

# Package ‘fgga’

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**Type** Package

**Title** Hierarchical ensemble method based on factor graph

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**biocViews** Software, StatisticalMethod, Classification, Network,  
NetworkInference, SupportVectorMachine, GraphAndNetwork, GO

**Description** Package that implements the FGGA algorithm. This package provides a hierarchical ensemble method based on factor graphs for the consistent cross-ontology annotation of protein coding genes. FGGA embodies elements of predicate logic, communication theory, supervised learning and inference in graphical models.

**Depends** R (>= 4.3), RBGL

**Imports** graph, stats, e1071, methods, gRbase, jsonlite, BiocFileCache,  
curl, igraph

**Suggests** knitr, rmarkdown, GOstats, GO.db, BiocGenerics, pROC, RUnit,  
BiocStyle

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 fgga-package

*FGGA: Factor Graph Gene ontology Annotation.*


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## Description

FGGA is a graph-based machine learning approach for the automated and consistent GO, PO, HPO and ZFA annotation of protein coding genes. The input is a set of ontological-terms annotated protein coding genes previously characterized in terms of a fixed number of user-defined features, including the presence/absence of PFAM domains, physical-chemical properties, presence of signal peptides, among others. The set of ontological terms defines the output cross-ontology subgraph. A hierarchical ensemble (SVMs) machine learning model is generated. This model can be used to predict the cross-ontology subgraph annotations of uncharacterized protein coding genes. Individual ontological-term annotations are accompanied by maximum a posteriori probability estimates issued by the native message passing algorithm of factor graphs.

## Author(s)

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## References

Spetale F.E., et al. **A Factor Graph Approach to Automated GO Annotation.** *PLoS ONE* (2016). <https://doi.org/10.1371/journal.pone.0146986>.

Spetale Flavio E., et al. **Consistent prediction of GO protein localization.** *Scientific Report* (2018). <https://doi.org/10.1038/s41598-018-26041-z>.

**See Also**

[fgga](#), [fgga2bipartite](#), [sumProduct](#), [svm](#)

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CfData	<i>A set of characterized protein coding genes from the <i>Cannis familiaris</i> organism annotated to a target GO subgraph considering both experimental and electronic evidence.</i>
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**Description**

The CfData dataset consists of a list containing the following:

*\$dxCf*: characterizations of 6962 protein coding genes in terms of 72 physico-chemical properties of their amino acid sequences. These sequences, obtained from the Uniprot database, are annotated to 36 GO-terms of the GO Molecular Function (GO-MF) ontology subdomain.

*\$stableCfGO*: a set of 6962 protein coding genes annotated to GO-MF target classes. Genes are identified by their **Uniprot** ID mappings which are obtained with the org.Cf.eg.db annotation package set to work with both experimental and electronic evidence. Additionally, only those GO-MF terms with at least 500 annotated genes were preserved.

*\$graphCfGO*: the target **GO-MF** subgraph obtained with the org.Cf.eg.db annotation package set to work with the set of **GO-MF** target classes.

*\$indexGO*: two arrays of Uniprot ID mappings defining the train-test partition of the set 6962 protein coding genes annotated to **GO-MF** terms.

*\$nodesGO*: labels of the GO-MF subgraph.

*\$varianceGOs*: a vector labeled with the variance of each **GO-MF** term.

**Usage**

```
data("CfData")
```

**Format**

A list with five named entries containing:

**dxCf** A matrix (6962 rows x 72 columns) containing the characterized proteins.

**graphCfGO** An adjacency binary matrix (36 rows x 36 columns) corresponding to the GO-MF subgraph.

**indexGO** A list with two named entries: indexTrain and indexTest each containing a numeric vector.

**tableCfGO** A binary matrix (6962 rows x 36 columns) containing GOs associated with a protein.

**nodesGO** A numerical vector containing the nodes of the GO-MF subgraph.

**Source**

Uniprot Taxonomy: 9615

<https://www.uniprot.org/uniprot/?query=taxonomy:9615>

Package: org.Cf.eg.db - Version: 3.8.2

<https://bioconductor.org/packages/org.Cf.eg.db/>

**Examples**

```
data(CfData)

## list objects included
ls(CfData)
# [1] "dxCf" "graphCfGO" "indexGO" "nodesGO" "tableCfGO"

# Physico-chemical properties of each protein
head(CfData[["dxCf"]])

# GO-MF node labels, GO-terms, of each protein
head(CfData[["tableCfGO"]])
```

---

createFolds

*Data splitting function useful for binary classification tasks*

---

**Description**

createFolds splits binary classification data into k-folds.

**Usage**

```
createFolds(target, k_fold = 10)
```

**Arguments**

target	A binary vector of a Ontology class
k_fold	An integer for the number of folds

**Details**

A random sampling is performed on binary classification data. A set of k data folds reflecting the original class balance is obtained.

**Value**

list of row position integers corresponding to the training data

**Author(s)**

Flavio E. Spetale and Pilar Bulacio <spetale@cifasis-conicet.gov.ar>

**References**

Hyndman and Athanasopoulos (2013), Forecasting: principles and practice. <https://www.otexts.org/fpp>

**Examples**

```
data(CfData)

createFolds(CfData[["tableCfG0"]][ , "GO:0005515"], k_fold = 2)
```

---

 fgga

---

*Factor Graph Cross-Ontology Annotation model*


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**Description**

A hierarchical graph-based machine learning model for the consistent GO, PO, ZFA, HPO annotation of protein coding genes.

**Usage**

```
fgga(graphOnto, tableOntoTerms, dxCharacterized, dxTestCharacterized,
      kFold, kernelSVM, tmax, epsilon)
```

**Arguments**

graphOnto	A graphNEL graph with ‘m’ Ontology node labels.
tableOntoTerms	A binary matrix with ‘n’ proteins (rows) by ‘m’ Ontology node labels (columns).
dxCharacterized	A data frame with ‘n’ proteins (rows) by ‘f’ features (columns).
dxTestCharacterized	A data frame with ‘k’ proteins (rows) by ‘f’ features (columns).
kFold	An integer for the number of folds.
kernelSVM	The kernel used to calculate the variance (default: radial).
tmax	An integer indicating the maximum number of iterations (default: 200).
epsilon	A real value less than 1 that represents the convergence criteria (default: 0.001).

## Details

The **FGGA model** is built in two main steps. In the first step, a core Factor Graph (FG) modeling hidden Ontology-term predictions and relationships is created. In the second step, the FG is enriched with nodes modeling observable Ontology-term predictions issued by **binary SVM classifiers**. In addition, probabilistic constraints modeling learning gaps between hidden and observable Ontology-term predictions are introduced. These gaps are assumed to be independent among Ontology-terms, locally additive with respect to observed predictions, and zero-mean Gaussian. **FGGA predictions** are issued by the native iterative **message passing algorithm** of factor graphs.

## Value

A named matrix with ‘k’ protein coding genes (rows) by ‘m’ cross-Ontology node labels (columns) where each element indicates a probabilistic prediction value.

## Author(s)

Flavio E. Spetale and Elizabeth Tapia <spetale@cifasis-conicet.gov.ar>

## References

Spetale F.E., Tapia E., Krsticevic F., Roda F. and Bulacio P. “A Factor Graph Approach to Automated GO Annotation”. PLoS ONE 11(1): e0146986, 2016.

Spetale Flavio E., Arce D., Krsticevic F., Bulacio P. and Tapia E. “Consistent prediction of GO protein localization”. Scientific Report 7787(8), 2018

## See Also

[fgga2bipartite](#), [sumProduct](#), [svmOnto](#)

## Examples

```
data(CfData)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

dxCfTestCharacterized <- CfData[["dxCf"]][CfData[["indexGO"]]$indexTest[1:2], ]

myTableGO <- CfData[["tableCfGO"]][
  CfData[["indexGO"]]$indexTrain[1:300], ]

dataTrain <- CfData[["dxCf"]][
  CfData[["indexGO"]]$indexTrain[1:300], ]

fggaResults <- fgga(graphOnto = mygraphGO,
  tableOntoTerms = myTableGO, dxCharacterized = dataTrain,
  dxTestCharacterized = dxCfTestCharacterized, kFold = 2,
  tmax = 50, epsilon = 0.05)
```

---

fgga2bipartite	<i>Forney Factor Graph model</i>
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**Description**

fgga2bipartite builds a Forney Factor Graph from a FGGA model.

**Usage**

```
fgga2bipartite(graphOnto)
```

**Arguments**

graphOnto      A graphNEL graph with ‘m’ cross-Ontology node labels.

**Details**

The **Gene Ontology** (GO) is structured as a directed acyclic graph (DAG) with nodes (GO-terms) representing gene functions and edges characterizing relationships between nodes. A variety of relationships are possible (currently 8). To compute GO-term predictions perfectly aware of GO-term relationships, a Forney Factor Graph is required. Hence, GO-terms are mapped to binary variable nodes, and relationships to logical factor nodes.

**Value**

A binary matrix with  $2*m$  rows by  $2*m-1$  columns where  $m$  is the quantity of cross-Ontology node labels.

**Author(s)**

Flavio E. Spetale <spetale@cifasis-conicet.gov.ar>

**References**

F. Spetale, J. Murillo, E. Tapia, D. Arce, S. Ponce, and P. Bulacio, “Formal modeling of gene ontology annotation predictions based on factor graphs,” *Journal of Physics: Conference Series*, vol. 705, no. 1, p. 012001, 2016.

Spetale F.E., Tapia E., Krsticevic F., Roda F. and Bulacio P. “A Factor Graph Approach to Automated GO Annotation”. *PLoS ONE* 11(1): e0146986, 2016.

Spetale Flavio E., Arce D., Krsticevic F., Bulacio P. and Tapia E. “Consistent prediction of GO protein localization”. *Scientific Report* 7787(8), 2018

**Examples**

```
data(CfData)
```

```
graphGO <- as(CfData$graphCfGO, "graphNEL")  
fgga2bipartite(graphGO)
```

fMeasure

*Individual and hierarchical F-measures***Description**

Set of functions to compute the individual and hierarchical F-score, precision, recall.

**Usage**

```
fMeasures(target, predicted, cutoff = 0.5)
fMeasuresByLevel(target, predicted, graphOnto, cutoff = 0.5)
fHierarchicalMeasures(target, predicted, graphOnto, cutoff = 0.5)
```

**Arguments**

target	A binary matrix with 'n' proteins (rows) by 'm' Ontology node labels (columns) corresponding to the target of ontology terms where 0 stands for negative and 1 for positive.
predicted	A real matrix with 'n' proteins (rows) by 'm' Ontology node labels (columns) corresponding to the predicted terms.
graphOnto	A graphNEL graph with 'm' Ontology node labels.
cutoff	A real value to divide the predicted terms into positive and negative. The predicted values higher than the cutoff will be taken as positive.

**Details**

fMeasures computes the F-score, precision, recall, specificity and accuracy for each ontological term.

fMeasuresByLevel computes F-score, precision, recall, specificity and accuracy for all ontological terms belongs to graph. The levels are calculated as the maximum distance between two terms of the graph.

fHierarchicalMeasures computes the hierarchical F-score, precision, recall for the predicted terms of a set of proteins.

**Value**

fMeasures and fMeasuresByLevel returns a list of two elements where the first element is a named vector with six attributes while the second element is an array of 'm' ontological terms by six attributes. The 6 attributes are:

Prec:	Precision
Recall:	Recall
Specif:	Specificity
Fmeasure:	F-score
Acc:	Accuracy



nPositive: Number of positive samples

fHierarchicalMeasures returns a list of five elements:

HP: Hierarchical Precision

HR: Hierarchical Recall

HF: Hierarchical F-score

nSample: Number of proteins evaluated

noEvalSample: Named vector of proteins not evaluated

### Author(s)

Flavio E. Spetale <spetale@cifasis-conicet.gov.ar>

### References

Verspoor K, Cohn J, Mnizewski S, C J. A categorization approach to automated ontological function annotation. Protein Science. 2006;15:1544–1549.

### Examples

```
data(CfData)

predGO <- matrix(runif(360, 0, 1),10,36, dimnames=list(rownames(
  CfData[["tableCfGO"]][seq_len(10)], colnames(CfData[["tableCfGO"]]))))

fMeasures(CfData[["tableCfGO"]][seq_len(10), ], predGO, cutoff = 0.5)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

fHierarchicalMeasures(CfData[["tableCfGO"]][seq_len(10), ], predGO, mygraphGO,
  cutoff = 0.5)
```

---

maxDistancegraphOnto *Maximum distance for a graph*

---

### Description

Computes the maximum distance from any node to the root of the graph

### Usage

```
maxDistancegraphOnto(graphOnto)
```

### Arguments

graphOnto A graphNEL graph with ‘m’ Ontology node labels.

**Details**

This function computes a distance matrix for a graph

**Value**

Named numeric array containing the distance from any node to the root.

**Author(s)**

Flavio E. Spetale <spetale@cifasis-conicet.gov.ar>

**See Also**

[fMeasure](#)

**Examples**

```
data(CfData)
mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")
maxDistancegraphOnto(mygraphGO)
```

---

```
preCoreFG
```

*Transitive closure processing of a cross-ontology DAG*

---

**Description**

preCoreFG ensures the transitive closure of inference paths -serial concatenation of relationships- in a cross-ontology DAG.

**Usage**

```
preCoreFG(ontoTerms, domains = "GO")
```

**Arguments**

ontoTerms	A vector with ‘m’ cross-ontology node labels
domains	A string that indicates which subdomains or ontologies will be used. Values: “GOBP”, “GOMF”, “GOCC”, “GOCC-PO”, “GOCC-ZFA”, “GOBP-HPO”, “GOMF-HPO”, “GOCC-HPO”, “GO-PO”, “GO-ZFA”, “GO-HPO”, “GO” (default, “BP-MF-CC”)

**Details**

Non-transitive relationships in cross-ontology DAG's may lead to non-transitive inference paths precluding the free propagation and consistency checking of ontology annotations. A transitive closure screening process over cross-ontology DAG's relationships is required before the construction of Forney Factor Graphs. Serial concatenation of relationships leading to non-transitive inference paths in a cross-ontology DAG are conformed by removing the most specific relationship.

**Value**

A graphNEL graph with 'm' node labels belong to ontologies used.

**Author(s)**

Flavio E. Spetale <spetale@cifasis-conicet.gov.ar>

**References**

Spetale Flavio E., Arce D., Krsticevic F., Bulacio P. and Tapia E. "Consistent prediction of GO protein localization". Scientific Report 7787(8), 2018

**See Also**

[fgga2bipartite](#)

**Examples**

```
data(CfData)

myGOs <- c(CfData[["nodesGO"]], "GO:1902494", "GO:0032991", "GO:1990234",
          "GO:0005575")

# mygraphGO <- preCoreFG(myGOs, domains = "GOMF")
```

---

sumProduct

*Message passing algorithm between nodes of the Forney Factor Graph*

---

**Description**

msgFGGA operates in Forney Factor Graphs and computes approximate maximum a posteriori (MAP) estimates of hidden Ontology variable nodes (Ontology-terms).

**Usage**

```
msgFGGA(matrixFGGA, obsValueOntoTerms, graphOnto, tmax = 200,
        epsilon = 0.001)
```

**Arguments**

matrixFGGA	A binary matrix with FGGA model of the class ‘fgga.’
obsValueOntoTerms	A named vector with ‘m’ probabilistic prediction values for a protein coding gene.
graphOnto	A graphNEL graph with ‘m’ Ontology node labels.
tmax	An integer indicating the maximum number of iterations (default: 200).
epsilon	An integer that represents the convergence criteria (default: 0.001)

**Details**

Starting from Ontology-term predictions at observable variable nodes, probability distribution functions modelling the learning noise of individual Ontology-terms, a user-defined number of iterations (maximum 200), a user-defined threshold for the convergence of predictions (maximum 0.001), and the structure of the Forney Factor Graph, the **msgFGGA** delivers approximate maximum a posteriori (MAP) estimates of hidden GO variable nodes (GO-terms).

**Value**

A named vector with ‘m’ consistent probabilistic predictions for a protein coding genes.

**Author(s)**

Flavio E. Spetale and Elizabeth Tapia <spetale@cifasis-conicet.gov.ar>

**References**

- Kschischang FR, Frey BJ, Loeliger H.-A. Factor graphs and the sum-product algorithm. *IEEE Trans. Inf. Theor.* 47, 498–519 (2001).
- Yedidia JS. Message-passing algorithms for inference and optimization. *Journal of Statistical Physics* 145, 860–890 (2011).
- Spetale FE, Tapia E, Krsticevic F, Roda F, Bulacio P (2016). A Factor Graph Approach to Automated GO Annotation. *PLOS ONE* 11(1): e0146986

**See Also**

[tableTPG](#)

**Examples**

```
data(CfData)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

myTableGO <- CfData[["tableCfGO"]][
  CfData[["indexGO"]]$indexTrain[1:500], ]

modelSVMs <- lapply(CfData[["nodesGO"]], FUN = svmTrain,
```

```

tableOntoTerms = myTableGO,
dxCharacterized = CfData[["dxCf"]],
graphOnto = mygraphGO, kernelSVM = "radial")

rootGO <- leaves(mygraphGO, "in")

varianceGOs <- CfData[["varianceGOs"]]

dxTestCharacterized <- CfData[["dxCf"]][
  sample(1:dim(CfData[["dxCf"]])[2], 2), ]

matrixGOTest <- svmOnto(svmModel = modelSVMs,
  dxCharacterized = dxTestCharacterized,
  rootNode = rootGO, varianceSVM = varianceGOs)

modelFGGA <- fgga2bipartite(mygraphGO)

matrixFGGATest <- t(apply(matrixGOTest, MARGIN = 1, FUN = msgFGGA,
  matrixFGGA = modelFGGA, graphOnto= mygraphGO,
  tmax = 50, epsilon = 0.1))

```

svmOnto

*Ontology-term predictions by binary SVM classifiers***Description**

svmOnto delivers soft Ontology-term predictions based on binary SVM classification models.

**Usage**

```
svmOnto(svmModel, dxCharacterized, rootNode, varianceSVM)
```

**Arguments**

svmModel	A list of object of class "svm" created by svm.
dxCharacterized	A data frame with 'n' protein coding genes (rows) by 'f' features (columns).
rootNode	A character indicating the root of the graph.
varianceSVM	A vector named with the variance of cross-Ontology node labels.

**Details**

Binary SVM predictions are supplemented with their corresponding margins. These margins are used to model the additive zero-mean Gaussian learning noise that corrupts ideal but hidden Ontology-term predictions. These ideal predictions are embedded in hidden variable nodes of the Forney Factor Graph.

**Value**

svmOnto            A named vector of predicted values for a protein sequence.

**Author(s)**

Flavio E. Spetale, Pilar Bulacio and Javier Murillo <spetale@cifasis-conicet.gov.ar>

**References**

Chang, Chih-Chung and Lin, Chih-Jen: LIBSVM: a library for Support Vector Machines <http://www.csie.ntu.edu.tw/~cjlin/libsvm>

Eisner R, Poulin B, Szafron D, Lu P, Greiner R. Improving protein function prediction using the hierarchical structure of the Gene Ontology. In: Proc. IEEE CIBCB; 2005. p. 1–1

Spetale FE, Tapia E, Krsticevic F, Roda F, Bulacio P (2016). A Factor Graph Approach to Automated GO Annotation. PLOS ONE 11(1): e0146986

**See Also**

[svmTrain](#)

**Examples**

```
data(CfData)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

modelSVMs <- lapply(CfData[["nodesGO"]][1:4], FUN = svmTrain,
                   tableOntoTerms = CfData[["tableCfGO"]],
                   dxCharacterized = CfData[["dxCf"]],
                   graphOnto = mygraphGO, kernelSVM = "radial")

rootGO <- leaves(mygraphGO, "in")

varianceGOs <- CfData[["varianceGOs"]]

# SVM testing in four GO-terms
dxTestCharacterized <- CfData[["dxCf"]][
  sample(1:dim(CfData[["dxCf"]])[1], 20), ]

matrixGOTest <- svmOnto(svmModel = modelSVMs,
                       dxCharacterized = dxTestCharacterized,
                       rootNode = rootGO, varianceSVM = varianceGOs)
```

---

svmTrain	<i>Binary SVM classification models for individual Ontology-term predictions</i>
----------	--

---

## Description

svmTrain delivers a set of binary SVM classifiers for different Ontology-terms.

## Usage

```
svmTrain(nodeGraph, tableOntoTerms, dxCharacterized, graphOnto,
         kernelSVM = "radial")
```

## Arguments

nodeGraph	A character indicating a GO node label
tableOntoTerms	A binary matrix with ‘n’ proteins (rows) by ‘m’ Ontology node labels (columns).
dxCharacterized	A data frame with ‘n’ protein coding genes (rows) by ‘f’ features (columns).
graphOnto	A graphNEL graph with ‘m’ Ontology node labels.
kernelSVM	The kernel used to calculate the variance (default: radial).

## Details

Starting from sets of positively annotated protein sequences to different GO-terms in a GO sub-graph, corresponding sets of negatively annotated protein sequences are computed using the inclusive separation policy proposed by Eisner et al. Training datasets for each GO-term are used to train binary Support Vector Machine (SVM) classifiers with a variety of kernel options.

## Value

svmTrain	A list of objects of “svm” class containing the fitted model.
----------	---

## Author(s)

Flavio E. Spetale, Pilar Bulacio and Javier Murillo <spetale@cifasis-conicet.gov.ar>

## References

- Chang, Chih-Chung and Lin, Chih-Jen: LIBSVM: a library for Support Vector Machines <http://www.csie.ntu.edu.tw/~cjlin/libsvm>
- Eisner R, Poulin B, Szafron D, Lu P, Greiner R. Improving protein function prediction using the hierarchical structure of the Gene Ontology. In: Proc. IEEE CIBCB; 2005. p. 1–1
- Spetale FE, Tapia E, Krsticevic F, Roda F, Bulacio P (2016). A Factor Graph Approach to Automated GO Annotation. PLOS ONE 11(1): e0146986

**See Also**[svmOnto](#)**Examples**

```

data(CfData)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

# SVM training in four GO-terms
modelSVMs <- lapply(CfData[["nodesGO"]][1:4], FUN = svmTrain,
                    tableOntoTerms = CfData[["tableCfGO"]],
                    dxCharacterized = CfData[["dxCf"]],
                    graphOnto = mygraphGO, kernelSVM = "radial")

```

---

tableTPG	<i>Valid configurations for hidden variable nodes in a Forney Factor Graph</i>
----------	--

---

**Description**

tableTPG provides valid configurations of hidden variable nodes at logical function nodes in a Forney Factor Graph under the True Path Graph (TPG) constraint.

**Usage**

```
tableTPG(att)
```

**Arguments**

`att` An integer indicating the number of cross-Ontology nodes involved

**Details**

Valid configurations of hidden variable nodes at logical function nodes enable messaging passing across the Forney Factor Graph. The TPG constraint is defined as: “If the child Ontology node describes the protein, then all its parent terms must also apply to that protein; and if a Ontology node does not describe a protein, then all its descendant Ontology nodes must not describe it”. The TPG constraint governs the structure of the Ontology-DAG and the inference process in the associated Forney Factor Graph.

**Value**

A binary matrix with  $(n-1)^2+1$  rows by  $n+1$  columns where  $n = attr$

**Author(s)**

Flavio E. Spetale, Pilar Bulacio and Javier Murillo <spetale@cifasis-conicet.gov.ar>



## References

- Tanoue J, Yoshikawa M, Uemura S (2012). The Gene Around GO viewer. *Bioinformatics* 18(12): 1705–1706.
- Spetale FE, Tapia E, Krsticevic F, Roda F, Bulacio P (2016). A Factor Graph Approach to Automated GO Annotation. *PLOS ONE* 11(1): e0146986

## Examples

```
tableTPG(3)
```

---

varianceOnto	<i>The variance of the gaussian learning noise at individual Ontology-terms</i>
--------------	---

---

## Description

varianceOnto estimates the variance of gaussian distributions modeling the additive learning noise that corrupts ideal Ontology-term predictions.

## Usage

```
varianceOnto(tableOntoTerms, dxCharacterized, kFold, graphOnto, rootNode,
             kernelSVM = "radial")
```

## Arguments

- `tableOntoTerms` A binary matrix with ‘n’ protein coding genes (rows) by ‘m’ cross-Ontology node labels (columns).
- `dxCharacterized` A data frame with ‘n’ protein coding genes (rows) by ‘f’ features (columns).
- `kFold` An integer for the number of folds.
- `graphOnto` A graphNEL graph with ‘m’ cross-Ontology node labels.
- `rootNode` A character indicating the root of the graph.
- `kernelSVM` The kernel used to calculate the variance (default: radial).

## Details

Under the assumption of symmetrical (Gaussian) conditional probability distributions for observable variable node predictions  $y_i$  over a hidden variable node annotations  $x_i$ , variances  $\eta_i$  can be estimated using a validation dataset of positively annotated samples. Let  $D$  be a validation dataset with  $L^+$  positively annotated samples

$$\hat{\eta}_i = 1/(L^+ - 1) * \sum_{i=1}^L (x_i - y_i)$$

where  $x_i = 1$  is the positive annotation of the  $i$ -th data sample to the  $i$ th Ontology-term and  $y_i$  is the corresponding real-valued classifier (SVM) prediction.

**Value**

A vector named with the variance of each cross-Ontology node.

**Author(s)**

Flavio E. Spetale <spetale@cifasis-conicet.gov.ar>

**References**

Spetale FE, Tapia E, Krsticevic F, Roda F, Bulacio P (2016). A Factor Graph Approach to Automated GO Annotation. PLOS ONE 11(1): e0146986

**Examples**

```
data(CfData)

mygraphGO <- as(CfData[["graphCfGO"]], "graphNEL")

rootGO <- leaves(mygraphGO, "in")

mygraphGO <- subGraph(c("GO:0140110", "GO:0098772", "GO:0003674"), mygraphGO)

myTableGO <- CfData[["tableCfGO"]][
  CfData[["indexGO"]]$indexTrain,
  c("GO:0140110", "GO:0098772", "GO:0003674")]

varianceGOs <- varianceOnto(tableOntoTerms = myTableGO,
  dxCharacterized = CfData[["dxCf"]],
  kFold = 2, graphOnto = mygraphGO,
  rootNode = rootGO, kernelSVM = "radial")
```

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