VRIJE UNIVERSITEIT BRUSSEL

Hydra GPU System Test

3D CNN

Michiel Jacobs
02/02/2021

Run information

Model:

Author: Michiel Jacobs
Version: 0.1.0
Type: 3D CNN
Feature: Coulomb Matrix
Label: Zero point energy

Data:

Maximum heavy atoms: 20
Maximum molecule size: 62
Split ratio: 0.8
Molecules for training: 80
Molecules for testing: 19

Neural Network

Network settings

	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6	Layer 7
Input shape	(6, 62, 62, 1)						
Batch size							
kernel size	(1, 3, 3)		(1, 3, 3)		(1, 3, 3)		
pool size							
filters	64		64		64		
dropout		0.2		0.2		0.2	

NN summary

Model: "sequential"

Layer (type)	Output Shape	Param #
conv3d (Conv3D)	(None, 6, 60, 60, 64)	640
max_pooling3d (MaxPooling3D)	(None, 3, 30, 30, 64)	0
conv3d_1 (Conv3D)	(None, 3, 28, 28, 64)	36928
max_pooling3d_1 (MaxPooling3	(None, 1, 14, 14, 64)	0
conv3d_2 (Conv3D)	(None, 1, 12, 12, 64)	36928
flatten (Flatten)	(None, 9216)	0
dropout (Dropout)	(None, 9216)	0
dense (Dense)	(None, 1)	9217

Total params: 83,713
Trainable params: 83,713
Non-trainable params: 0

Results

Results and graphs comming soon.

Log

```
2021-02-02 13:43:34,234:INFO:Starting model 3D_CNN_0.1.0_on_02-02-2021_13.43.34
2021-02-02 13:43:34,234:INFO:==================== Model info ====================
2021-02-02 13:43:34,234:INFO:Author: Michiel Jacobs
2021-02-02 13:43:34,234:INFO:Version: 0.1.0
2021-02-02 13:43:34,234:INFO:Modeltype: 3D CNN
2021-02-02 13:43:34,234:INFO:Maximum heavy atoms: 20
2021-02-02 13:43:34,234:INFO:Feature: Coulomb Matrix
2021-02-02 13:43:34,234:INFO:Labels: Zero point energy
2021-02-02 13:43:34,234:INFO:DEVELOPMENT: True
2021-02-02 13:43:34,234:INFO:============== Step 1: loading data ==============
2021-02-02 13:43:41,248:INFO:Data loaded
2021-02-02 13:43:41,249:INFO:============== Step 2: data preprocessing ==============
2021-02-02 13:43:41,249:INFO:Trimming dataset...
2021-02-02 13:43:41,524:INFO:Loading arrays...
2021-02-02 13:43:41,531:INFO:Shuffeling data...
2021-02-02 13:43:41,532:INFO:Calculating maximum size of molecules...
2021-02-02 13:43:41,532:INFO:The maximumsize of molecules is 62
2021-02-02 13:43:41,532:INFO:Normalizing data...
2021-02-02 13:43:41,536:INFO:Tensorisation of the coulomb matrices...
2021-02-02 13:43:44,409:INFO:Building channels...
2021-02-02 13:43:44,410:INFO:Calculating train test split...
2021-02-02 13:43:44,410:INFO:There are 100 entries in this dataset.
2021-02-02 13:43:44,410:INFO:Split ratio set to 0.8.
2021-02-02 13:43:44,410:INFO:Trainingset contains 80 molecules.
2021-02-02 13:43:44,410:INFO:Building train and test sets...
2021-02-02 13:43:44,411:INFO:Converting train features to tf.tensors...
2021-02-02 13:47:32,432:INFO:Converting test features to tf.tensors...
2021-02-02 13:48:26,367:INFO:Converting train labels to array...
2021-02-02 13:48:26,367:INFO:Converting test labels to array...
2021-02-02 13:48:26,367:INFO:============== Step 3: Model compilation ==============
2021-02-02 13:48:26,368:INFO:Building model...
2021-02-02 13:48:28,276:INFO:Model: "sequential"
2021-02-02
13:48:28,277:INFO:_________________________________________________________________
2021-02-02 13:48:28,277:INFO:Layer (type)                 Output Shape              Param #
2021-02-02
13:48:28,277:INFO:=================================================================
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2021-02-02 13:48:28,277:INFO:conv3d (Conv3D)              (None, 6, 60, 60, 64)     640
2021-02-02
13:48:28,277:INFO:_________________________________________________________________
2021-02-02 13:48:28,277:INFO:max_pooling3d (MaxPooling3D) (None, 3, 30, 30, 64)     0
2021-02-02
13:48:28,277:INFO:_________________________________________________________________
2021-02-02 13:48:28,277:INFO:conv3d_1 (Conv3D)            (None, 3, 28, 28, 64)     36928
2021-02-02
13:48:28,277:INFO:_________________________________________________________________
2021-02-02 13:48:28,277:INFO:max_pooling3d_1 (MaxPooling3 (None, 1, 14, 14, 64)     0
2021-02-02
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13:48:28,277:INFO:_____
2021-02-02 13:48:28,277:INFO:conv3d_2 (Conv3D) (None, 1, 12, 12, 64) 36928
2021-02-02
13:48:28,278:INFO:_____
2021-02-02 13:48:28,278:INFO:flatten (Flatten) (None, 9216) 0
2021-02-02
13:48:28,278:INFO:_____
2021-02-02 13:48:28,278:INFO:dropout (Dropout) (None, 9216) 0
2021-02-02
13:48:28,278:INFO:_____
2021-02-02 13:48:28,278:INFO:dense (Dense) (None, 1) 9217
2021-02-02
13:48:28,278:INFO:===
==========
2021-02-02 13:48:28,278:INFO:Total params: 83,713
2021-02-02 13:48:28,278:INFO:Trainable params: 83,713
2021-02-02 13:48:28,278:INFO:Non-trainable params: 0
2021-02-02
13:48:28,278:INFO:_____
2021-02-02 13:48:28,280:INFO:Compiling the model...
2021-02-02 13:48:28,286:INFO:============== Step 4: Model training ==============
2021-02-02 13:48:36,222:INFO:============== Step 5: Model evaluation ==============
2021-02-02 13:48:36,437:INFO:============== Step 6: Saving, reporting and cleanup
==============
2021-02-02 13:48:36,437:INFO:Saving model...
2021-02-02 13:48:36,793:WARNING:From
/apps/brussel/CO7/skylake/software/TensorFlow/2.3.1-foss-2020a-Python-3.8.2/lib/python3.8/site-packages/
tensorflow/python/training/tracking/tracking.py:111: Model.state_updates □□□□□□
tensorflow.python.keras.engine.training) is deprecated and will be removed in a future version.
Instructions for updating:
This property should not be used in TensorFlow 2.0, as updates are applied automatically.
2021-02-02 13:48:36,797:WARNING:From
/apps/brussel/CO7/skylake/software/TensorFlow/2.3.1-foss-2020a-Python-3.8.2/lib/python3.8/site-packages/
tensorflow/python/training/tracking/tracking.py:111: Layer.updates □□□□□□
tensorflow.python.keras.engine.base_layer) is deprecated and will be removed in a future version.
Instructions for updating:
This property should not be used in TensorFlow 2.0, as updates are applied automatically.
2021-02-02 13:48:37,970:INFO:Assets written to:
/scratch/brussel/102/vsc10255/Experimental-Reactivity-Prediction/code/models/../../models/3D_CNN_0.1.0_
on_02-02-2021_13.43.34.tf/assets
2021-02-02 13:48:38,175:INFO:Model saved.
2021-02-02 13:48:38,176:INFO:Generating report...