
K-CHAIN Documentation

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MODULE: KCHAIN

This module consists of `kChainModel` class to create, fit, append, and update K-CHAIN models in TensorFlow

class `kChain.kChainModel` (*debug=False*)

__init__ (*debug=False*)

Initialize object of type K-CHAIN model.

Parameters *debug* (*bool*) – various print statements throughout the code execution will be executed to help in debugging.

_createEqnModel (*inputVar, outputVar, mdlName, eqMdl*)

Build a K-CHAIN model using input and output variables from the KG and the physics equation.

Parameters

- **inputVar** (*JSON array*) – array of JSON variable objects with name, type, and value fields
- **outputVar** (*JSON array*) – array of JSON variable objects with name, type, and value fields
- **mdlName** (*string*) – Name to assign to the final model (E.g.: ‘Newtons2ndLaw’)
- **eqMdl** (*string*) – Equation relating inputs to output (E.g.: “c = a * b”)

Returns

- TensorFlow Graph: Computational graph of the physics equation
- *metagraphLoc*: string of location on disk where computational model was stored

Return type (TensorFlow Graph, string)

_createNNModel (*inputVar, outputVar, mdlName*)

Build a K-CHAIN model as a neural network using input and output variables from the KG.

Parameters

- **inputVar** (*JSON array*) – array of JSON variable objects with name (as in dataset) and type fields
- **outputVar** (*JSON array*) – array of JSON variable objects with name (as in dataset) and type fields
- **mdlName** (*string*) – Name to assign to the final model (E.g.: ‘Newtons2ndLaw’)

Returns

- TensorFlow Graph: computational graph of the neural network

- `metagraphLoc`: string of location on disk where computational model is stored

Return type (TensorFlow Graph, string)

`__getDefaultValues` ()

Reads json from file and return if exists, else create new and return empty

`__getVarType` (*typeStr*)

Obtain tensorflow datatypes for variable type information from KG

Parameters **`typeStr`** (*string*) – String denoting type of variable with possible values of bool, integer, float, and double (default).

Returns datatype in TensorFlow (e.g. `tf.bool`)

`__makePyFile` (*stringfun*)

Write the formatted code into a python module for conversion to tensorflow graph

Parameters **`stringfun`** (*string*) – formatted python code as string to be written in python file

`__runSessionWithDefaults` (*sess, mdl, inputVar, output, fd, defaultValues, defaultValuesUsed*)

Run a TensorFlow session with given inputs and fill in missing values from defaults or inform user about missing information

Parameters

- **`sess`** (*TF Session*) – TensorFlow session to run the computation
- **`mdl`** (*TF Graph*) – TensorFlow Graph to run the session
- **`inputVar`** (*JSON array*) – array of JSON variable objects with name, type, and value fields
- **`output`** (*TF Graph Node*) – TensorFlow Graph node for output from computation
- **`feed_dict`** (*Dictionary*) – Feed dictionary for TF placeholders and their values
- **`defaultValues`** (*JSON*) – Name:Value pairs of default values from model build stage
- **`defaultValuesUsed`** (*JSON Array*) – array of default variable JSON objects with name and value fields (empty initially)

Returns

- output: value(s) of output variable.
- Default JSON array : array of default variable JSON objects with name and value fields.
- string : Name of missing variable, which is needed for inference

Return type (output type, Default JSON array, string)

`__setDefaultValues` (*defValues*)

Writes json with provided values back to file

`build` (*inputVar, outputVar, mdlName, dataLoc=None, eqMdl=None*)

Build a K-CHAIN model using input and output variables from the KG.

Parameters

- **`inputVar`** (*JSON array*) – array of JSON variable objects with name (as in dataset), type, and value fields
- **`outputVar`** (*JSON array*) – array of JSON variable objects with name (as in dataset), type, and value fields

- **mdlName** (*string*) – Name to assign to the final model (E.g.: ‘Newtons2ndLaw’)
- **dataLoc** (*string*) – Location of dataset as .csv with Row 1 - Variables names, Row 2 - Units, Row 3 onwards - data (default = None)
- **eqMdl** (*string*) – python TF eager-compatible code (e.g: “c = a * b” or “a = tf.math.sqrt(x*y)”)

evaluate (*inputVar, outputVar, mdlName*)

Evaluates a model with given inputs to compute output values

Parameters

- **inputVar** (*JSON array*) – array of JSON variable objects with name, type, and value fields
- **outputVar** (*JSON array*) – array of JSON variable objects with name, type, and value fields
- **mdlName** (*string*) – Name to model to use (E.g.: ‘Newtons2ndLaw’)

Returns

- Output JSON array : array of output variable JSON objects with name, type, and value fields. The resulting output of the computation is assigned to the value field of the JSON object.
- Default JSON array : array of default variable JSON objects with name and value fields.
- string : Name of missing variable, which is needed for inference

Return type (Output JSON array, Default JSON array, string)

fitModel (*dataset, inputVar, outputVar, mdlName*)

Fit a K-CHAIN model using input and output variables from the KG and the corresponding dataset.

Parameters

- **dataset** (*Pandas Dataframe*) – dataset with inputs and outputs
- **inputVar** (*JSON array*) – array of JSON variable objects with name (as in dataset) and type fields
- **outputVar** (*JSON array*) – array of JSON variable objects with name (as in dataset) and type fields
- **mdlName** (*string*) – Name to assign to the final model (E.g.: ‘Newtons2ndLaw’)

Returns Location on disk where computational model and trained parameters are stored

Return type string

getDataset (*dataLoc=None*)

Create Pandas DataFrame from identified csv.

Parameters **dataLoc** (*string*) – Location of dataset as .csv with Row 1 - Variables names, Row 2 - Units, Row 3 onwards - data (default = None)

Returns DataFrame with values read from csv file

Return type df (Pandas DataFrame)

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