A PRIMER ON GRAPH KERNELS

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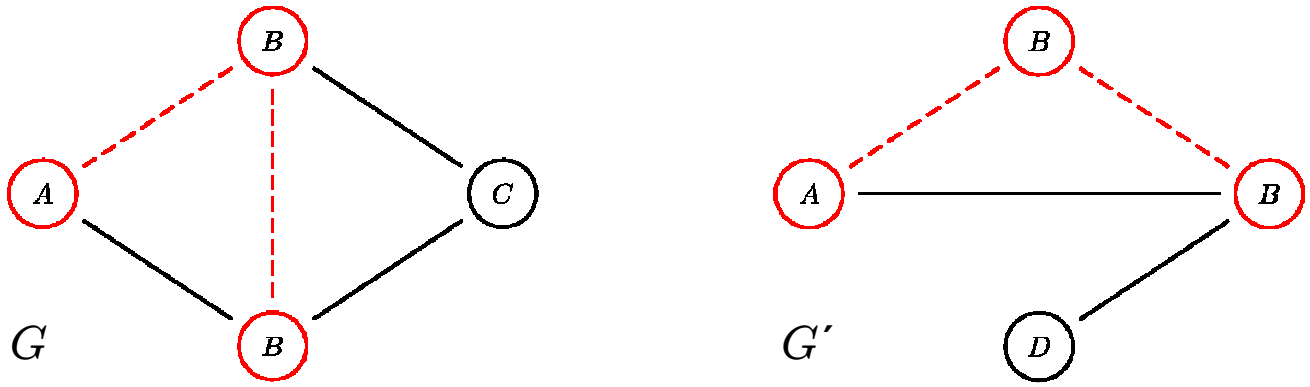
Graph Comparison

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*

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

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

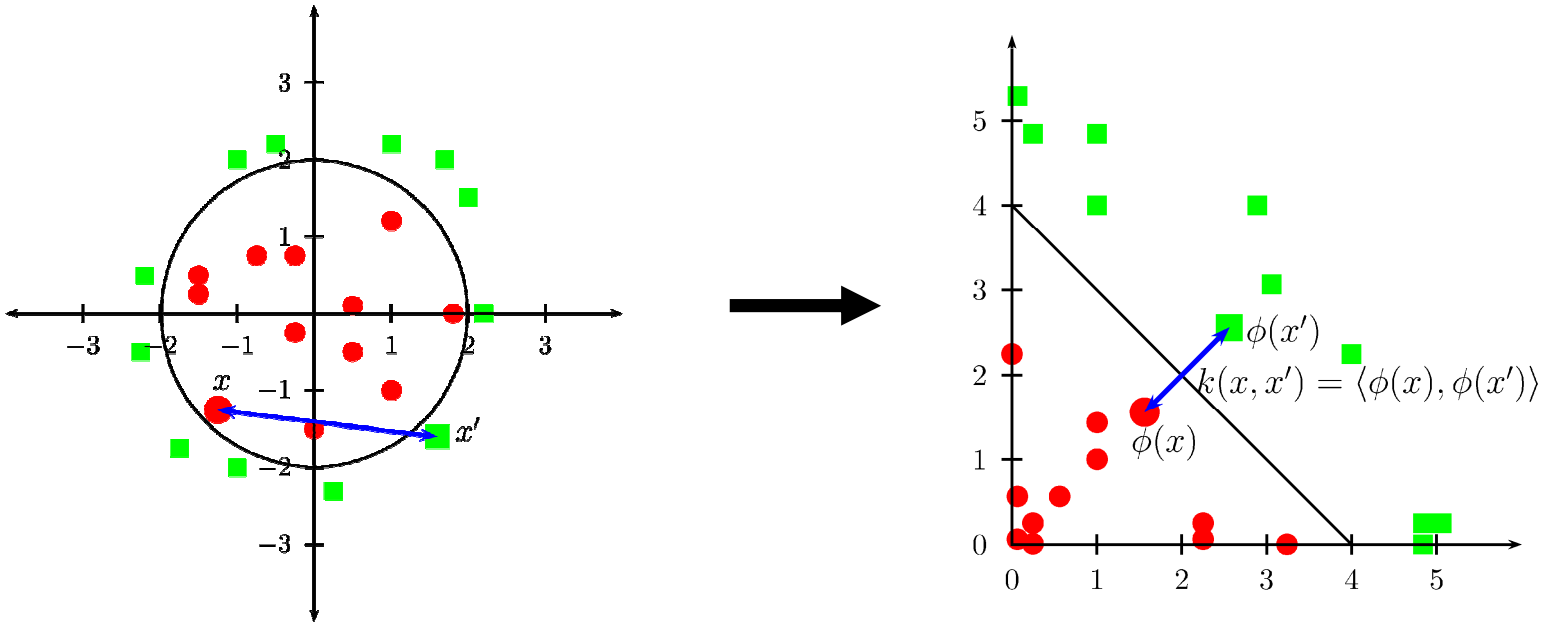
- Compare substructures of graphs that are computable in polynomial time.

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 on Graph Kernels

(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

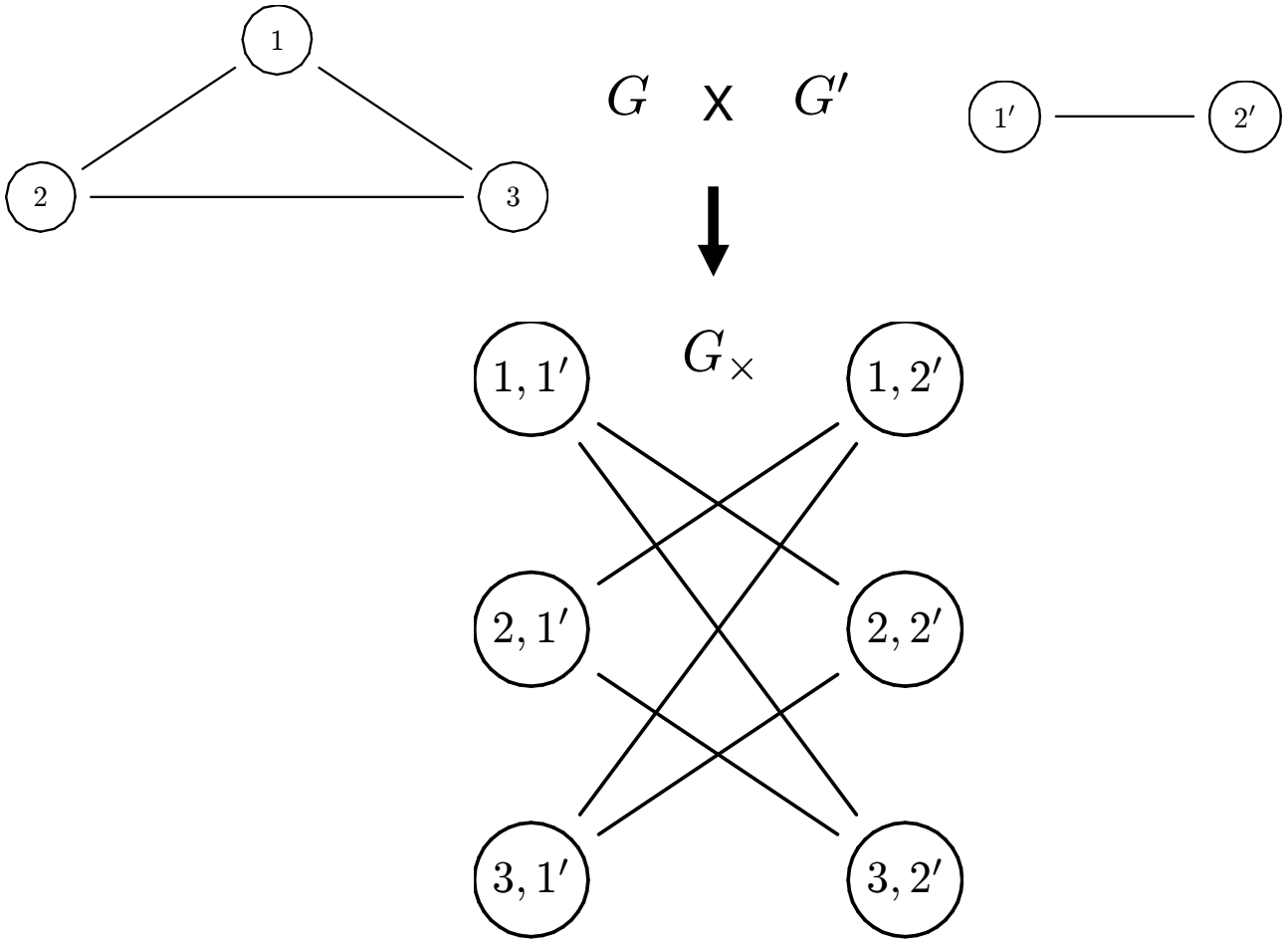
- Count common walks in two input graphs G and G'
- Walks are sequences of nodes that allow repetitions of nodes

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 $G_\times=(V_\times,E_\times)$
- 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 Computation of 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

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

- One then exploits the well-known fact

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

  to rewrite the above question as

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

- Now one has to solve

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

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

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

From Sylvester Equations to Random Walk Kernels

- In

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

one substitutes

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

and obtain

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

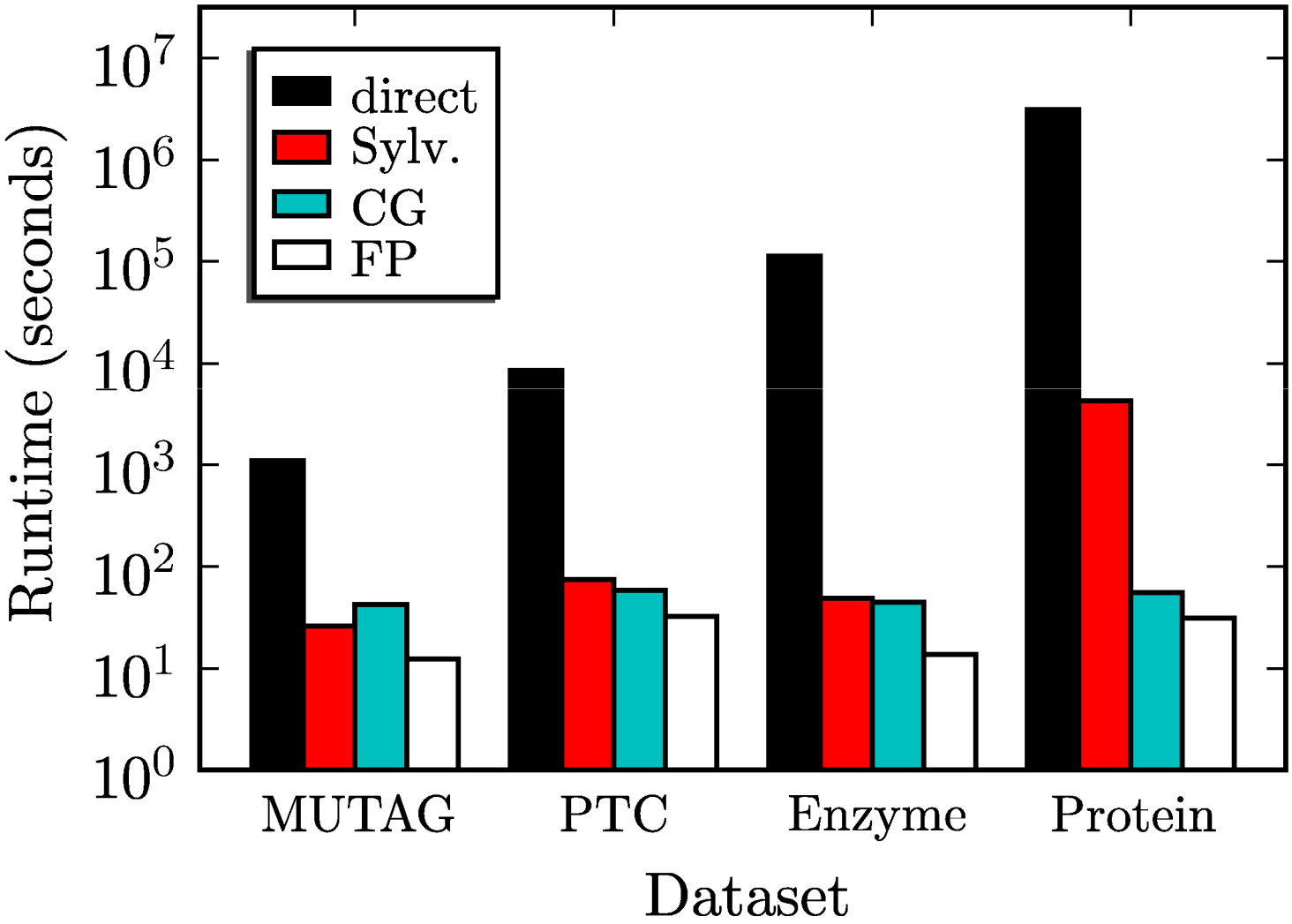
Further Speed-ups for Sparse Graphs

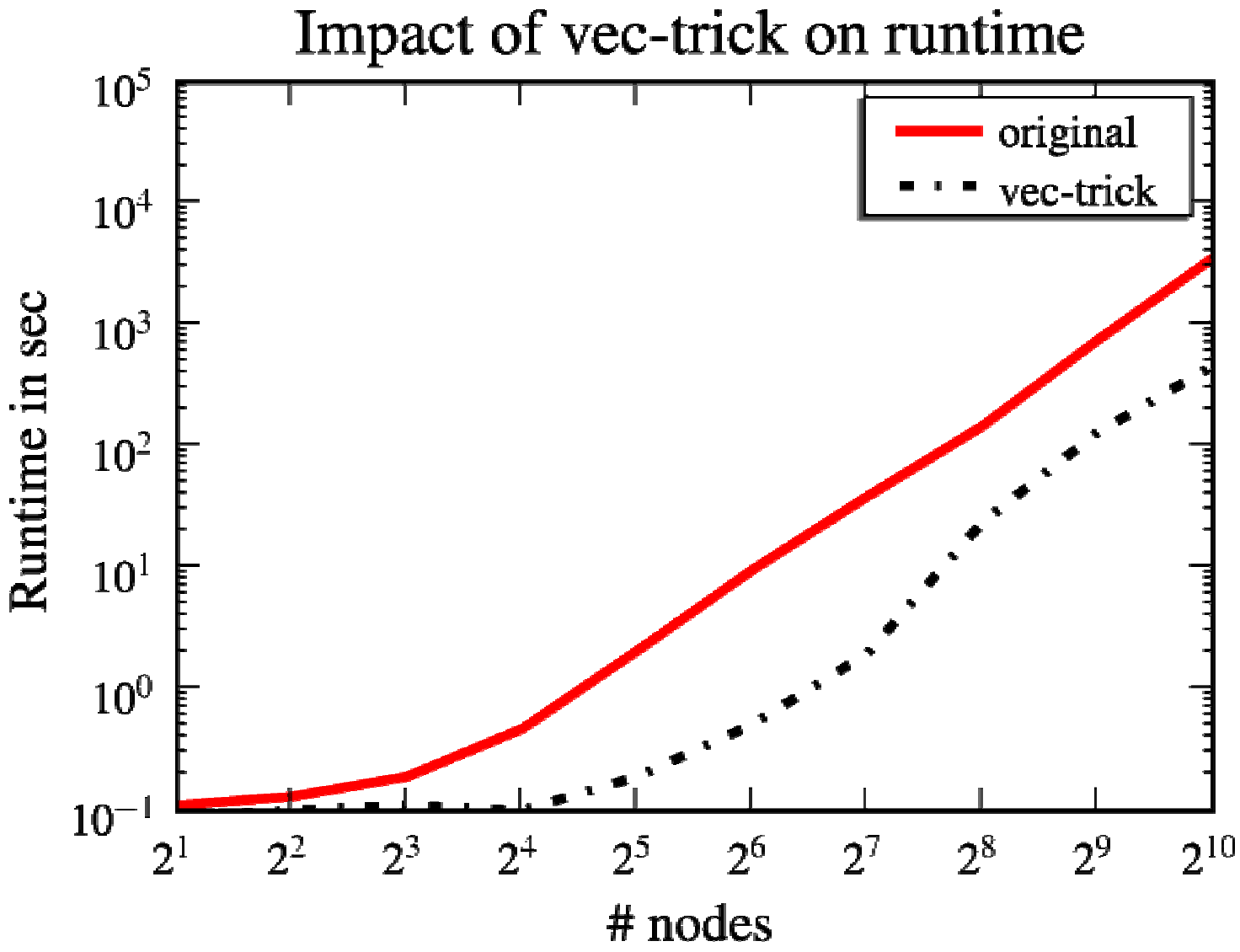
- Vec-Trick
  - Let S and T be sparse.
  - We can efficiently compute $(T^\top \otimes S)\,\mathrm{vec}\,X$ for each X as $\mathrm{vec}(SXT)$.
  - How to exploit this fact?
- Fix-Point Iteration (FP)
  - Determine a fix point (Kashima et. al, 2003):

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

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

Impact on Runtime for Kernel Computation




Impact of vec-trick on runtime
Runtime in sec
10^5
10^4
10^3
10^2
10^1
10^0
10^{-1}
original
vec-trick
2^1
2^2
2^3
2^4
2^5
2^6
2^7
2^8
2^9
2^{10}
nodes

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

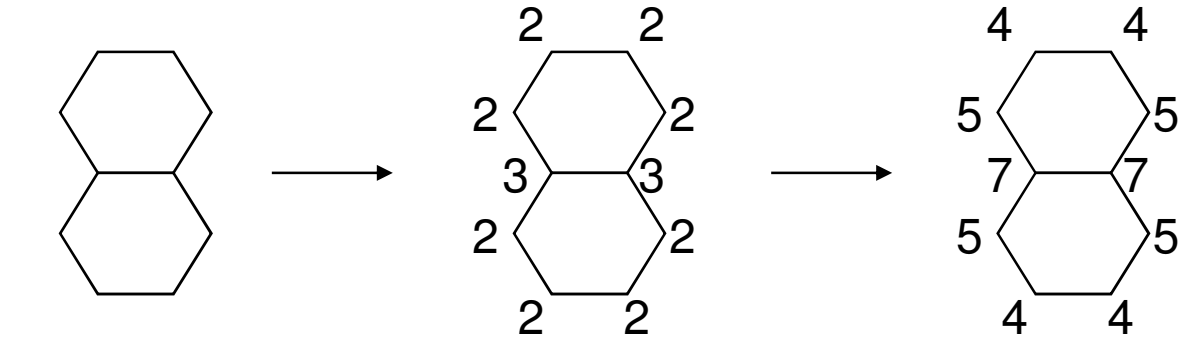
- Walks in G_T correspond to walks in G, but it is not possible to totter between 2 nodes

  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

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

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 $O(n^k)$

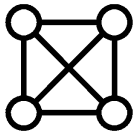
Two solutions on unlabeled graphs

- Precompute isomorphisms
- Sample graphlets

Disadvantage

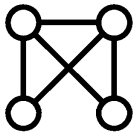
- Same solutions not feasible on labeled graphs

Graphlet Kernel



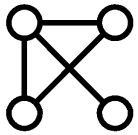
1
clique

111111



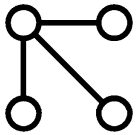
2
diamond

111110



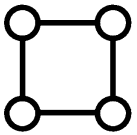
3
flower

111100



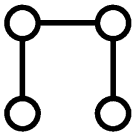
4
star

111000



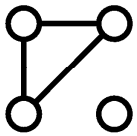
5
square

110011



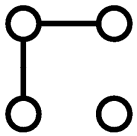
6
line

110010



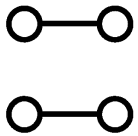
7
triangle

110100



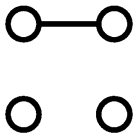
8
3-line

110000



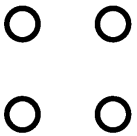
9
2 separate edges

100001



10
1 edge

100000



11
no edge

000000

Recent Trends

Combine graph kernels with graphical models (Bach, ICML 2008)

- Presents a new kernel for 2D or 3D point clouds
- Compares local subsets of the point clouds
- Considers subsets based on subtrees and walks
- Uses a specific factorized form for the local kernels between subtrees.

Combine graph kernels with group theory (Kondor and B., ICML 2008)

- Represent graph as a function over the symmetric group
- Derive invariants for that function called the *skew spectrum*
- Use subset of these invariants that is computable in $O(n^3)$ as feature representation of the graph

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

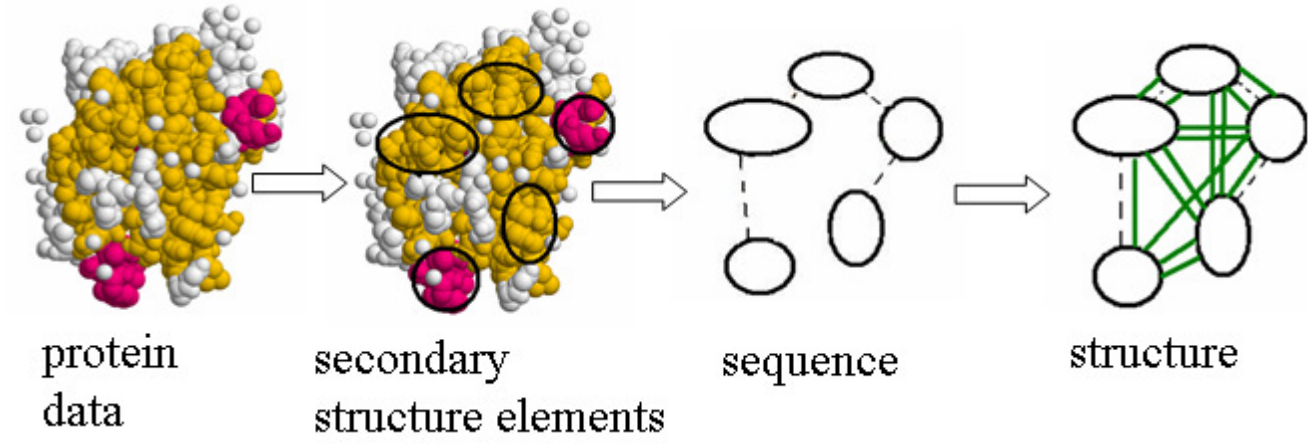
- Define a kernel that considers *graph fragments*: Subgraphs with a maximum of l edges
- Fragment-based kernels outperform kernels using frequent subgraphs and walk-based kernels

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

References

- Francis Bach: Graph kernels between point clouds. ICML 2008
- Karsten M. Borgwardt, Hans-Peter Kriegel: Shortest-Path Kernels on Graphs. ICDM 2005: 74-81
- Karsten M. Borgwardt, Cheng Soon Ong, Stefan Schönauer, S. V. N. Vishwanathan, Alexander J. Smola, Hans-Peter Kriegel: Protein function prediction via graph kernels. ISMB (Supplement of Bioinformatics) 2005: 47-56
- Karsten M. Borgwardt, Tobias Petri, S. V. N. Vishwanathan, Hans-Peter Kriegel: An Efficient Sampling Scheme For Comparison of Large Graphs. MLG 2007
- Mukund Deshpande, Michihiro Kuramochi, Nikil Wale, George Karypis: Frequent Substructure-Based Approaches for Classifying Chemical Compounds. IEEE Trans. Knowl. Data Eng. 17(8): 1036-1050 (2005)
- Holger Fröhlich, Jörg K. Wegner, Florian Sieker, Andreas Zell: Optimal assignment kernels for attributed molecular graphs. ICML 2005: 225-232

References

- Thomas Gärtner, Peter A. Flach, Stefan Wrobel: On Graph Kernels: Hardness Results and Efficient Alternatives. COLT 2003: 129-143
- David Haussler. Convolution kernels on discrete structures. UCSC-CRL-99-10,1999.
- Tamás Horváth, Thomas Gärtner, Stefan Wrobel: Cyclic pattern kernels for predictive graph mining. KDD 2004: 158-167
- Hisashi Kashima, Koji Tsuda, Akihiro Inokuchi: Marginalized Kernels Between Labeled Graphs. ICML 2003: 321-328
- Imre Risi Kondor, Karsten M. Borgwardt: The skew spectrum of graphs. ICML 2008
- Pierre Mahé, Nobuhisa Ueda, Tatsuya Akutsu, Jean-Luc Perret, Jean-Philippe Vert: Extensions of marginalized graph kernels. ICML 2004

References

- Sauro Menchetti, Fabrizio Costa, Paolo Frasconi: Weighted decomposition kernels. ICML 2005:585-592
- Michel Neuhaus, Horst Bunke: A Random Walk Kernel Derived from Graph Edit Distance. SSPR/SPR 2006: 191-199
- Liva Ralaivola, Sanjay Joshua Swamidass, Hiroto Saigo, Pierre Baldi: Graph kernels for chemical informatics. Neural Networks 18(8): 1093-1110 (2005)
- Jan Ramon, Thomas Gärtner: Expressivity versus Efficiency of Graph Kernels. First International Workshop on Mining Graphs, Trees and Sequences 2003
- S.V.N. Vishwanathan, Karsten M. Borgwardt, Nicol N. Schraudolph: Fast Computation of Graph Kernels. NIPS 2006:1449-1456
- Nikil Wale, George Karypis: Comparison of Descriptor Spaces for Chemical Compound Retrieval and Classification. ICDM 2006: 678-689