

Predicting Point energies

Zero

3D CNN



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 | | |

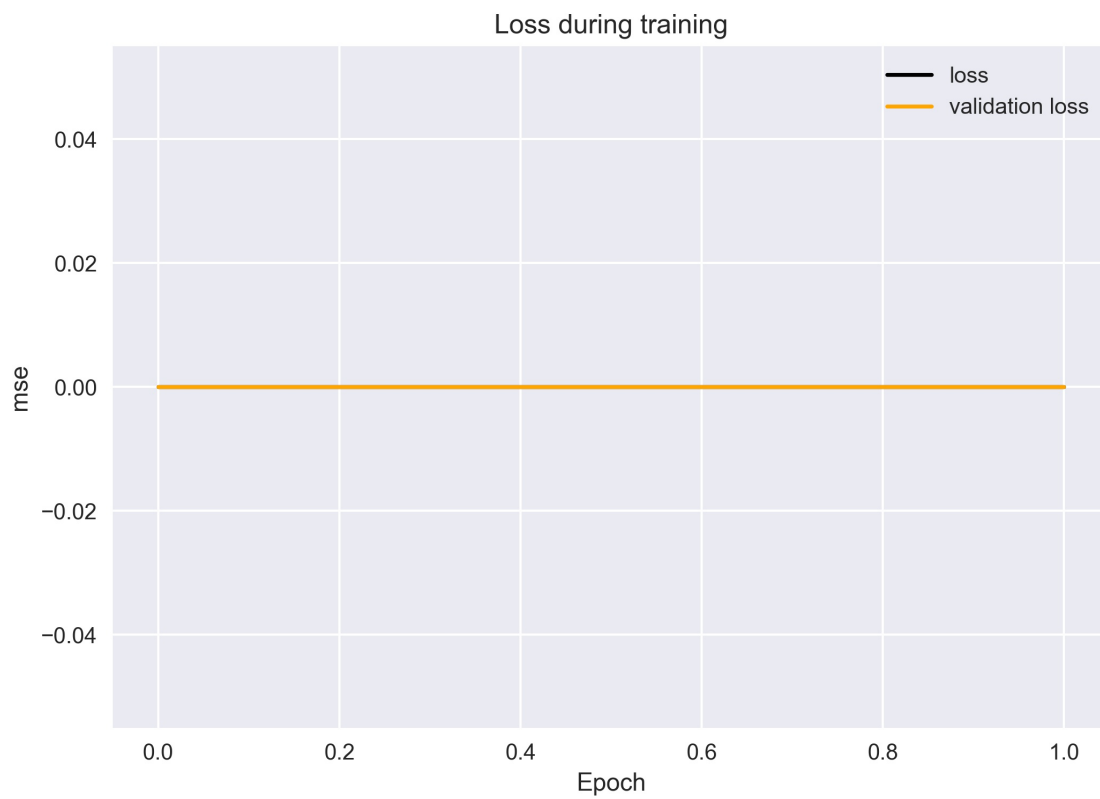
NN summary

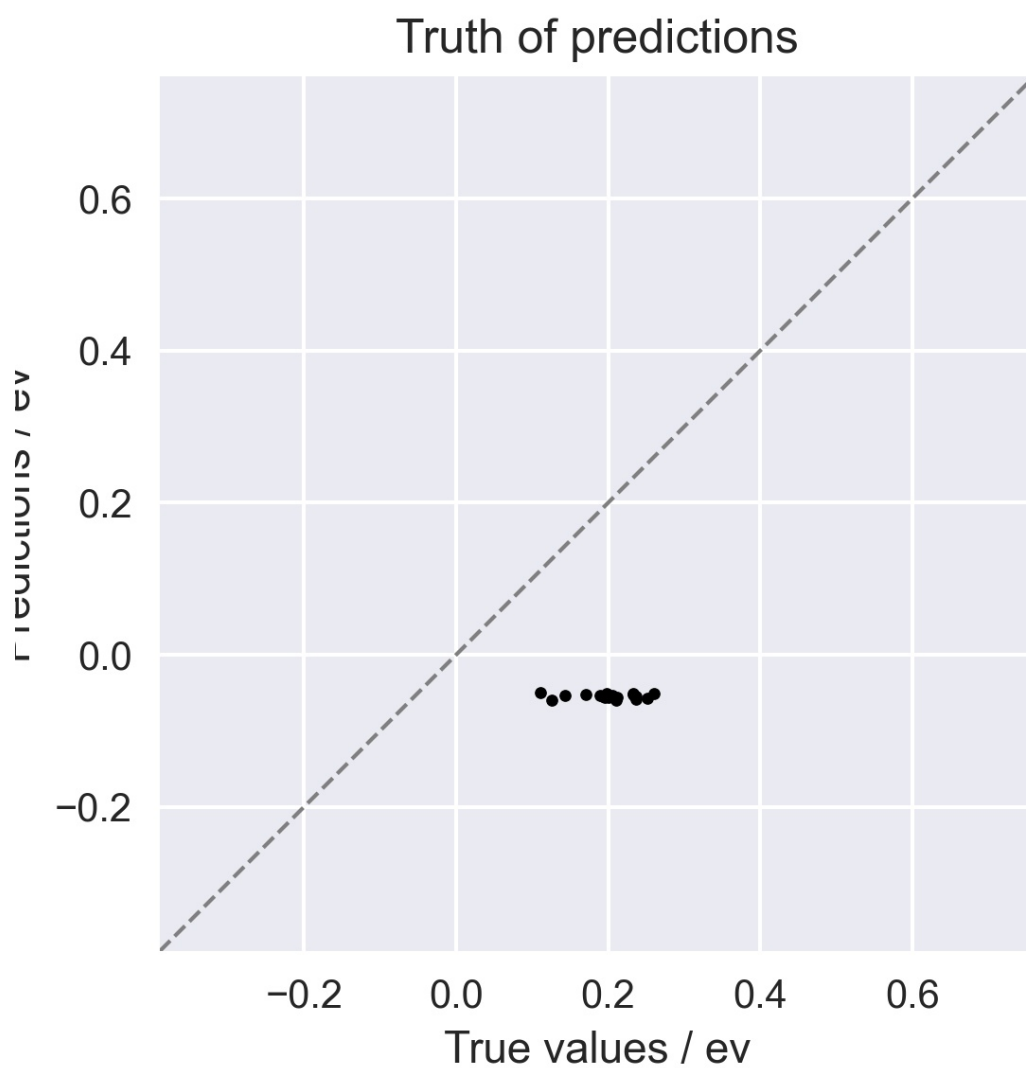
Model: "sequential"

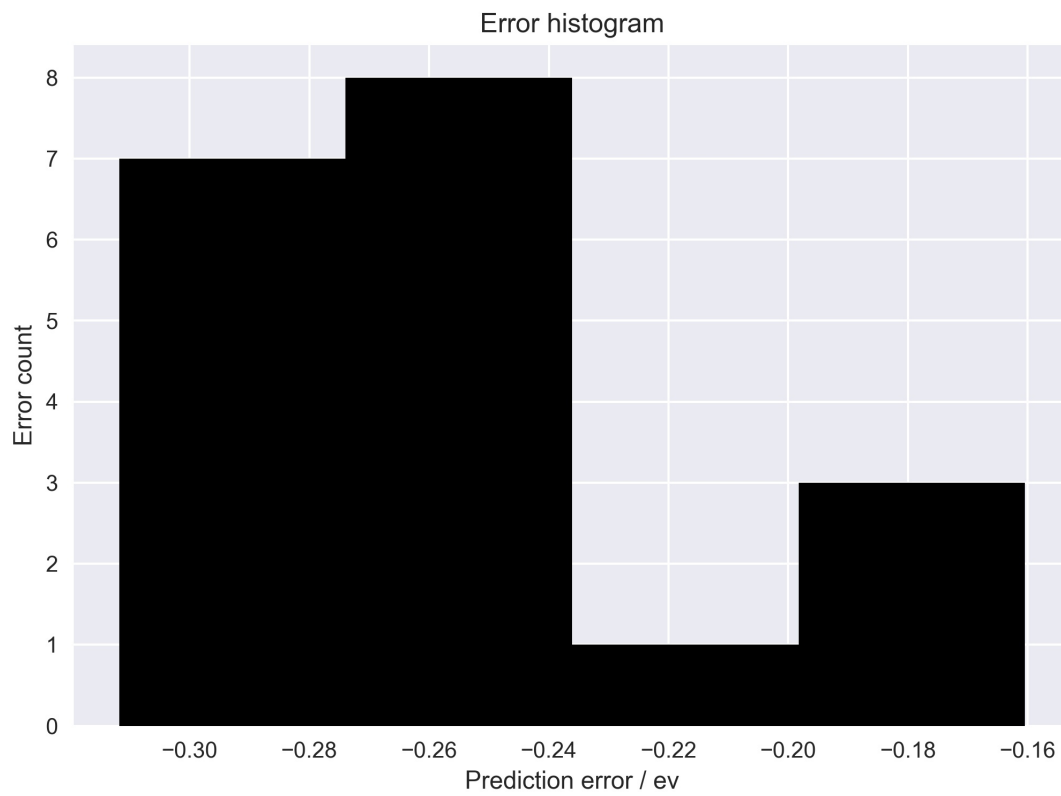
| Layer (type) | Output Shape | Param # |
|--------------------------------|-----------------------|---------|
| ===== | | |
| conv3d (Conv3D) | (None, 6, 60, 60, 64) | 640 |
| ----- | | |
| max_pooling3d (MaxPooling3D) | (None, 3, 30, 30, 64) | 0 |
| ----- | | |
| conv3d_1 (Conv3D) | (None, 3, 28, 28, 64) | 36928 |
| ----- | | |
| max_pooling3d_1 (MaxPooling3D) | (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

Training evaluation








Log

```
2021-02-03 12:46:36,876:INFO:Starting model 3D_CNN_0.1.0_on_02-03-2021_12.46.36
2021-02-03 12:46:36,876:INFO:===== Model info =====
2021-02-03 12:46:36,876:INFO:Author: Michiel Jacobs
2021-02-03 12:46:36,876:INFO:Version: 0.1.0
2021-02-03 12:46:36,876:INFO:Modeltype: 3D CNN
2021-02-03 12:46:36,877:INFO:Maximum heavy atoms: 20
2021-02-03 12:46:36,877:INFO:Feature: Coulomb Matrix
2021-02-03 12:46:36,877:INFO:Labels: Zero point energy
2021-02-03 12:46:36,877:INFO:DEVELOPMENT: True
2021-02-03 12:46:36,877:INFO:===== Step 1: loading data =====
2021-02-03 12:46:43,824:INFO:Data loaded
2021-02-03 12:46:43,825:INFO:===== Step 2: data preprocessing =====
2021-02-03 12:46:43,825:INFO:Trimming dataset...
2021-02-03 12:46:44,127:INFO>Loading arrays...
2021-02-03 12:46:44,132:INFO:Shuffling data...
2021-02-03 12:46:44,133:INFO:Calculating maximum size of molecules...
2021-02-03 12:46:44,133:INFO:The maximumsize of molecules is 62
2021-02-03 12:46:44,133:INFO:Normalizing data...
2021-02-03 12:46:44,138:INFO:Tensorisation of the coulomb matrices...
2021-02-03 12:46:47,431:INFO:Building channels...
2021-02-03 12:46:47,432:INFO:Calculating train test split...
2021-02-03 12:46:47,432:INFO:There are 100 entries in this dataset.
2021-02-03 12:46:47,432:INFO:Split ratio set to 0.8.
2021-02-03 12:46:47,432:INFO:Trainingset contains 80 molecules.
2021-02-03 12:46:47,432:INFO:Building train and test sets...
2021-02-03 12:46:47,433:INFO:Converting train features to tf.tensors...
2021-02-03 12:46:47,591:INFO:Converting test features to tf.tensors...
2021-02-03 12:46:47,595:INFO:Converting train labels to array...
2021-02-03 12:46:47,595:INFO:Converting test labels to array...
2021-02-03 12:46:47,595:INFO:===== Step 3: Model compilation =====
2021-02-03 12:46:47,598:INFO:Building model...
2021-02-03 12:46:47,674:INFO:Model: "sequential"
2021-02-03
12:46:47,674:INFO:_____
2021-02-03 12:46:47,674:INFO:Layer (type)           Output Shape           Param #
2021-02-03
12:46:47,674:INFO:=====
=====
2021-02-03 12:46:47,674:INFO:conv3d (Conv3D)         (None, 6, 60, 60, 64)   640
2021-02-03
12:46:47,674:INFO:_____
2021-02-03 12:46:47,674:INFO:max_pooling3d (MaxPooling3D) (None, 3, 30, 30, 64)   0
2021-02-03
12:46:47,674:INFO:_____
2021-02-03 12:46:47,674:INFO:conv3d_1 (Conv3D)       (None, 3, 28, 28, 64)   36928
2021-02-03
12:46:47,675:INFO:_____
2021-02-03 12:46:47,675:INFO:max_pooling3d_1 (MaxPooling3 (None, 1, 14, 14, 64)   0
2021-02-03
```



```

12:46:47,675:INFO:_____
2021-02-03 12:46:47,675:INFO:conv3d_2 (Conv3D)      (None, 1, 12, 12, 64)   36928
2021-02-03
12:46:47,675:INFO:_____
2021-02-03 12:46:47,675:INFO:flatten (Flatten)      (None, 9216)           0
2021-02-03
12:46:47,675:INFO:_____
2021-02-03 12:46:47,675:INFO:dropout (Dropout)      (None, 9216)           0
2021-02-03
12:46:47,675:INFO:_____
2021-02-03 12:46:47,675:INFO:dense (Dense)          (None, 1)              9217
2021-02-03
12:46:47,675:INFO:=====
=====
2021-02-03 12:46:47,676:INFO:Total params: 83,713
2021-02-03 12:46:47,676:INFO:Trainable params: 83,713
2021-02-03 12:46:47,676:INFO:Non-trainable params: 0
2021-02-03
12:46:47,676:INFO:_____
2021-02-03 12:46:47,676:INFO:Compiling the model...
2021-02-03 12:46:47,685:INFO:===== Step 4: Model training =====
2021-02-03 12:47:12,909:INFO:===== Step 5: Model evaluation =====
2021-02-03 12:47:13,384:INFO:Test scores: [0.0, 0.0]
2021-02-03 12:47:14,625:INFO:===== Step 6: Saving, reporting and cleanup
=====
2021-02-03 12:47:14,625:INFO:Saving model...
2021-02-03 12:47:16,053: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_12.46.36.tf\assets
2021-02-03 12:47:16,334:INFO:Model saved.
2021-02-03 12:47:16,334:INFO:Generating report...

```