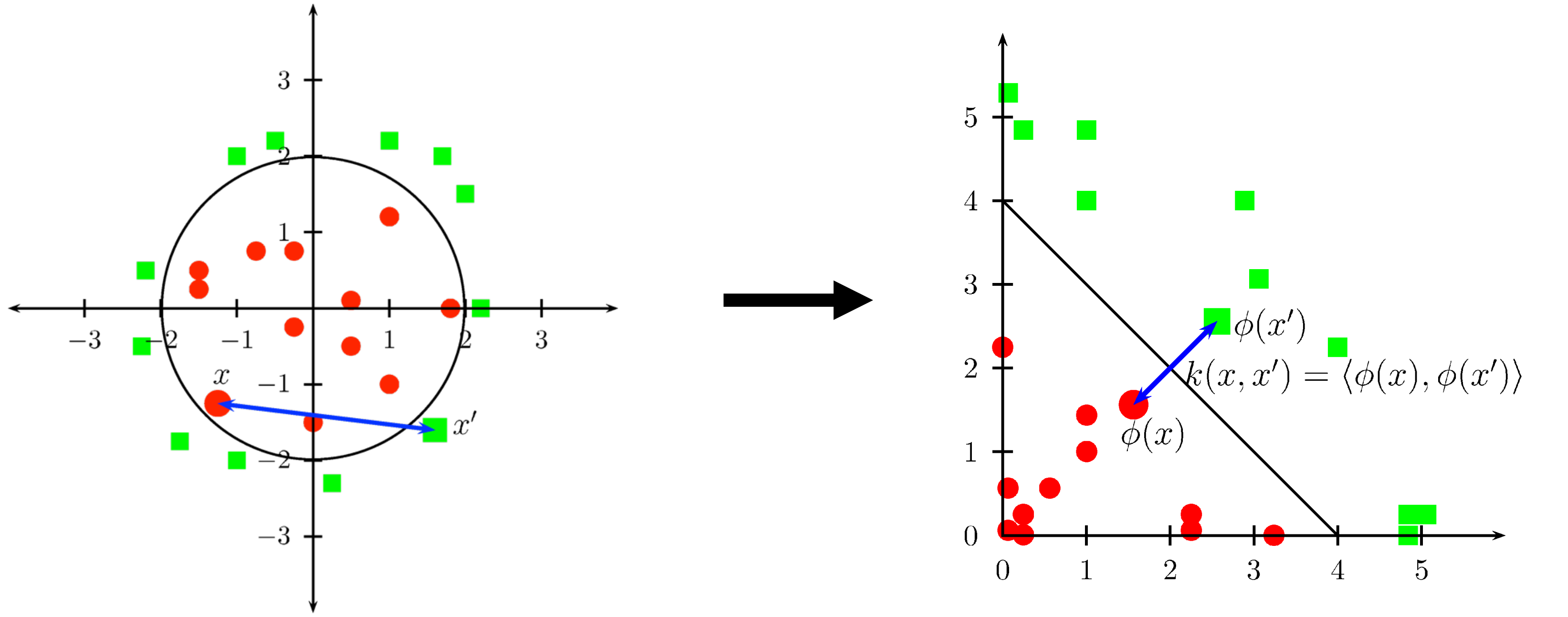
- Compare substructures of graphs that are computable in polynomial time.

Criteria for a good graph kernel

- Expressive
- Efficient to compute
- Positive definite
- Applicable to wide range of graphs

What is a Kernel? (Schölkopf ,1997)

- Map two objects x and x' via mapping ϕ into feature space $\mathcal{H}$.
- Measure their similarity in $\mathcal{H}$ as $\langle \phi(x), \phi(x') \rangle$.
- **Kernel Trick**: Compute inner product in $\mathcal{H}$ as kernel in input space $k(x, x') = \langle \phi(x), \phi(x') \rangle$.



What is a Graph Kernel?

Instance of R-convolution kernels by Haussler (1999)

- R-convolution kernels compare decompositions of two structured objects

$$k_{convolution}(x, x') = \sum_{(x_d, x) \in \mathrm{R}} \sum_{(x'_d, x') \in \mathrm{R}} k_{parts}(x_d, x'_d)$$

- Graph kernels are convolution kernels on pairs of graphs
  (**not** pairs of nodes, though this is a common use in the literature)
- A new decomposition relation R results in a new graph kernel.
- A graph kernel makes the whole family of kernel methods applicable to graphs (e.g. for classification, clustering, feature selection, two-sample tests).

Hardness Results (Gaertner, Flach, Wrobel, COLT 2003)

Link to graph isomorphism

- Let k(G,G') = $\langle \phi(G), \phi(G') \rangle$ be a graph kernel.
- If ϕ is injective, k is called a complete graph kernel.

Proposition 1 *Computing any complete graph kernel is at least as hard as deciding whether two graphs are isomorphic.*

Proof As ϕ is injective,

$$\begin{aligned}&\sqrt{k(G,G) - 2k(G,G') + k(G',G')}\\ &= \sqrt{\langle \phi(G) - \phi(G'), \phi(G) - \phi(G') \rangle}\\ &= \|\phi(G) - \phi(G')\| = 0\end{aligned}$$

if and only if G is isomorphic to G'. ■

Random Walks (Kashima et al., ICML 2003, Gaertner et al., COLT 2003)

Principle

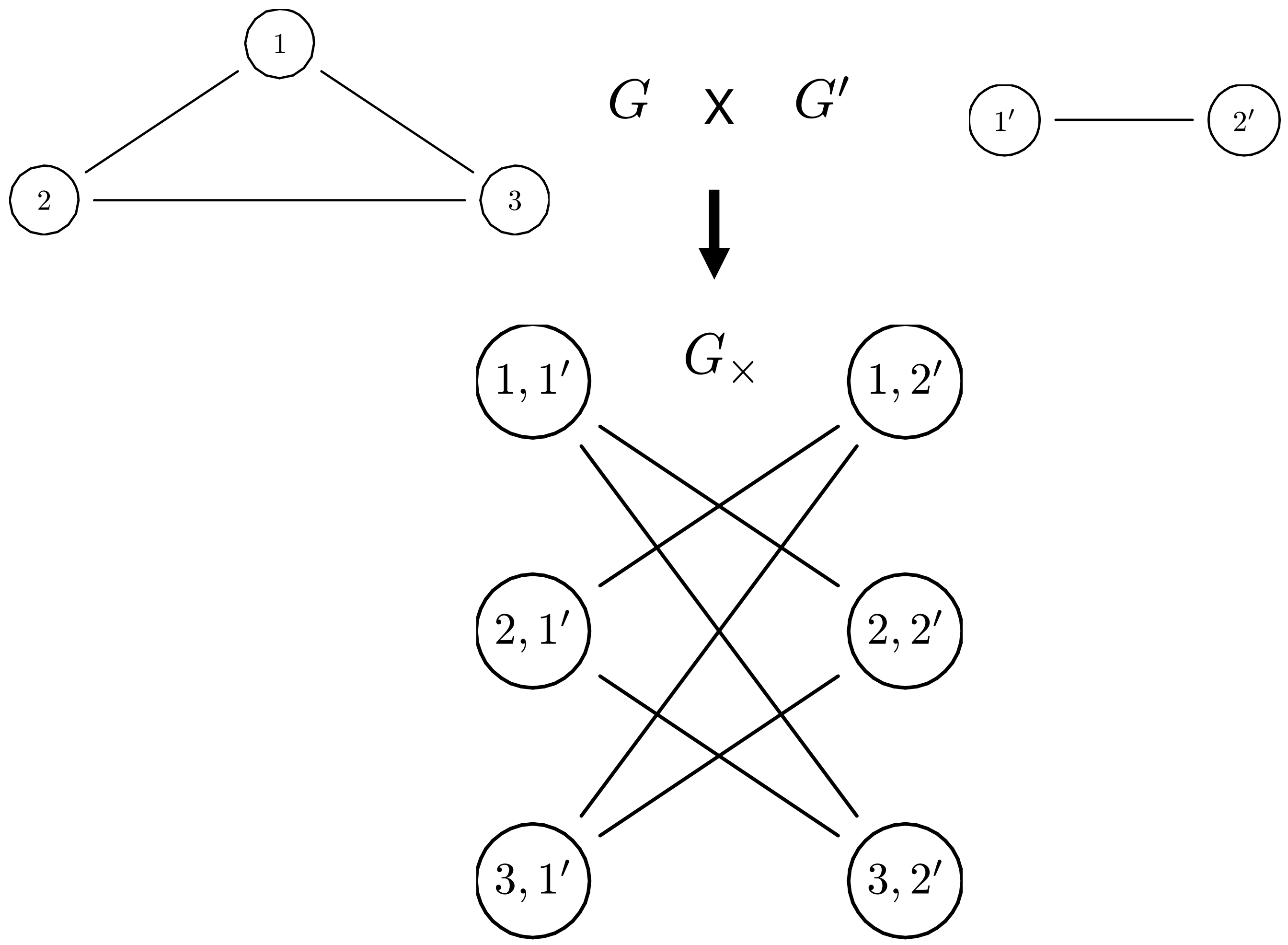
- Count common walks in two input graphs G and G'
- Walks are sequences of nodes that allow repetitions of nodes

Elegant computation

- Walks of length *k* can be computed by looking at the *k*-th power of the adjacency matrix
- Construct direct product graph of G and G'
- Count walks in this product graph $G_x=(V_x,E_x)$
- Each walk in the product graph corresponds to one walk in G and G'

$$k_\times(G,G') = \sum_{i,j=1}^{|V_\times|} [\sum_{k=0}^{\infty} \lambda^k A_\times^k]_{ij}$$

Random Walks – Direct Product Graph



Setbacks of Random Walk Kernels

Disadvantages

- Runtime problems
- Tottering
- 'Halting'

Potential solutions

- Fast computation of random walk graph kernels (Vishwanathan et al., NIPS 2006)
- Preventing tottering and label enrichment (Mahe et al., ICML 2004)
- Graph kernels based on shortest paths (B. and Kriegel, ICDM 2005)

Fast Random Walk Kernels

(Vishwanathan et al., NIPS 2006)

Direct computation: O(n^6)

$$k_\times(G,G') = \sum_{i,j=1}^{|V_\times|} [\sum_{k=0}^{\infty} \lambda^k A_\times^k]_{ij} = \mathbf{e}^\top \underbrace{(\mathbf{1} - \lambda A_\times)^{-1}}_{n^2 \times n^2} \mathbf{e}$$

Solution

- Cast computation of random walk kernel as Sylvester Equation
- These can be solved in O(n^3)

Vec-Operator and Kronecker Products

Vec-Operator

- vec flattens an n x n matrix A into an n^2 x 1 vector vec(A).
- It stacks the columns of the matrix on top of each other, from left to right.

Kronecker Product

- Product of two matrices A and B
- Each element of A is multiplied with the full matrix B:

$$A \otimes B := \begin{bmatrix} A_{1,1}B & A_{1,2}B & \dots & A_{1,n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{n,1}B & A_{n,2}B & \dots & A_{n,m}B \end{bmatrix}$$

Sylvester Equations

- Equations of the form

$$X = SXT + X_0$$

- Given three $n \times n$ matrices S, T, and X_0.
- One wants to solve for X.
- Solvable in $O(n^3)$.
- It is possible to turn Sylvester equations into graph kernels.

From Sylvester Equations to Random Walk Kernels

- First, the Sylvester equation is rewritten as

$$\operatorname{vec}(X) = \operatorname{vec}(SXT) + \operatorname{vec}(X_0)$$

- One then exploits the well-known fact

$$\operatorname{vec}(SXT) = (T^\top \otimes S)\operatorname{vec}(X)$$

  to rewrite the above question as

$$(\mathbf{I} - T^\top \otimes S)\operatorname{vec}(X) = \operatorname{vec}(X_0).$$

- Now one has to solve

$$\operatorname{vec}(X) = (\mathbf{I} - T^\top \otimes S)^{-1}\operatorname{vec}(X_0).$$

- One multiplies both sides by $\operatorname{vec}(X_0)^\top$

$$\operatorname{vec}(X_0)^\top\operatorname{vec}(X) = \operatorname{vec}(X_0)^\top(\mathbf{I} - T^\top \otimes S)^{-1}\operatorname{vec}(X_0).$$

From Sylvester Equations to Random Walk Kernels

- In

$$\operatorname{vec}(X_0)^\top \operatorname{vec}(X) = \operatorname{vec}(X_0)^\top (\mathbf{I} - T^\top \otimes S)^{-1} \operatorname{vec}(X_0)$$

one substitutes

$$\begin{aligned} X_0 &= \mathbf{e}\,\mathbf{e}^\top \\ T &= \lambda A(G)^\top \\ S &= A(G') \end{aligned}$$

and obtain

$$\begin{aligned} \mathbf{e}^\top \operatorname{vec}(X) &= \mathbf{e}^\top (\mathbf{I} - \lambda A(G) \otimes A(G'))^{-1}\,\mathbf{e} \\ &= \mathbf{e}^\top (\mathbf{I} - \lambda A_\times)^{-1}\,\mathbf{e}\,. \end{aligned}$$

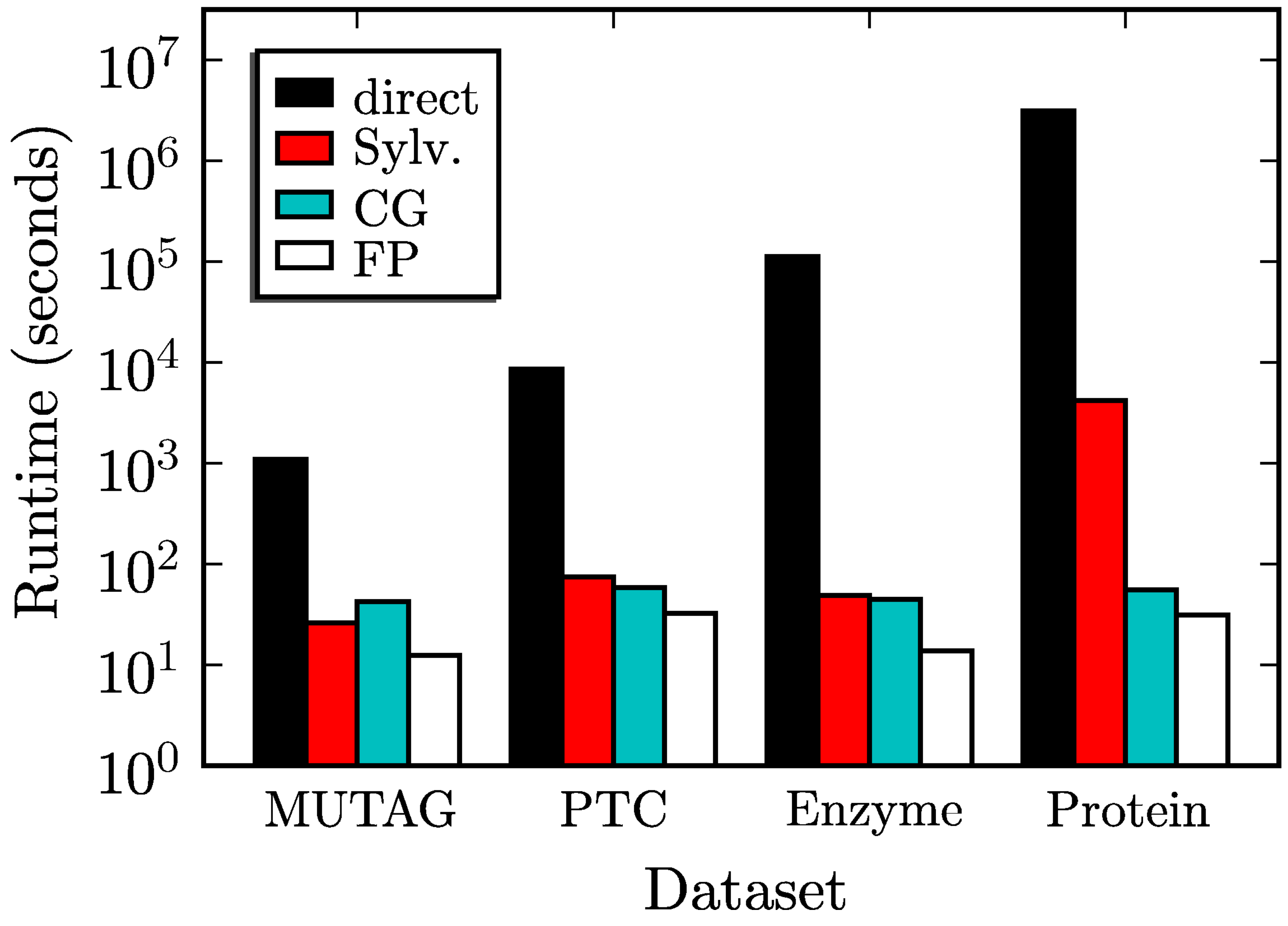
Further Speed-ups for Sparse Graphs

- Vec-Trick
  - Let S and T be sparse.
  - We can efficiently compute $(T^\top \otimes S) \operatorname{vec} X$ for each X as $\operatorname{vec}(SXT)$.
  - How to exploit this fact?
- Fix-Point Iteration (FP)
  - Determine a fix point (Kashima et. al, 2003):

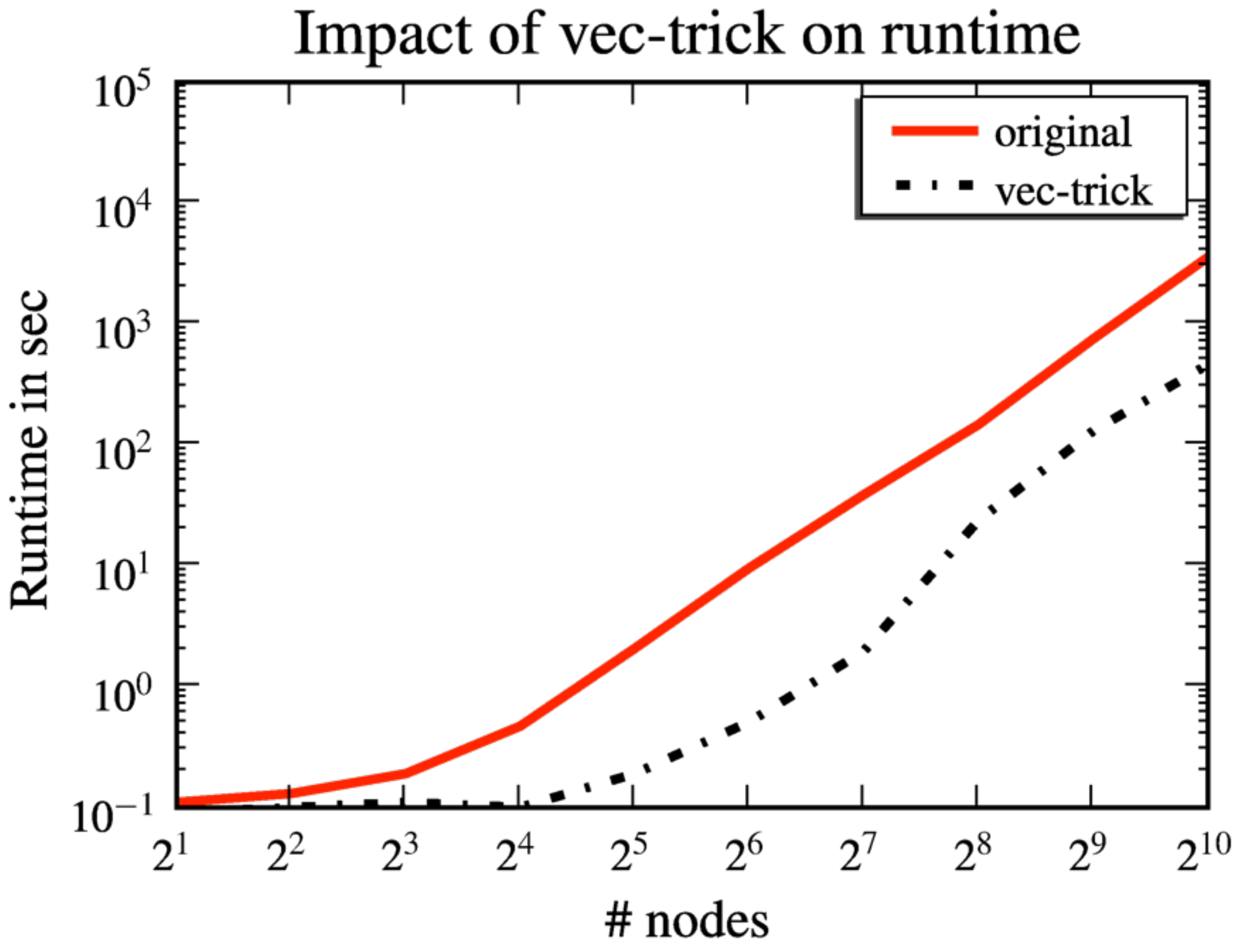
$$\operatorname{vec} X_{k+1} = \mathbf{e} + (T^\top \otimes S) \operatorname{vec} X_k$$

- Conjugate Gradient (GC)
  - Use conjugate gradient solver to compute X in $(\mathbf{I} - T^\top \otimes S) \operatorname{vec} X = \mathbf{e}$.
  - Requires computation of $(T^\top \otimes S) \operatorname{vec} X_k$ for the residuum R in each step.

Impact on Runtime for Kernel Computation



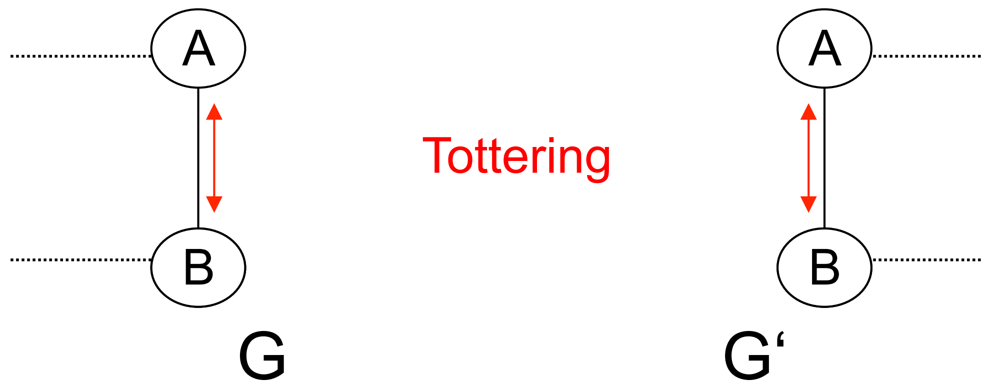
Impact of vec-trick



Tottering (Mahe et al., ICML 2004)

Phenomenon of tottering

- Walks allow for repetitions of nodes
- A walk can visit the same cycle of nodes all over again
- Kernel measures similarity in terms of common walks
- Hence a small structural similarity can cause a huge kernel value



Preventing Tottering

- Explicitly forbid tottering between 2 nodes, that is any walk $(v_1, \ldots, v_l)$ such that $v_i = v_{i+2}$ for any $i \in \{1, \ldots, l-2\}$.
- Special transformation of each of the input graphs $G = (V, E)$ allows for this modification:
  - Create a new graph G_T with $V_T = V \cup E$ and $E_T = \{(v, (v, t)) | v \in V, (v, t) \in E\} \cup \{((u, v), (v, t)) | (u, v), (v, t) \in E, u \neq t\}$
  - The node set of G_T is the set of vertices and edges of G
  - In G_T, there are directed edges between each node from G and each adjacent edge, and between edges from G that share exactly one node (that is target node in one edge, and source node in the other)

Preventing Tottering

- Walks in G_T correspond to walks in G, but it is not possible to totter between 2 nodes

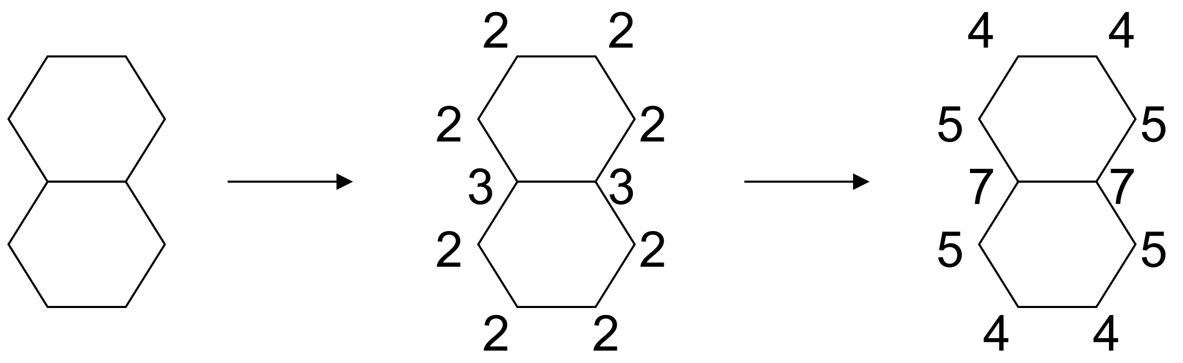
  Limitations

  – Modification increases graph size from $O(n)$ to $O(n^2)$ with adverse effects on kernel computation runtime

  – Experimental evidence does not show a uniform improvement of classification accuracy

Label Enrichment: Morgan Index (1965)

- Size of product graph affects runtime of kernel computation
- The more node labels, the smaller the product graph
- Trick: Introduce new artificial node labels
- Topological descriptors of nodes are natural extra labels
- For instance, the Morgan Index that counts k-th order neighbours of a node:



Original graph

1st order Morgan Index

2nd order Morgan Index

Replacing Walks by Paths

Underlying idea

- Paths do not suffer from tottering
- Define a graph kernel based on paths

Setbacks

- All paths are NP-hard to compute
- Longest paths are NP-hard to compute
- But shortest paths are computable in $O(n^3)$!

Pitfall

- Number of shortest paths in a graph may be exponential in the number of nodes (in pathological cases)

Workaround

- Shortest paths need not be unique, but shortest path distances are
- Define graph kernel based on shortest path distances

Shortest-Path Kernel on Graphs (B. and Kriegel, ICDM 2005)

- Compute all-pairs-shortest-paths for G and G' via Floyd-Warshall
- Define a kernel by comparing all pairs of shortest path lengths from G and G':

$$k(G, G') = \sum_{v_i, v_j \in G} \sum_{v'_k, v'_l \in G'} k_{length}(d(v_i, v_j), d(v'_k, v'_l))$$

- $d(v_i, v_j)$ is the length of the shortest path between node v_i and v_j
- k_{length} is a kernel that compares the lengths of two shortest paths, for instance,
  - a linear kernel $k(d(v_i, v_j), d(v'_k, v'_l)) = d(v_i, v_j) * d(v'_k, v'_l)$, or
  - a delta kernel $k(d(v_i, v_j), d(v'_k, v'_l)) = \begin{cases} 1 & \text{if } d(v_i, v_j) = d(v'_k, v'_l) \\ 0 & \text{otherwise} \end{cases}$

Link to Wiener Index (Wiener, 1947)

Definition 1 (Wiener Index) *Let $G = (V, E)$ be a graph. Then the Wiener Index $W(G)$ of G is defined as*

$$W(G) = \sum_{v_i \in G} \sum_{v_j \in G} d(v_i, v_j), \tag{1}$$

where $d(v_i, v_j)$ is defined as the length of the shortest path between nodes v_i and v_j from G.

Link to Wiener Index

- Compute the product of the Wiener Indices $W(G)$ and $W(G')$ as

$$\begin{aligned}
W(G) * W(G') &= (\sum_{v_i \in G} \sum_{v_j \in G} d(v_i, v_j))(\sum_{v'_k \in G'} \sum_{v'_l \in G'} d(v'_k, v'_l)) \\
&= \sum_{v_i \in G} \sum_{v_j \in G} \sum_{v'_k \in G'} \sum_{v'_l \in G'} d(v_i, v_j) d(v'_k, v'_l) \\
&= \sum_{v_i, v_j \in G} \sum_{v'_k, v'_l \in G'} k_{linear}(d(v_i, v_j), d(v'_k, v'_l)) \\
&= k_{shortest\ path}(G, G')
\end{aligned}$$

Properties of Shortest-Path Kernel

Advantages

- No tottering, better accuracy on classification benchmarks
- Runtime is in O(n^4) and includes
  - Computing all-pairs-shortest-paths for G and for G‘: O(n^3)
  - Comparing all pairs of shortest paths from G and G‘: O(n^4)
- Empirically faster than (fast) random walk kernels (probably due to graph size)

Disadvantages

- O(n^4) too slow for large graphs
- Dense matrix representation for connected graphs, may lead to memory problems on large graphs

Optimal Assignment Kernel (Froehlich et al., ICML 2005)

- G and G' are graphs
- $\{x_1, \ldots, x_{|G|}\}$ are substructures of G, e.g. nodes
- $\{y_1, \ldots, y_{|G'|}\}$ are substructures of G', e.g. nodes
- k_1 is a non-negative kernel comparing substructures
- π is a permutation of the natural numbers $\{1, \ldots, \min(|G|, |G'|)\}$
- Then
  $$k_A(G, G') := \begin{cases} \max_\pi \sum_{i=1}^{|G|} k_1(x_i, y_{\pi(i)}), & \text{if } |G'| \geq |G| \\ \max_\pi \sum_{j=1}^{|G'|} k_1(x_{\pi(j)}, y_j), & \text{otherwise} \end{cases}$$
  is the **optimal assignment kernel** (Froehlich et al, ICML 2005)
- Not positive definite in general (Vert, 2008)

Weighted Decomposition Kernel (Menchetti et al., ICML 2005)

- $G = (V, E)$ and $G' = (V', E')$ are graphs
- Idea is to define two different types of substructures
- s is a subgraph of G called a **selector**, with associated kernel δ
- $z = (z_1, ..., z_D)$ is a tuple of subgraphs of G called the **contexts of occurrence** of s in x, with associated kernel κ
- Then

$$k(G, G') := \sum_{(s,z) \in R^{-1}(G), (s',z') \in R^{-1}(G')} \delta(s, s') \sum_{d=1}^{D} \kappa(z_d, z'_d) \qquad (1)$$

  is the **weighted decomposition kernel** (Menchetti et al., ICML 2005)

- Example: s can be a node and z the neighbourhood of s in G

Edit-Distance Kernel (Neuhaus and Bunke, 2006)

Principle

- Tries to combine the power of graph kernels and edit distances
- Random walk kernel that uses a modified product graph:
- It only contains pairs of nodes that were matched by a graph edit-distance beforehand

Advantage

- Edit-distance kernels outperform random walks and edit distances in their experimental evaluation

Disadvantage

- These edit-distance kernels are not positive definite in general

Subtree Kernel (Ramon and Gaertner, 2004)

Principle

- Compare subtree-like patterns in two graphs
- Subtree-like pattern is a subtree that allows for repetitions of nodes and edges (similar to walk versus path)
- For all pairs of nodes v from G and u from G‘:
  - Compare u and v via a kernel function
  - Recursively compare all sets of neighbours of u and v via a kernel function

Advantages

- Richer representation of graph structure than walk-based approach

Disadvantages

- Runtime grows exponentially with the recursion depth of the subtree-like patterns

Cyclic Pattern Kernel (Horvath et al., KDD 2004)

Principle

- Compare simple cycles in two graphs (paths where start node equals end node)
- Number of simple cycles is exponential in the number n of vertices in worst case
- Define canonical string representation of each simple cycle, referred to as a cyclic pattern

Advantages

- Interesting alternative to walk-based kernels

Disadvantages

- Cyclic pattern kernel on general graphs is NP-hard to compute
- Restrict their attention to scenarios where the number of simple cycles in a graph dataset is bounded by a constant

Graphlet Kernel (B., Petri, et al., MLG 2007)

Principle

- Count subgraphs of limited size *k* in *G* and *G'*
- These subgraphs are referred to as **graphlets** (Przulj, Bioinformatics 2007)
- Define graph kernel that counts isomorphic graphlets in two graphs

Runtime problems

- Pairwise test of isomorphism is expensive
- Number of graphlets scales as $O(n^k)$

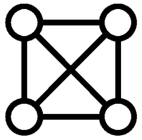
Two solutions on unlabeled graphs

- Precompute isomorphisms
- Sample graphlets

Disadvantage

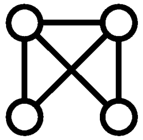
- Same solutions not feasible on labeled graphs

Graphlet Kernel



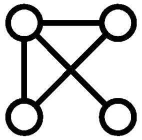
1
clique

111111



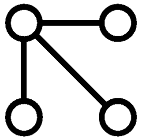
2
diamond

111110



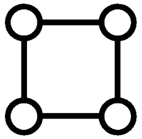
3
flower

111100



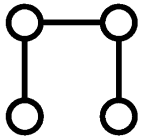
4
star

111000



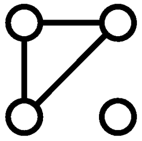
5
square

110011



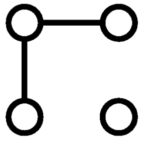
6
line

110010



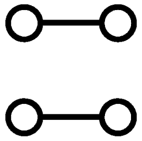
7
triangle

110100



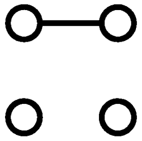
8
3-line

110000



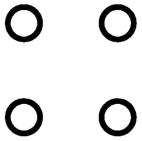
9
2 separate edges

100001



10
1 edge

100000



11
no edge

000000

Applications: Chemoinformatics (Ralaivola et al., 2005)

Graph kernels inspired by concepts from chemoinformatics

- Define three new kernels (Tanimoto, MinMax, Hybrid) for function prediction of chemical compounds
- Based on the idea of molecular fingerprints and
- Counting labeled paths of depth up to *d* using depth-first search from each possible vertex

Properties

- Tailored for applications in chemical informatics,
- Exploit the small size and
- Low average degree of these molecular graphs.

Chemical Compound Classification (Wale et al, ICDM 2006)

New kernels and experimental comparison of existing techniques

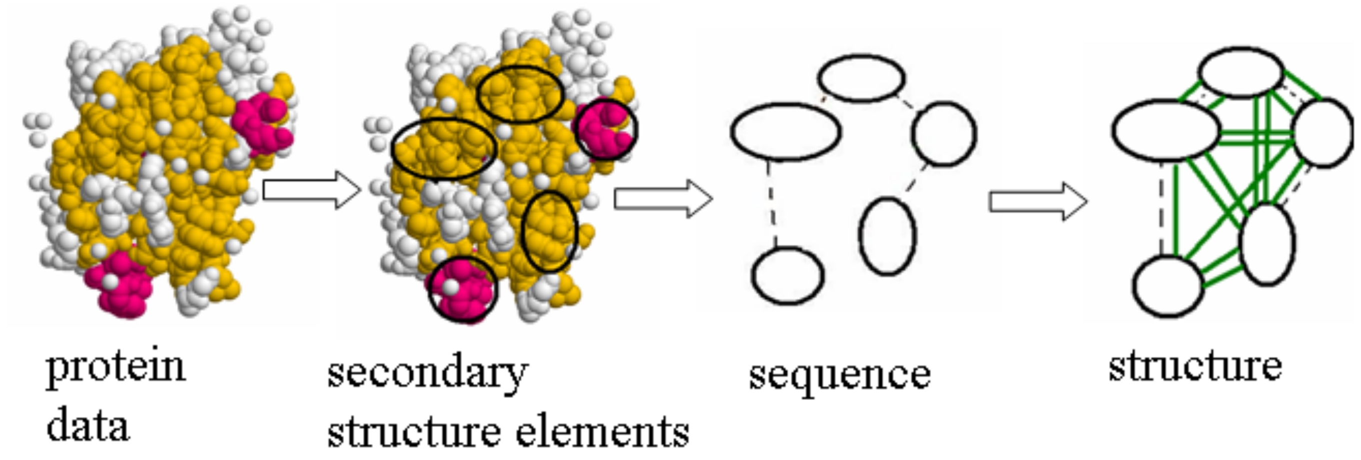
- Define a kernel that considers *graph fragments*: Subgraphs with a maximum of l edges
- Fragment-based kernels outperform kernels using frequent subgraphs and walk-based kernels

Four choices in kernel design for chemical compounds

- Generation of patterns (learnt from dataset versus defined by expert)
- ‘Preciseness‘ of the patterns (whether subgraph features map to the same dimension in feature space)
- Complete coverage (whether the patterns occur in all of the instances of the dataset)
- Complexity of patterns (walks and cycles versus frequent subgraphs)

Applications: Protein Function Prediction (B. et al, ISMB 2005)

- Predict the function of a protein from its structure
- Model protein structure as graph
- Use graph kernels to measure structural similarity and SVM to predict functional class
- Reaches competitive results on benchmark datasets



Future Challenges for Graph Kernel Research

Data level

- Larger and more graph data
- More dynamic graph data

Algorithmic level

- Feature selection on graphs
- Scalability and efficiency
- Automatic choice of complexity of representation

Interdisciplinary level

- Link to graph mining, both current research and literature
- Applications in bioinformatics and the Internet

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