Documentation

1 QuantumModelMaker

1.1 quantum-rescale Function

- **Objective**: Prepare a given dataset for quantum encoding by rescaling it to be within range of 0 and 1.
- Input Parameter(s): Pandas Dataset
- **Return**: Returns x as input features and y as output label.

1.2 smooth Function

- **Objective**: Make a given dataset stationary by applying exponential smoothing to each of the columns to its training subset.
- Input Parameter(s): Pandas Dataset: Input for smoothing.

'train-split': An integer value to split the dataset into a training set that is smoothed while preserving the test set.

'smooth-level': Alpha value for smoothing the dataset.

• Return: Returns the smoothed dataset

1.3 create-discrete-circuits Function

- Objective: Generate quantum circuits compatible with discrete-data QCNN models.
- Input Parameter(s): Data: Pandas Dataset

Qubits: Cirq.GridQubit Object.

Test: Boolean present for investigating process of circuit generation. Set to False. 'smooth-level': Alpha value for smoothing the dataset.

• Return: Returns a tensor of quantum circuits for each input datapoint within the dataset.

1.4 encode-discrete-data Function

- **Objective**: Split dataset into Train, Validation, and Test and create return output labels and quantum circuits of input features compatible with discrete-data models.
- Input Parameter(s): data: Pandas Dataset

labels: Output Labels (Biogas Production).

Qubits: Cirq.GridQubit Object.

• **Return**: Returns output labels and quantum-encoded input features for discrete-data models for each of the train, validation, and test sets.

1.5 create-time-window-circuits Function

- Objective: Generate quantum circuits compatible with time-window QCNN models.
- Input Parameter(s): Data: Pandas Dataset
 Qubits: Cirq.GridQubit Object.

Test: Boolean present for investigating process of circuit generation. Set to False. 'smooth-level': Alpha value for smoothing the dataset.

• Return: Returns a tensor of quantum circuits for each input datapoint within the dataset.

1.6 encode-time-window-data Function

- **Objective**: Split dataset into Train, Validation, and Test and create return output labels and quantum circuits of input features compatible with time-window models.
- Input Parameter(s): data: Pandas Dataset labels: Output Labels (Biogas Production).

Qubits: Cirq.GridQubit Object.

• **Return**: Returns output labels and quantum-encoded input features for time-window models for each of the train, validation, and test sets.

1.7 create-model-circuit Function

• Objective: Create QCNN Architecture model

• Input Parameter(s): Qubits: Cirq.GridQubit Object.

• Return: Return a circuit representation of a QCNN model

1.8 prepare-quantum-states Function

- **Objective**: Prepare quantum-circuits for inputs and model depending on the model-type passed in as an input.
- Input Parameter(s): X: Input Feature Dataset

y: Output Label Pandas Series

feature-count: Number of features being used for model development.

type: Type of model being built. Can be either 'time-window' or 'discrete'.

• Return: QCNN model circuit, qubit object, X, and y for train, test, and validation.

1.9 get-callbacks Function

- **Objective**: Create Callbacks that the model can use during training for creating model checkpoints
- Input Parameter(s): Patience: Number of epochs that the model can wait to verify if the validation loss descreases. Set to 5 by default.
- **Return**: Return es-callback which is an early stopping callback, and modelckpt-callback, which is a model checkpoint callback.

1.10 build-model Function

- Objective: Concatenate QCNN Model with PQC layer and compile an executeable model.
- Input Parameter(s):qcnn-circuit: Circuit version of QCNN Qubits: Cirq.GridQubit object.
- Return: a compiled executeable tefq model.

1.11 make-q-cnn-model Function

- **Objective**: A wrapper that utilises all prior functions to create an executeable model for a given model type and train it.
- Input Parameter(s):type: 'discrete' or 'time-window' String object

retrain: Boolean value to continue training if model does not train to a low enough val-loss

model: Model Object

history: History Object containing a model object's history.

• Return: Model Object and History

2 Quantum Model Validator

2.1 visualize-loss Function

• Objective: Visualize a model's training and validation loss

• Input Parameter(s): History: 'A model's training history object

Title: String Object.

• Return: None

3 ModelMaker

3.1 smooth Function

- **Objective**: Make a given dataset stationary by applying exponential smoothing to each of the columns to its training subset.
- Input Parameter(s): Pandas Dataset: Input for smoothing.

'train-split': An integer value to split the dataset into a training set that is smoothed while preserving the test set.

'smooth-level': Alpha value for smoothing the dataset.

• Return: Returns the smoothed dataset

3.2 Generate-Classical-Dataset Function

- Objective: Create Train, Test, and Validation Datasets
- Return: Returns Train, Test, and Validation Datasets.

3.3 build-model Function

- Objective: Build an executeable tensorflow CNN model for given data-type
- Input Parameter(s): mtype: Model Type, either 'discrete' or 'time-window'. inputs: Input object for executeable model. 'smooth-level': Alpha value for smoothing the dataset.
- Return: Returns an executeable tensorflow CNN model for given data-type.

3.4 get-callbacks Function

• **Objective**: Create Callbacks that the model can use during training for creating model checkpoints

- Input Parameter(s): Patience: Number of epochs that the model can wait to verify if the validation loss descreases. Set to 5 by default.
- **Return**: Return es-callback which is an early stopping callback, and modelckpt-callback, which is a model checkpoint callback.

3.5 train-model Function

• Objective: Train the created 'time-window' or 'discrete' model

• Input Parameter(s): model: model object

dataset-train: Training Dataset dataset-val: Validation Dataset es-callback: EarlyStopping Callback

modelckpt-callback: Model Checkpoint Callback

• Return: Return return a trained model and it's history.

3.6 make-discrete-data-cnn-model Function

• **Objective**: A wrapper that utilises all prior functions to create an executeable discrete-data model for a given model type and train it.

• Input Parameter(s): :retrain: Boolean value to continue training if model does not train to a low enough val-loss

model: Model Object

history: History Object containing a model object's history.

• Return: Return return a trained model and it's history.

3.7 make-time-window-cnn-model Function

• **Objective**: A wrapper that utilises all prior functions to create an executeable time-window model for a given model type and train it.

• Input Parameter(s): :retrain: Boolean value to continue training if model does not train to a low enough val-loss

model: Model Object

history: History Object containing a model object's history.

• Return: Return return a trained model and it's history.

3.8 Model Validator

3.9 visualize-loss Function

• Objective: Visualize a model's training and validation loss

• Input Parameter(s): History: 'A model's training history object

Title: String Object.

• Return: None

3.10 show-plot Function

• Objective: Visualize a model's Predictions against expected values

• Return: None