VRIJE UNIVERSITEIT BRUSSEL

Predicting Zero Point energies

3D CNN

Michiel Jacobs
03/02/2021

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: 400
Molecules for testing: 99

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

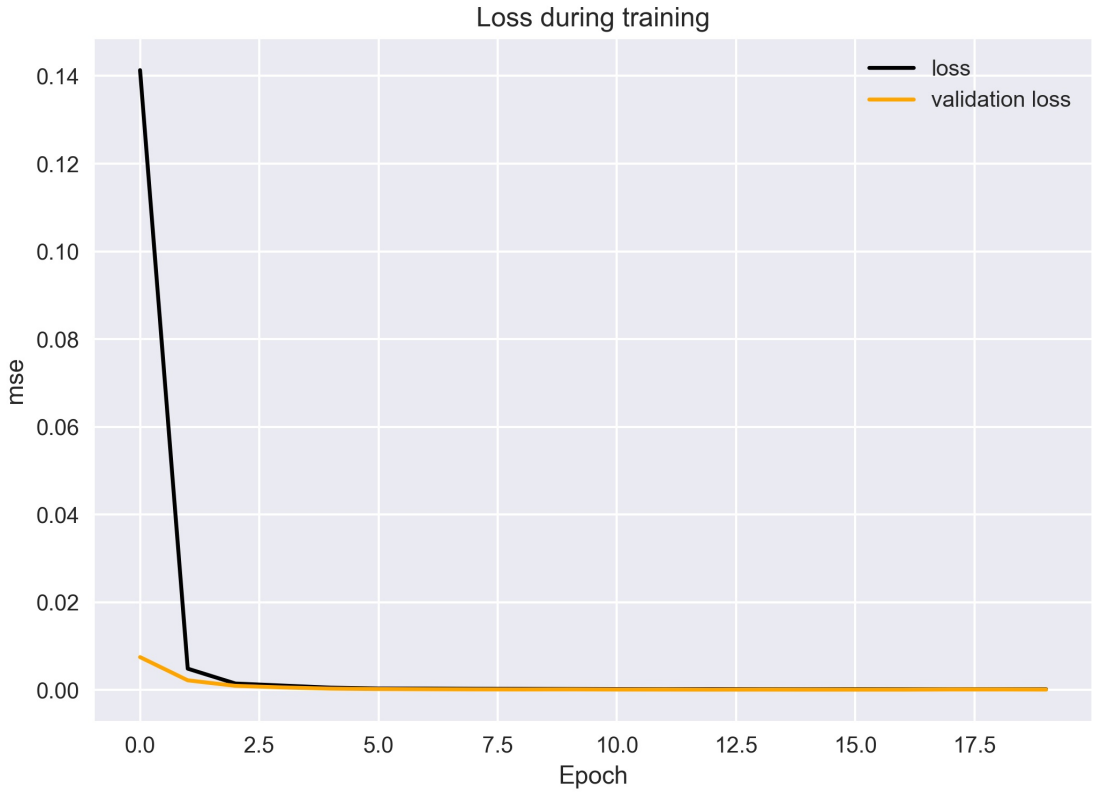
Model: "sequential"

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, 32)	294944
dense_1 (Dense)	(None, 32)	1056
dense_2 (Dense)	(None, 1)	33

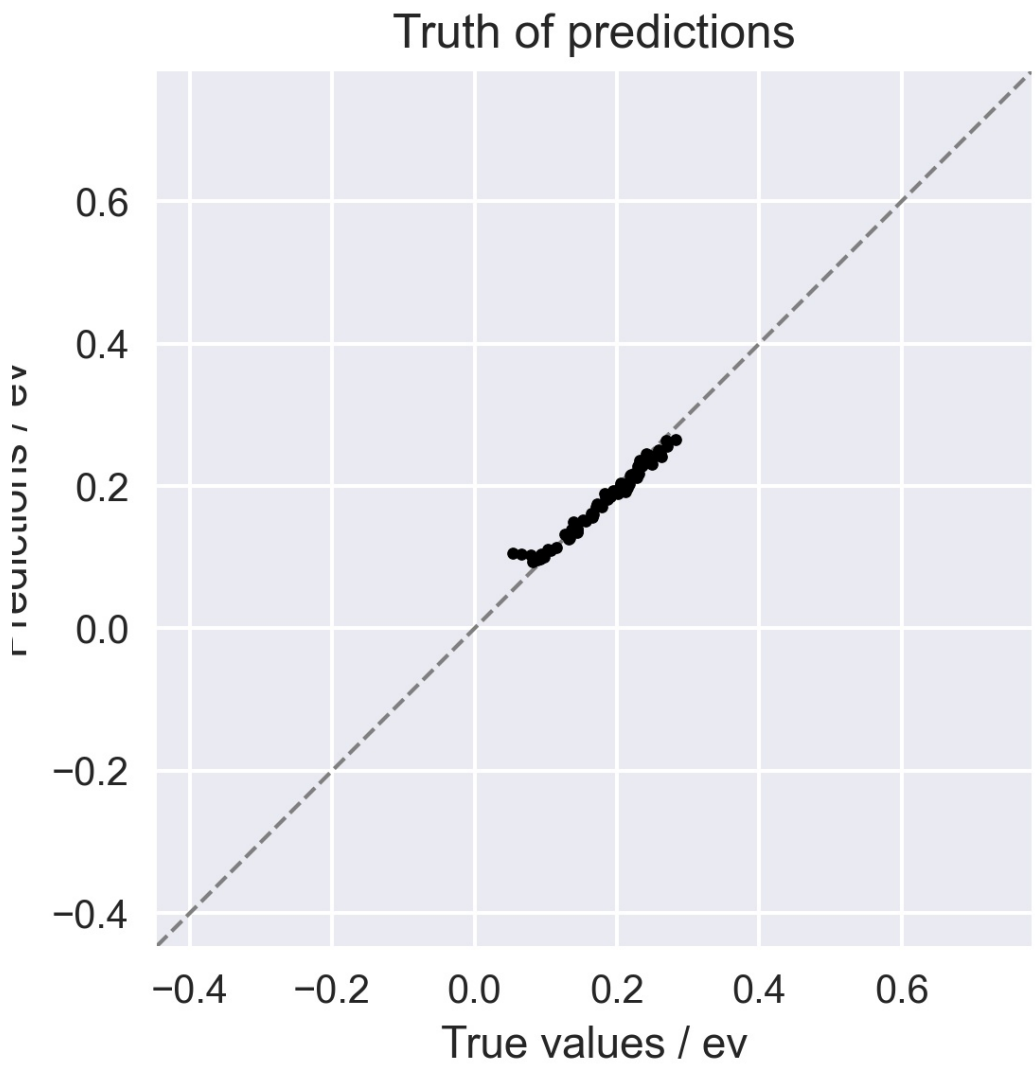
Total params: 370,529
Trainable params: 370,529
Non-trainable params: 0

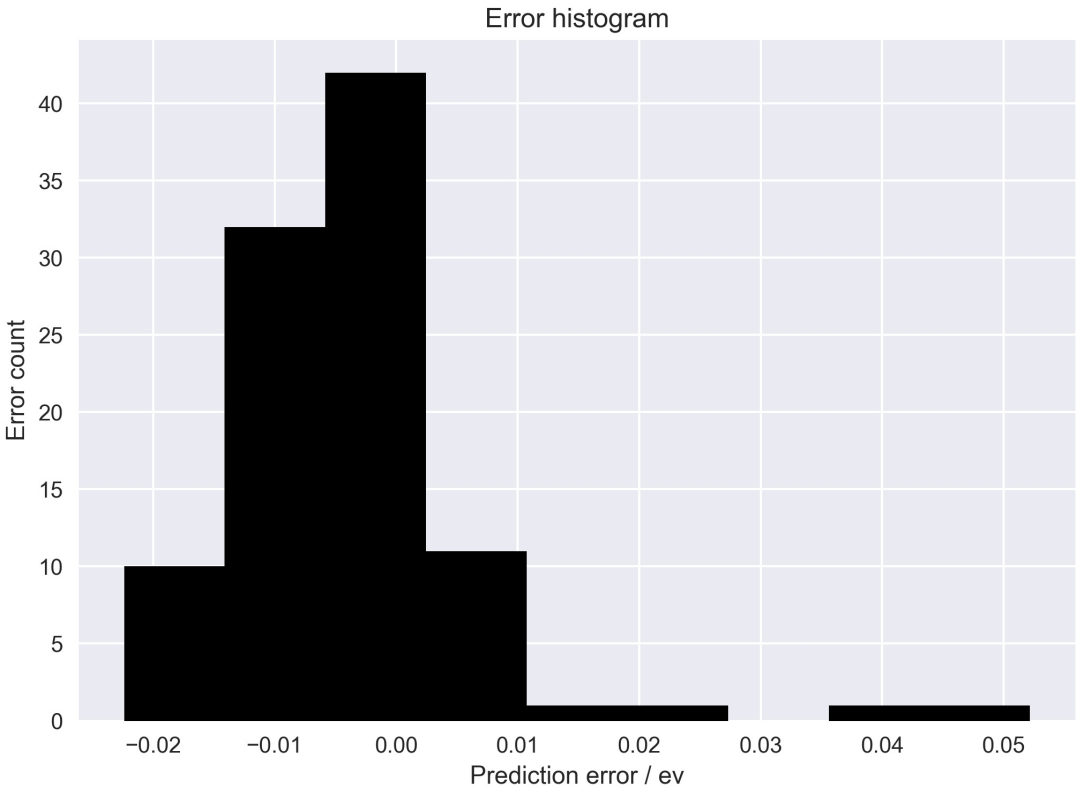
Results

Training evaluation



Model evaluation





Log

```
2021-02-03 14:29:30,116:INFO:Starting model 3D_CNN_0.1.0_on_02-03-2021_14.29.30
2021-02-03 14:29:30,116:INFO:==================== Model info ====================
2021-02-03 14:29:30,116:INFO:Author: Michiel Jacobs
2021-02-03 14:29:30,116:INFO:Version: 0.1.0
2021-02-03 14:29:30,117:INFO:Modeltype: 3D CNN
2021-02-03 14:29:30,117:INFO:Maximum heavy atoms: 20
2021-02-03 14:29:30,117:INFO:Feature: Coulomb Matrix
2021-02-03 14:29:30,117:INFO:Labels: Zero point energy
2021-02-03 14:29:30,117:INFO:DEVELOPMENT: True
2021-02-03 14:29:30,117:INFO:============== Step 1: loading data ==============
2021-02-03 14:29:36,359:INFO:Data loaded
2021-02-03 14:29:36,359:INFO:============== Step 2: data preprocessing ==============
2021-02-03 14:29:36,359:INFO:Trimming dataset...
2021-02-03 14:29:36,631:INFO:Loading arrays...
2021-02-03 14:29:36,652:INFO:Shuffeling data...
2021-02-03 14:29:36,653:INFO:Calculating maximum size of molecules...
2021-02-03 14:29:36,653:INFO:The maximumsize of molecules is 62
2021-02-03 14:29:36,653:INFO:Normalizing data...
2021-02-03 14:29:36,684:INFO:Tensorisation of the coulomb matrices...
2021-02-03 14:29:52,877:INFO:Building channels...
2021-02-03 14:29:52,881:INFO:Calculating train test split...
2021-02-03 14:29:52,881:INFO:There are 500 entries in this dataset.
2021-02-03 14:29:52,881:INFO:Split ratio set to 0.8.
2021-02-03 14:29:52,881:INFO:Trainingset contains 400 molecules.
2021-02-03 14:29:52,881:INFO:Building train and test sets...
2021-02-03 14:29:52,881:INFO:Converting train features to tf.tensors...
2021-02-03 14:29:53,048:INFO:Converting test features to tf.tensors...
2021-02-03 14:29:53,063:INFO:Converting train labels to array...
2021-02-03 14:29:53,063:INFO:Converting test labels to array...
2021-02-03 14:29:53,063:INFO:============== Step 3: Model compilation ==============
2021-02-03 14:29:53,064:INFO:Building model...
2021-02-03 14:29:53,137:INFO:Model: "sequential"
2021-02-03
14:29:53,137:INFO:_________________________________________________________________
2021-02-03 14:29:53,137:INFO:Layer (type)                 Output Shape              Param #
2021-02-03
14:29:53,138:INFO:=================================================================
==========
2021-02-03 14:29:53,138:INFO:conv3d (Conv3D)              (None, 6, 60, 60, 64)     640
2021-02-03
14:29:53,138:INFO:_________________________________________________________________
2021-02-03 14:29:53,138:INFO:max_pooling3d (MaxPooling3D) (None, 3, 30, 30, 64)     0
2021-02-03
14:29:53,138:INFO:_________________________________________________________________
2021-02-03 14:29:53,138:INFO:conv3d_1 (Conv3D)            (None, 3, 28, 28, 64)     36928
2021-02-03
14:29:53,138:INFO:_________________________________________________________________
2021-02-03 14:29:53,138:INFO:max_pooling3d_1 (MaxPooling3 (None, 1, 14, 14, 64)     0
2021-02-03
```

14:29:53,138:INFO:_____
2021-02-03 14:29:53,138:INFO:conv3d_2 (Conv3D) (None, 1, 12, 12, 64) 36928
2021-02-03
14:29:53,139:INFO:_____
2021-02-03 14:29:53,139:INFO:flatten (Flatten) (None, 9216) 0
2021-02-03
14:29:53,139:INFO:_____
2021-02-03 14:29:53,139:INFO:dropout (Dropout) (None, 9216) 0
2021-02-03
14:29:53,139:INFO:_____
2021-02-03 14:29:53,139:INFO:dense (Dense) (None, 32) 294944
2021-02-03
14:29:53,139:INFO:_____
2021-02-03 14:29:53,139:INFO:dense_1 (Dense) (None, 32) 1056
2021-02-03
14:29:53,139:INFO:_____
2021-02-03 14:29:53,139:INFO:dense_2 (Dense) (None, 1) 33
2021-02-03
14:29:53,139:INFO:===
==========
2021-02-03 14:29:53,140:INFO:Total params: 370,529
2021-02-03 14:29:53,140:INFO:Trainable params: 370,529
2021-02-03 14:29:53,140:INFO:Non-trainable params: 0
2021-02-03
14:29:53,140:INFO:_____
2021-02-03 14:29:53,140:INFO:Compiling the model...
2021-02-03 14:29:53,147:INFO:============== Step 4: Model training ==============
2021-02-03 14:48:52,498:INFO:============== Step 5: Model evaluation ==============
2021-02-03 14:48:55,070:INFO:Test scores: [0.00012014201638521627, 0.007941341027617455,
0.00012014201638521627]
2021-02-03 14:48:58,613:INFO:============== Step 6: Saving, reporting and cleanup
==============
2021-02-03 14:48:58,613:INFO:Saving model...
2021-02-03 14:49:00,727:INFO:Assets written to: c:\□□□□□□□Michiel Jacobs\□□□□□□□□□□
Thesis\Experimental-Reactivity-Prediction\code\models\..\..\models\CM_ZPE_3DCNN\3D_CNN_0.1.0_on_02-0
3-2021_14.29.30.tf\assets
2021-02-03 14:49:01,067:INFO:Model saved.
2021-02-03 14:49:01,067:INFO:Generating report...