Package ‘graphkernels’

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Description A fast C++ implementation for computing various graph kernels including (1) simple kernels between vertex and/or edge label histograms, (2) graphlet kernels, (3) random walk kernels (popular baselines), and (4) the Weisfeiler-Lehman graph kernel (state-of-the-art).

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`graphkernels-package` *Graph Kernels*

Description

A fast C++ implementation for computing various graph kernels including (1) simple kernels between vertex and/or edge label histograms, (2) graphlet kernels, (3) random walk kernels (popular baselines), and (4) the Weisfeiler-Lehman graph kernel (state-of-the-art).

Details

This library provides the following graph kernels:

- the linear kernel between vertex label histograms
- the linear kernel between edge label histograms
- the linear kernel between vertex-edge label histograms
- the linear kernel combination vertex label histograms and vertex-edge label histograms
- the Gaussian RBF kernel between vertex label histograms
- the Gaussian RBF kernel between edge label histograms
- the Gaussian RBF kernel between vertex-edge label histograms
- the graphlet kernel
- the k-step random walk kernel
- the geometric random walk kernel
- the exponential random walk kernel
- the shortest-path kernel
- the Weisfeiler-Lehman subtree kernel

Given a list of **igraph** graphs, each function calculates the corresponding kernel (Gram) matrix.

Author(s)

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References

Borgwardt, K. M., Kriegel, H.-P.: **Shortest-Path Kernels on Graphs**, *Proceedings of the 5th IEEE International Conference on Data Mining (ICDM'05)*, 74-81 (2005) https://ieeexplore.ieee.org/document/1565664/.

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Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
KEH <- CalculateEdgeHistKernel(mutag)
  ## compute linear kernel between edge histograms
KWL <- CalculateWLKernel(mutag, 5)
  ## compute Weisfeiler-Lehman subtree kernel
```

CalculateConnectedGraphletKernel

Connected graphlet kernel

Description

This function calculates a kernel matrix of the graphlet kernel with connected graphlets K_{CGL} between unlabeled graphs.

Usage

```
CalculateConnectedGraphletKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	the number k of graphlet nodes ($k = 3$, 4, or 5 is supported)

Value

a kernel matrix of the connected graphlet kernel K_{CGL}

Author(s)

Mahito Sugiyama

References

Shervashidze, N., Vishwanathan, S. V. N., Petri, T., Mehlhorn, K., Borgwardt, K. M.: **Efficient Graphlet Kernels for Large Graph Comparison**, *Proceedings of the 12th International Conference on Artificial Intelligence and Statistics (AISTATS)*, 5, 488-495 (2009) https://proceedings.mlr.press/v5/shervashidze09a.html.

Examples

```
data(mutag)
K <- CalculateConnectedGraphletKernel(mutag, 4)
```

CalculateEdgeHistGaussKernel

Gaussian RBF kernel between edge label histograms

Description

This function calculates a kernel matrix of the Gaussian RBF kernel $K_{EH,G}$ between edge label histograms.

Usage

```
CalculateEdgeHistGaussKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	σ in the Gaussian RBF kernel

Value

a kernel matrix of the Gaussian RBF kernel $K_{EH,G}$ between edge label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateEdgeHistGaussKernel(mutag, .1)
```

`CalculateEdgeHistKernel` *Linear kernel between edge label histograms*

Description

This function calculates a kernel matrix of the linear kernel K_{EH} between edge label histograms.

Usage

```
CalculateEdgeHistKernel(G)
```

Arguments

`G`	a list of `igraph` graphs

Value

a kernel matrix of the linear kernel K_{EH} between edge label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateEdgeHistKernel(mutag)
```

CalculateExponentialRandomWalkKernel
Exponential random walk kernel

Description

This function calculates a kernel matrix of the exponential random walk kernel K_{ER}.

Usage

```
CalculateExponentialRandomWalkKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	a coefficient β, with which the weight λ_k for each step k is given as $\lambda_k = \beta^k / k!$

Value

a kernel matrix of the exponential random walk kernel K_{ER}

Author(s)

Mahito Sugiyama

References

Gartner, T., Flach, P., Wrobel, S.: **On graph kernels: Hardness results and efficient alternatives**, *Learning Theory and Kernel Machines (LNCS 2777)*, 129-143 (2003) https://link.springer.com/chapter/10.1007/978-3-540-45167-9_11.

Examples

```
data(mutag)
K <- CalculateExponentialRandomWalkKernel(mutag[1:5], .1)
```

`CalculateGeometricRandomWalkKernel`
Geometric random walk kernel

Description

This function calculates a kernel matrix of the geometric random walk kernel K_{GR}.

Usage

```
CalculateGeometricRandomWalkKernel(G, par)
```

Arguments

`G`	a list of `igraph` graphs
`par`	a coefficient λ, with which the weight λ_k for each step k is given as $\lambda_k = \lambda^k$

Value

a kernel matrix of the geometric random walk kernel K_{GR}

Author(s)

Mahito Sugiyama

References

Gartner, T., Flach, P., Wrobel, S.: **On graph kernels: Hardness results and efficient alternatives**, *Learning Theory and Kernel Machines (LNCS 2777)*, 129-143 (2003) https://link.springer.com/chapter/10.1007/978-3-540-45167-9_11.

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateGeometricRandomWalkKernel(mutag, .1)
```

`CalculateGraphletKernel` *Graphlet kernel*

Description

This function calculates a kernel matrix of the graphlet kernel K_{GL} between unlabeled graphs.

Usage

```
CalculateGraphletKernel(G, par)
```

Arguments

`G`	a list of `igraph` graphs
`par`	the number k of graphlet nodes ($k = 3$ or 4 is supported)

Value

a kernel matrix of the graphlet kernel K_{GL}

Author(s)

Mahito Sugiyama

References

Shervashidze, N., Vishwanathan, S. V. N., Petri, T., Mehlhorn, K., Borgwardt, K. M.: **Efficient Graphlet Kernels for Large Graph Comparison**, *Proceedings of the 12th International Conference on Artificial Intelligence and Statistics (AISTATS)*, 5, 488-495 (2009) https://proceedings.mlr.press/v5/shervashidze09a.html.

Examples

```
data(mutag)
K <- CalculateGraphletKernel(mutag, 4)
```

`CalculateGraphletKernelCpp` *An C++ implementation of graphlet kernels*

Description

This function calculates a graphlet kernel matrix.

Usage

```
CalculateGraphletKernelCpp(graph_adj_all, graph_adjlist_all, k, connected)
```

Arguments

`graph_adj_all`	a list of adjacency matrices
`graph_adjlist_all`	a list of adjacency lists
`k`	the number k of graphlet nodes
`connected`	whether or not graphlets are conneceted

Value

a kernel matrix of the respective graphlet kernel

Author(s)

Mahito Sugiyama

References

Shervashidze, N., Vishwanathan, S. V. N., Petri, T., Mehlhorn, K., Borgwardt, K. M.: **Efficient Graphlet Kernels for Large Graph Comparison**, *Proceedings of the 12th International Conference on Artificial Intelligence and Statistics (AISTATS)*, 5, 488-495 (2009) https://proceedings.mlr.press/v5/shervashidze09a.html.

Examples

```
data(mutag)
al.list <- as.list(rep(NA, length(mutag)))
for (i in 1:length(mutag)) { al.list[[i]] <- as_adj_list(mutag[[i]]) }
K <- CalculateGraphletKernelCpp(list(), al.list, 4, 0)
```

`CalculateKernelCpp` *An C++ implementation of graph kernels*

Description

This function calculates a kernel matrix.

Usage

```
CalculateKernelCpp(graph_info_list, par_r, kernel_type)
```

Arguments

`graph_info_list`	a list of `igraph` graphs
`par_r`	parameters of kernels
`kernel_type`	type of kernel

Value

a kernel matrix of the respective kernel

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
graph.info.list <- vector("list", length(mutag))
for (i in 1:length(mutag)) { graph.info.list[[i]] <- GetGraphInfo(mutag[[i]]) }
K <- CalculateKernelCpp(graph.info.list, 5, 11)
```

CalculateKStepRandomWalkKernel
k-step random walk kernel

Description

This function calculates a kernel matrix of the k-step random walk kernel $K^k_\times$.

Usage

```
CalculateKStepRandomWalkKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	a vector of coefficients $\lambda_0, \lambda_1, \ldots, \lambda_k$

Value

a kernel matrix of the k-step random walk kernel $K^k_\times$

Author(s)

Mahito Sugiyama

References

Gartner, T., Flach, P., Wrobel, S.: **On graph kernels: Hardness results and efficient alternatives**, *Learning Theory and Kernel Machines (LNCS 2777)*, 129-143 (2003) https://link.springer.com/chapter/10.1007/978-3-540-45167-9_11.

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateKStepRandomWalkKernel(mutag, rep(1, 2))
```

CalculateShortestPathKernel

Shortest-path kernel

Description

This function calculates a kernel matrix of the shortest-path kernel K_{SP}.

Usage

```
CalculateShortestPathKernel(G)
```

Arguments

G	a list of igraph graphs

Value

a kernel matrix of the shortest-path kernel K_{SP}

Author(s)

Mahito Sugiyama

References

Borgwardt, K. M., Kriegel, H.-P.: **Shortest-Path Kernels on Graphs**, *Proceedings of the 5th IEEE International Conference on Data Mining (ICDM'05)*, 74-81 (2005) https://ieeexplore.ieee.org/document/1565664/.

Examples

```
data(mutag)
K <- CalculateShortestPathKernel(mutag)
```

CalculateVertexEdgeHistGaussKernel

Gaussian RBF kernel between vertex-edge label histograms

Description

This function calculates a kernel matrix of the Gaussian RBF kernel $K_{VEH,G}$ between vertex-edge label histograms.

Usage

```
CalculateVertexEdgeHistGaussKernel(G, par)
```

Arguments

`G`	a list of `igraph` graphs
`par`	σ in the Gaussian RBF kernel

Value

a kernel matrix of the Gaussian RBF kernel $K_{VEH,G}$ between vertex-edge label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateVertexEdgeHistGaussKernel(mutag, .1)
```

`CalculateVertexEdgeHistKernel`

Linear kernel between vertex-edge label histograms

Description

This function calculates a kernel matrix of the linear kernel K_{VEH} between vertex-edge label histograms.

Usage

```
CalculateVertexEdgeHistKernel(G)
```

Arguments

`G`	a list of `igraph` graphs

Value

a kernel matrix of the linear kernel K_{VEH} between vertex-edge label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateVertexEdgeHistKernel(mutag)
```

CalculateVertexHistGaussKernel

Gaussian RBF kernel between vertex label histograms

Description

This function calculates a kernel matrix of the Gaussian RBF kernel $K_{VH,G}$ between vertex label histograms.

Usage

```
CalculateVertexHistGaussKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	σ in the Gaussian RBF kernel

Value

a kernel matrix of the Gaussian RBF kernel $K_{VH,G}$ between vertex label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateVertexHistGaussKernel(mutag, .1)
```

`CalculateVertexHistKernel` *Linear kernel between vertex label histograms*

Description

This function calculates a kernel matrix of the linear kernel K_{VH} between vertex label histograms.

Usage

```
CalculateVertexHistKernel(G)
```

Arguments

G	a list of `igraph` graphs

Value

a kernel matrix of the linear kernel K_{VH} between vertex label histograms

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateVertexHistKernel(mutag)
```

`CalculateVertexVertexEdgeHistKernel` *Linear kernel combination of vertex label histograms and vertex-edge label histograms*

Description

This function calculates a kernel matrix of the linear kernel combination K_H of vertex label histograms K_{VH} and vertex-edge label histograms K_{VEH}.

Usage

```
CalculateVertexVertexEdgeHistKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	a coefficient λ, with which the resulting kernel is given as $K_{VH} + \lambda K_{VEH}$

Value

a kernel matrix that is equivalent to $K_{VH} + \lambda K_{VEH}$

Author(s)

Mahito Sugiyama

References

Sugiyama, M., Borgwardt, K. M.: **Halting in Random Walk Kernels**, *Advances in Neural Information Processing Systems (NIPS 2015)*, 28, 1630-1638 (2015) https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf.

Examples

```
data(mutag)
K <- CalculateVertexVertexEdgeHistKernel(mutag, .1)
```

CalculateWLKernel *Weisfeiler-Lehman subtree kernel*

Description

This function calculates a kernel matrix of the Weisfeiler-Lehman subtree kernel K_{WL}.

Usage

```
CalculateWLKernel(G, par)
```

Arguments

G	a list of igraph graphs
par	the number h of iterations

Value

a kernel matrix of the Weisfeiler-Lehman subtree kernel K_{WL}

Author(s)

Mahito Sugiyama

References

Shervashidze, N., Schweitzer, P., van Leeuwen, E. J., Mehlhorn, K., Borgwardt, K. M.: **Weisfeiler-Lehman Graph Kernels**, *Journal of Machine Learning Research*, 12, 2359-2561 (2011) https://www.jmlr.org/papers/volume12/shervashidze11a/shervashidze11a.pdf.

Examples

```
data(mutag)
K <- CalculateWLKernel(mutag, 5)
```

`GetGraphInfo` *Necessary information of graphs for kernel computation*

Description

This function extracts necessary information of graphs for kernel computation.

Usage

```
GetGraphInfo(g)
```

Arguments

`g`	an `igraph` graph

Value

a list of graph information with the following elements:

`edge`	a matrix of edges with their labels
`vlabel`	a vector of vertex labels
`vsize`	the number of vertices
`esize`	the number of edges
`maxdegree`	the maximum degree

Author(s)

Mahito Sugiyama

Examples

```
data(mutag)
ginfo <- GetGraphInfo(mutag[[1]])
```

graphkernels_CalculateGraphletKernelCpp
Symbol registration

Description

This is a supplement for symbol registration.

Author(s)

Mahito Sugiyama

graphkernels_CalculateKernelCpp
Symbol registration

Description

This is a supplement for symbol registration.

Author(s)

Mahito Sugiyama

mutag *The mutag dataset*

Description

This is the mutag dataset, a well known benchmark dataset for graph processing algorithms.

Usage

```
data(mutag)
```

Author(s)

Mahito Sugiyama

References

Debnath, A. K., Lopez de Compadre, R. L., Debnath, G., Shusterman, A. J., Hansch, C.: **Structure-activity relationship of mutagenic aromatic and heteroaromatic nitro compounds. correlation with molecular orbital energies and hydrophobicity**, *Journal of Medicinal Chemistry*, 34(2), 786-797 (1991) https://pubs.acs.org/doi/abs/10.1021/jm00106a046.

Examples

```
data(mutag)
K <- CalculateWLKernel(mutag, 5)
```

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