# PySCMs Release 2.0.0

**Black-Swan-ICL** 

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CHAPTER

ONE

### STRUCTURALCAUSALMODELS

### 1.1 StructuralCausalModels package

#### 1.1.1 Submodules

#### 1.1.2 StructuralCausalModels.dag module

exception StructuralCausalModels.dag.TopologicalOrderingMethodNotImplemented
Bases: Exception

Raised when the requested topological ordering method is not implemented.

exception StructuralCausalModels.dag.InvalidOrdering
 Bases: Exception

Raised when an ordering is not a valid causal ordering for a given DAG.

class StructuralCausalModels.dag.DirectedAcyclicGraph(adjacency\_matrix, name=")
 Bases: StructuralCausalModels.directed\_graph.DirectedGraph

A class to represent Directed Acyclic Graphs (DAGs).

A DirectedAcyclicGraph object is a representation of a DAG. It is defined by the adjacency matrix of the graph ; validation will be performed to check that the graph defined is directed and acyclic. An exception will be raised otherwise.

#### **Parameters**

- adjacency\_matrix (array\_like) The adjacency matrix of the graph.
- **name** (*str, optional*) The name of the object created (default is '').
- **Raises** *InvalidAdjacencyMatrix* If the adjacency matrix does not define a directed and acyclic graph.

#### static validate\_dag\_adjacency\_matrix (matrix, atol=1e-06)

Checks that a matrix is a valid adjacency matrix for a directed acyclic graph. Uses the characterisation of acyclicity established by D. Wei, T. Gao and Y. Yu in<sup>1</sup> : a directed graph is acyclic if and only if its adjacency matrix is nilpotent.

#### Parameters

• **matrix** (*array\_like*) – The matrix to check.

<sup>&</sup>lt;sup>1</sup> Wei, D., Gao, T. and Yu, Y. "DAGs with No Fears : A Closer Look at Continuous Optimization for Learning Bayesian Networks". *Advances in Neural Information Processing Systems*, volume 33, pp. 3895-3906, 2020.

- **atol** (*float, optional*) The absolute tolerance used to check that the eigenvalues are all equal to 0 (default is  $10^{-6}$ ).
- **Returns** *bool* Whether the matrix to check is a valid adjacency matrix for a directed acyclic graph.

#### Notes

#### kahn\_algorithm()

An implementation of Kahn's algorithm for topological ordering of a graph.

**Returns** *list* – A topological ordering of the graph.

#### compute\_causal\_order(method='kahn')

Computes a causal order of the DAG using the method chosen by the user.

**Parameters method** (*str; optional*) – The method to use to compute the causal order (default is 'kahn').

**Returns** *list* – A causal order of the DAG.

**Raises** TopologicalOrderingMethodNotImplemented – If the method chosen by the usr is not implemented.

#### check\_topological\_ordering(ordering)

Checks whether an ordering is a correct topological ordering for the graph.

Parameters ordering (list) – The candidate ordering.

**Returns** *bool* – Whether the ordering is a correct topological ordering for the graph.

**Raises** *InvalidOrdering* – If the ordering passed is not a valid ordering for the graph.

#### static causal\_order\_to\_dag(causal\_order)

Generates the maximally connected DAG that is compatible with the causal order provided i.e. for all j such that j > i in the causal order, there will be an edge from  $X_i$  to  $X_j$  in the DAG (i.e. there will be a 1 in position [i, j] in the DAG's adjacency matrix).

**Parameters causal\_order** (*array\_like*) – The causal order.

**Returns** *DirectedAcyclicGraph* – The maximally connected DAG compatible with the causal order.

#### 1.1.3 StructuralCausalModels.directed\_graph module

class StructuralCausalModels.directed\_graph.DirectedGraph(adjacency\_matrix,

name = '')

Bases: StructuralCausalModels.graph.Graph

A class to represent directed graphs.

A DirectedGraph object is a representation of a directed graph. It is defined by the adjacency matrix of the graph ; validation will be performed to check that the graph defined is directed. An exception will be raised otherwise.

#### Parameters

- adjacency\_matrix (array\_like) The adjacency matrix of the graph.
- **name** (*str, optional*) The name of the object created (default is '').

Raises InvalidAdjacencyMatrix – If the adjacency matrix does not define a directed graph.

static validate\_directed\_graph\_adjacency\_matrix(matrix)

Checks that a matrix is a valid adjacency matrix for a directed graph.

Parameters matrix (array\_like) – The matrix to check.

**Returns** *bool* – Whether the matrix to check is a valid adjacency matrix for a directed graph.

### 1.1.4 StructuralCausalModels.graph module

class StructuralCausalModels.graph.Graph(adjacency\_matrix, name=")

Bases: object

A class to represent graphs.

A Graph object is a representation of the graph. The graph may be very general : it does not have to be directed, or acyclic for instance. It is arguably easiest to think of a graph in terms of its adjacency matrix which is why this implementation is 'adjacency matrix'-driven. Other representations can be more convenient depending on context, which is why these representations are automatically generated upon construction and stored as attributes of the Graph object.

#### Parameters

- adjacency\_matrix (array\_like) The adjacency matrix of the graph.
- **name** (*str*, *optional*) The name of the object created (default is ``).

#### adjacency\_matrix\_representation

The representation of the graph based on the adjacency matrix.

Type GraphViaAdjacencyMatrix

#### adjacency\_list\_representation

The representation of the graph based on the adjacency lists.

**Type** GraphViaAdjacencyLists

#### edge\_representation

The adjacency of the graph based on the typed (undirected, forward etc.) edges.

**Type** *GraphViaEdges* 

#### static validate\_binary\_matrix(matrix)

Validates that a matrix is a proper adjacency matrix.

A proper adjacency matrix contains only 0's and 1's.

**Parameters matrix** (*array\_like*) – The matrix to validate.

**Returns** *bool* – Whether the matrix is a valid adjacency matrix.

#### property name

the name of the graph.

Type str

#### property adjacency\_matrix

the adjacency matrix of the graph.

Type array\_like

#### **structural\_hamming\_distance** (*other*, *penalty\_edge\_mismatch\_func=None*) Computes the Structural Hamming Distance between two graphs.

By default, the Structural Hamming Distance (SHD) is equal to the number of edges in the graphs that are not of the same type. A different weighted scheme for penalty computation may be provided (we may

want to penalise the presence of an edge in the opposite direction more than the absence of an edge, for example).

#### **Parameters**

- other (*Graph*) The graph to compare.
- **penalty\_edge\_mismatch\_func** (*callable, optional*) The edge mismatch penalty scheme (default is None in which case a built-in function is used).
- **Returns** *float* The Structural Hamming Distance (SHD), in its default form or under a userprovided edge mismatch penalty scheme.

Raises GraphsCannotBeCompared - Raised if the graphs do not have the same vertex set.

#### static adjacency\_matrix\_to\_adjacency\_lists(adjacency\_matrix)

Converts an adjacency matrix to the corresponding adjacency lists.

Parameters adjacency\_matrix (array\_like) – The adjacency matrix.

**Returns** *list* – The adjacency lists.

**static adjacency\_lists\_to\_adjacency\_matrix** (*adjacency\_lists*) Converts adjacency lists to the corresponding adjacency matrix.

**Parameters adjacency\_lists** (*list*) – The adjacency lists.

**Returns** *array\_like* – The adjacency matrix.

#### static compute\_edge\_type (m\_ij, m\_ji)

Determines the type of the edge between two vertices.

Determines the type of the edge between  $X_i$  and  $X_j$  based on the values of  $M_{i,j}$  and  $M_{j,i}$  where M is the adjacency matrix of the graph.

#### **Parameters**

- **m\_ij** (*int*) The element in the adjacency matrix at the intersection of the i-th row and the j-th column.
- **m\_ji** (*int*) The element in the adjacency matrix at the intersection of the j-th row and the i-th column.

**Returns** *EdgeType* – The typed edge between  $X_i$  and  $X_j$  in the graph.

#### static adjacency\_matrix\_to\_edges(adjacency\_matrix)

Converts adjacency matrix to the corresponding typed edges.

Parameters adjacency\_matrix (array\_like) – The adjacency matrix.

#### Returns

*dict* – The typed edges.

The keys are tuples (i, j); they indicates the edge is between  $X_i$  and  $X_j$  in the graph. The values are EdgeType objects which indicate what type of edge is between  $X_i$  and  $X_j$  in the graph.

#### static edges\_to\_adjacency\_lists(edges)

Converts the typed edges to the corresponding adjacency lists.

**Parameters edges** (*dict*) – The typed edges.

The keys are tuples (i, j); they indicates the edge is between  $X_i$  and  $X_j$  in the graph. The values are EdgeType objects which indicate what type of edge is between  $X_i$  and  $X_j$  in the graph.

Returns list - The adjacency lists.

#### static edges\_to\_adjacency\_matrix(edges)

Converts the typed edges to the corresponding adjacency matrix.

**Parameters edges** (*dict*) – The typed edges.

The keys are tuples (i, j); they indicates the edge is between  $X_i$  and  $X_j$  in the graph. The values are EdgeType objects which indicate what type of edge is between  $X_i$  and  $X_j$  in the graph.

**Returns** *array\_like* – The adjacency matrix.

```
static adjacency_lists_to_edges(adjacency_lists)
```

Converts adjacency lists to the corresponding typed edges..

**Parameters adjacency\_lists** (*list*) – The adjacency lists.

Returns

dict – The typed edges.

The keys are tuples (i, j); they indicates the edge is between  $X_i$  and  $X_j$  in the graph. The values are EdgeType objects which indicate what type of edge is between  $X_i$  and  $X_j$  in the graph.

#### 1.1.5 StructuralCausalModels.graph\_via\_adjacency\_lists module

exception StructuralCausalModels.graph\_via\_adjacency\_lists.InvalidAdjacencyLists
 Bases: Exception

Raised when the adjacency lists are not valid for the graph.

**class** StructuralCausalModels.graph\_via\_adjacency\_lists.**GraphViaAdjacencyLists**(*nb\_vertices*,

adjacency\_lists, name=")

Bases: object

Implements a graph structure using an adjacency list representation.

As an "extra security", the number of vertices must be provided as well as the adjacency lists ; there must be as many vertices as there are adjacency lists.

#### Parameters

- **nb\_vertices** (*int*) The number of vertices in the graph.
- **adjacency\_lists** (*list*) The list of adjacency lists defining the graph. The ordering in the list is the natural one : adjacency\_lists[0] is the adjacency list for vertex X<sub>0</sub> etc.
- name (str, optional) The name of the object created (default is '').

#### indegrees

The list of in-degrees of the vertices i.e. the number of edges pointing to the vertices. The ordering in the list is the natural one : indegrees[0] is the in-degree for vertex  $X_0$  etc.

Type list

**Raises** *InvalidAdjacencyLists* – If the number of adjacency lists provided does not match the number of vertices in the graph.

#### 1.1.6 StructuralCausalModels.graph\_via\_adjacency\_matrix module

exception StructuralCausalModels.graph\_via\_adjacency\_matrix.InvalidAdjacencyMatrix
Bases: Exception

Raised if the adjacency matrix does not contain only 0's and 1's.

class StructuralCausalModels.graph\_via\_adjacency\_matrix.GraphViaAdjacencyMatrix(adjacency\_matrix)

name = '')

Bases: object

Implements a graph structure using an adjacency matrix representation.

#### Parameters

• adjacency\_matrix (array\_like) – The adjacency matrix of the graph.

• name (*str*, *optional*) – The name of the object created (default is '').

**Raises** *InvalidAdjacencyMatrix* – If the adjacency matrix provided does not contain only 0's and 1's.

```
static validate_binary_matrix(matrix)
```

Checks that a matrix is an adjacency matrix (i.e. a square matrix containing only 0's and 1's).

Parameters matrix (array\_like) – The matrix to check.

Returns *bool* – Whether the matrix is a valid adjacency matrix.

#### 1.1.7 StructuralCausalModels.graph\_via\_edges module

```
class StructuralCausalModels.graph_via_edges.EdgeType(value)
```

Bases: enum.Enum

An enumeration to represent possible types of edges between vertices.

NONE = 'no edge'

```
FORWARD = ' \rightarrow '
```

BACKWARD = ' < -'

UNDIRECTED = '--'

exception StructuralCausalModels.graph\_via\_edges.GraphsCannotBeCompared Bases: Exception

Raised when two graphs do not have the same vertex set.

exception StructuralCausalModels.graph\_via\_edges.ImpossibleEdgeConfiguration
 Bases: Exception

Raised when an edge is not one of the possible types of edges.

class StructuralCausalModels.graph\_via\_edges.GraphViaEdges(edges, name=")
 Bases: object

Implements a graph structure using a representation via typed edges.

Typed edges make it possible than  $X_i$  and  $X_j$  have no edge between them, or that they have an undirected edge, or a forward edge  $X_i \longrightarrow X_j$  or a backward edge  $X_i \longleftarrow X_j$ .

#### Parameters

- edges (dict) A dictionary defining the edges of the graph in the format (i, j) : EdgeType.FORWARD for  $X_i \longrightarrow X_j$ , for example.
- **name** (*str, optional*) The name of the object created (default is '').

#### static compute\_penalty(edge\_1, edge\_2)

Provides a default method to compute the penalty incurred when two edges are of a same type or of different types.

#### Parameters

- **edge\_1** (*EdgeType*) The first edge.
- **edge\_2** (*EdgeType*) The second edge.

**Returns** *float* – The penalty incurred.

**Raises** ImpossibleEdgeConfiguration – If one of the edges is not one of the possible types of edges.

#### structural\_hamming\_distance(other, penalty\_edge\_mismatch\_func=None)

Computes the Structural Hamming Distance between two graphs. By default it is equal to the number of edges in the graphs that are not of the same type. A different weighted scheme for penalty computation may be provided (we may want to penalise the presence of an edge in the opposite direction more than the absence of an edge, for example).

#### Parameters

- **other** (*GraphViaEdges*) The graph to compare.
- **penalty\_edge\_mismatch\_func** (*callable*) The edge mismatch penalty scheme.
- **Returns** *float* The Structural Hamming Distance (SHD), in its default form or under a userprovided edge mismatch penalty scheme.

**Raises** GraphsCannotBeCompared – Raised if the graphs do not have the same vertex set.

#### 1.1.8 StructuralCausalModels.linear\_structural\_causal\_model module

exception StructuralCausalModels.linear\_structural\_causal\_model.InvalidWeightedAdjacencyMat Bases: Exception

Raised if the weighted adjacency matrix does not define a directed graph.

exception StructuralCausalModels.linear\_structural\_causal\_model.InvalidNumberOfExogenousVas Bases: Exception

Raised if the number of exogenous variables provided is incorrect.

By incorrect is meant that the number of exogenous variables provided is inconsistent with the number of variables expected in the SCM.

class StructuralCausalModels.linear\_structural\_causal\_model.LinearStructuralCausalModel(name)

nb\_

strı ture

Bases: StructuralCausalModels.structural\_causal\_model.StructuralCausalModel

A class to represent linear Structural Causal Models.

Beware, does not check the equation are linear.

Parameters

- **nb\_var** (*int*) The number of variables in the SCM.
- structural\_equations (*list*) The list of the structural equations defining the SCM.
- name (*str*, *optional*) The name of the SCM (default is '').

static create\_from\_coefficient\_matrix (matrix, causal\_order, exogenous\_variables,

*name="*) Creates a linear SCM from a coefficient matrix.

The coefficient matrix is interpreted as the weighted adjacency matrix of the graph associated to a linear SCM.

#### **Parameters**

- **matrix** (*numpy.ndarray*) The weighted adjacency matrix of the graph associated to the linear SCM to build.
- causal\_order (array\_like) A causal order of the graph associated to the SCM.
- exogenous\_variables (*list*) The list of the exogenous variables. Note that the list must be ordered in the "natural" way not necessarily in the causal ordering. In other terms, exogenous\_varoables[0] contains the exogenous variables for the structural equation that has  $X_0$  on its left-hand side etc.
- name (str, optional) The name of the linear SCM created (default is '').

**Returns** *LinearStructuralCausalModel* – The linear SCM corresponding to the weighted adjacency matrix provided.

#### Raises

- *InvalidWeightedAdjacencyMatrix* If the weighted adjacency matrix provided defines a graph that is not a directed graph.
- InvalidNumberOfExogenousVariables If the number of exogenous variables provided does not correspond to the number of variables expected from the matrix provided.

#### 1.1.9 StructuralCausalModels.structural\_causal\_model module

exception StructuralCausalModels.structural\_causal\_model.InconsistentStructuralCausalModelN Bases: Exception

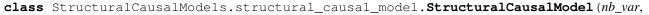
Raised if the Structural Causal Model is not defined in a consistent way.

exception StructuralCausalModels.structural\_causal\_model.CyclicityWarning
Bases: UserWarning

Raised if there is a high probability that the SCM contains a cycle.

exception StructuralCausalModels.structural\_causal\_model.InvalidIntervention
 Bases: Exception

Raised if the intervention attempted is invalid.



structural\_equations, name=")

Bases: object

A class to represent Structural Causal Models (SCMs).

As an "extra security", the number of variables must be provided in addition to the structural equations ; the number of variables must be equal to the number of structural equations.

#### **Parameters**

- **nb\_var** (*int*) The number of variables in the SCM.
- **structural\_equations** (*list*) The list of the structural equations defining the SCM.
- **name** (*str*; *optional*) The name of the SCM (default is '').

#### Raises

- *InconsistentStructuralCausalModelDefinition* If the number of structural equations provided does not correspond to the number of variables in the SCM.
- *CyclicityWarning* If the SCM defined is (highly likely to be) cyclic.

#### generate\_data (nb\_samples)

Generates samples from an SCM.

**Parameters nb\_samples** (*int*) – The number of samples to generate.

#### Returns

pandas.DataFrame – A dataframe containing the samples.

The column names correspond to the variables in the SCM. Thus column 0 contains the samples for  $X_0$ , column 1 the samples for  $X_1$  etc.

#### adjacency\_matrix()

Generates the adjacency matrix of the graph corresponding to the SCM.

Returns *numpy.ndarray* – The adjacency matrix of the graph corresponding to the SCM.

#### compute\_causal\_order()

Computes a causal order of the DAG associated to the SCM.

**Returns** *list* – A causal order of the DAG associated to the SCM.

#### order\_structural\_equations()

Returns structural equations, ordered to follow a causal order.

The structural equations may or may not be provided in an order that is consistent with a causal ordering of the DAG associated to the SCM. This function returns the list of structural equations ordered in a manner consistent with a causal ordering of the associated DAG.

**Returns** *list* – The structural equations making up the SCM, causally ordered.

#### check\_no\_cycles(atol=1e-06)

Checks that the SCM defined is not cyclic.

Note that this function is essentially a wrapper around static method DirectedAcyclic-Graph.validate\_dag\_adjacency\_matrix, which relies on characterisation of acyclicity by the nilpotence of the adjacency matrix.

As eigenvalues are only ever computed approximately, it is theoretically possible than an eigenvalue is computed as very small but non-zero even though it is actually zero hence the use of a tolerance.

**Parameters atol** (*float, optional*) – The absolute tolerance used to check that the eigenvalues are all equal to 0 (default is  $10^{-6}$ ).

Raises CyclicityWarning - If the SCM is (highly likely to be) cyclic.

**perform\_intervention** (*new\_structural\_equation*) Performs an intervention on the SCM.

Performs an intervention on the SCM by replacing one of its constitutive structural equations by a new structural equation.

**Parameters** new\_structural\_equation (*StructuralEquation*) – The new structural equation.

Returns StructuralCausalModel - The post-intervention SCM.

Raises

- **InvalidIntervention** If the new structural equation does not correspond to an existing one i.e. it has  $X_{i_0}$  on its left-hand side but there is no  $X_{i_0}$  variable in the SCM.
- CyclicityWarning If the post-intervention SCM is (highly likely to be) cyclic.

#### 1.1.10 StructuralCausalModels.structural\_equation module

class StructuralCausalModels.structural\_equation.StructuralEquation (index\_lhs,

indices\_rhs, exogenous\_variable, function)

Bases: object

A class to represent structural equations.

Structural Equations are assignments of the sort

$$X_i := g((X_j)_{j \in J}, U_i),$$

where  $U_i$  is an exogenous (random) variable.

#### Parameters

- **index\_lhs** (*int*) The index of the structural variable on the left-hand side of the structural equation (the "i").
- indices\_rhs (*list*) The indices of the structural variables on the right-hand side of the structural equation (the "j's in J").
- exogenous\_variable (*scipy.stats.rv\_continuous or scipy.stats.rv\_discrete*) The exogenous variable (the "U<sub>i</sub>").
- **function** (*callable*) The function defining the functional form of the assignment in the structural equation (the "g").

#### generate\_data(data)

Generates samples from a structural equation.

**Parameters data** (*pandas.DataFrame*) – A dataframe containing data at least for the structural variables on the right-hand side of the structural equation.

If it contains data for the structural variable on the left-hand side of the structural equation, that data will be overwritten.

**Returns** pandas.DataFrame – The samples.

### **1.1.11 Module contents**

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TWO

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