**B3BD REGRESSION (logBB prediction from SMILES)**

1. **Chemprop:**

**MoleculeModel**(

(encoder): MPN(

(encoder): ModuleList(

(0): MPNEncoder(

(dropout): Dropout(p=0.3, inplace=False)

(act\_func): ReLU()

(W\_i): Linear(in\_features=147, out\_features=256, bias=False)

(W\_h): Linear(in\_features=256, out\_features=256, bias=False)

(W\_o): Linear(in\_features=389, out\_features=256, bias=True)

)

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)

(readout): Sequential(

(0): Dropout(p=0.3, inplace=False)

(1): Linear(in\_features=256, out\_features=256, bias=True)

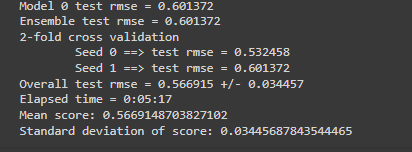
(2): ReLU()

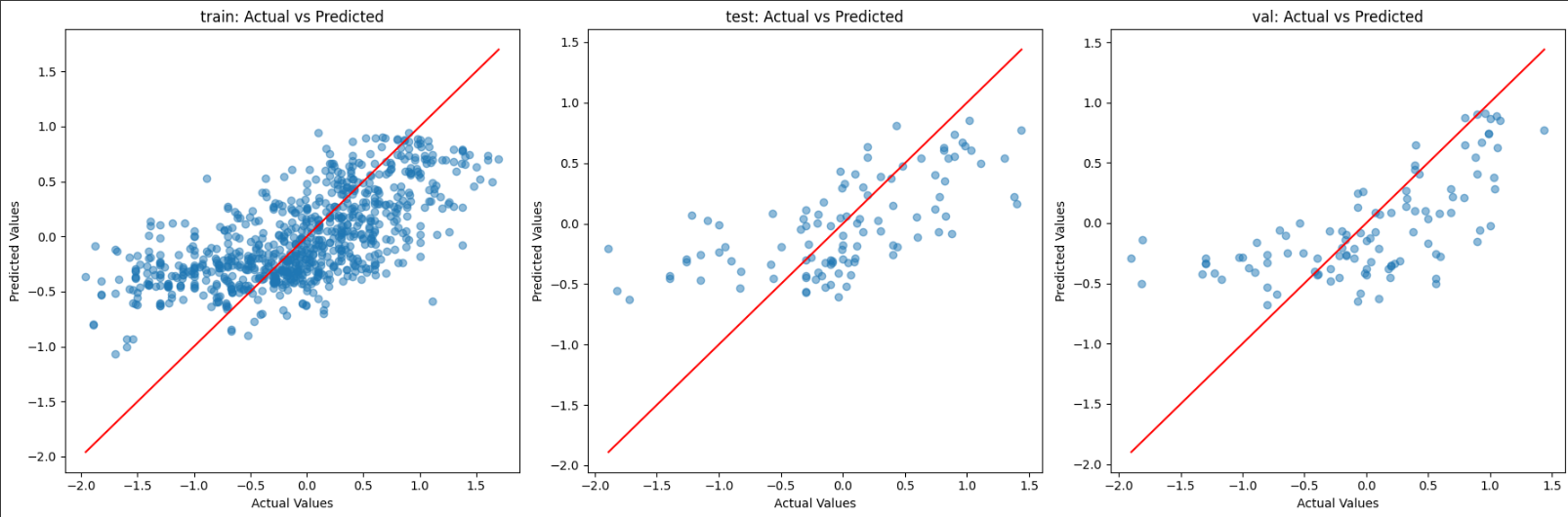
(3): Dropout(p=0.3, inplace=False)

(4): Linear(in\_features=256, out\_features=1, bias=True)

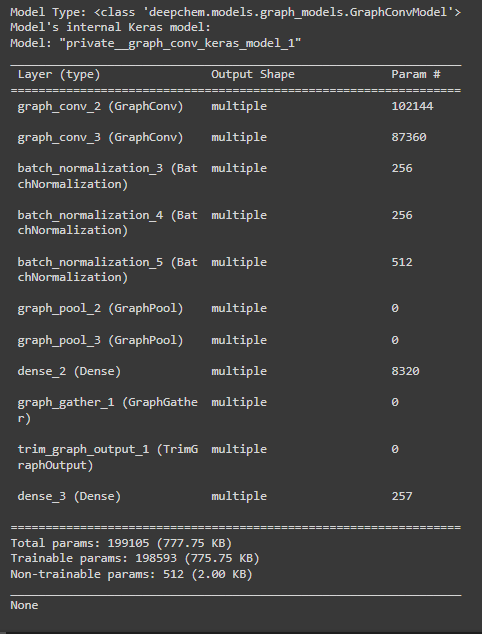
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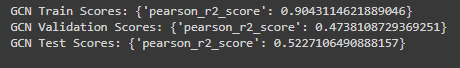
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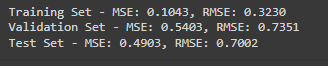


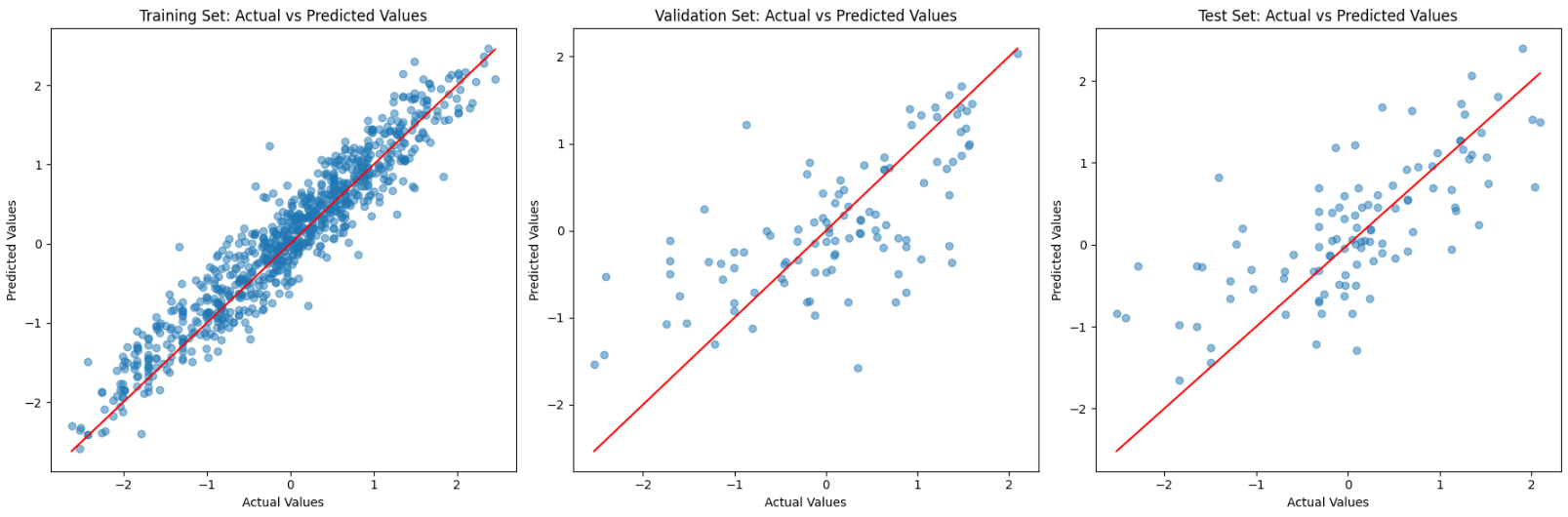


1. **GraphConvModel from deepchem:**

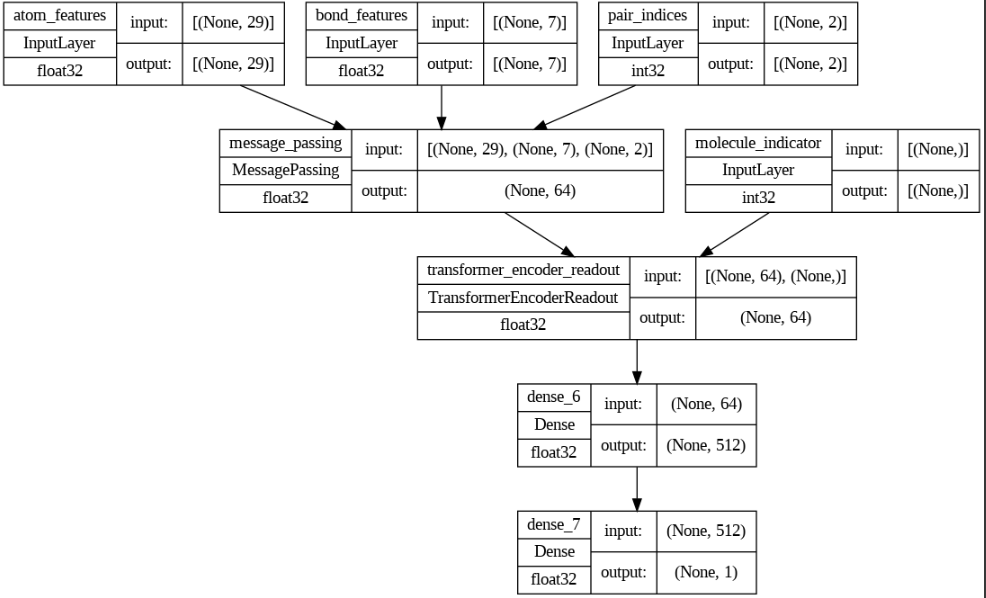
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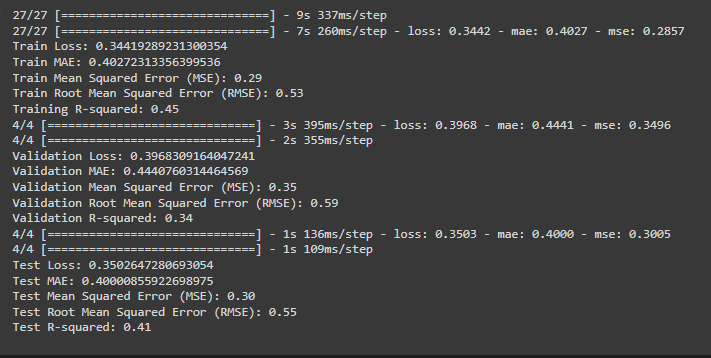
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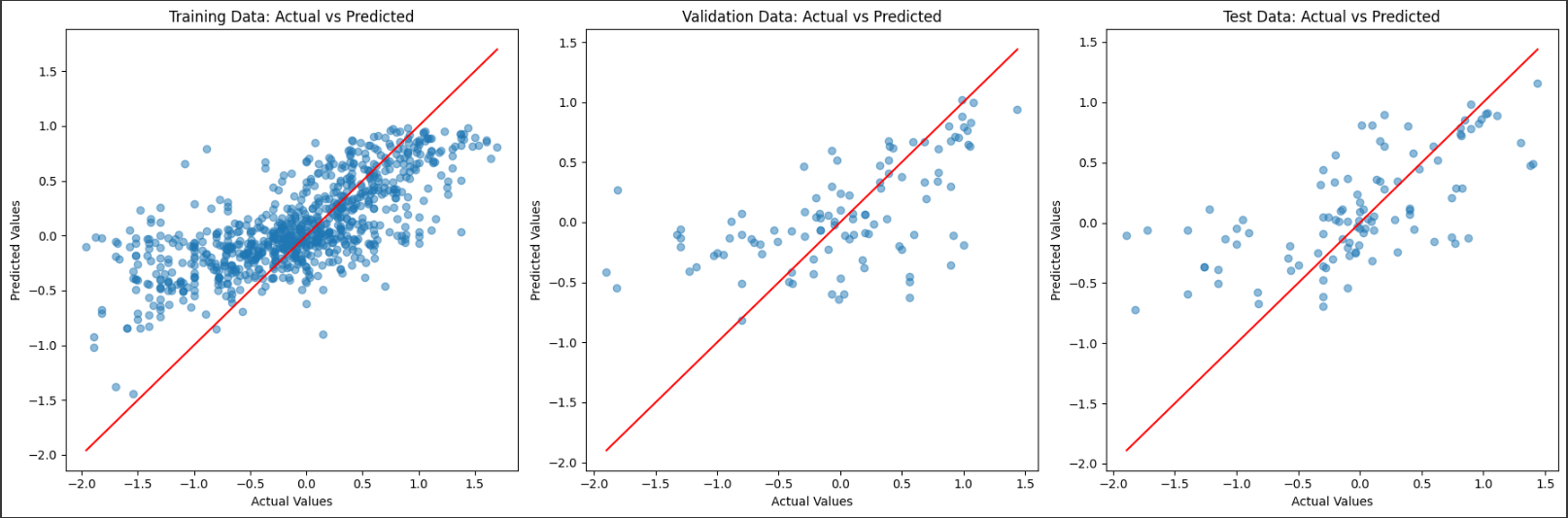
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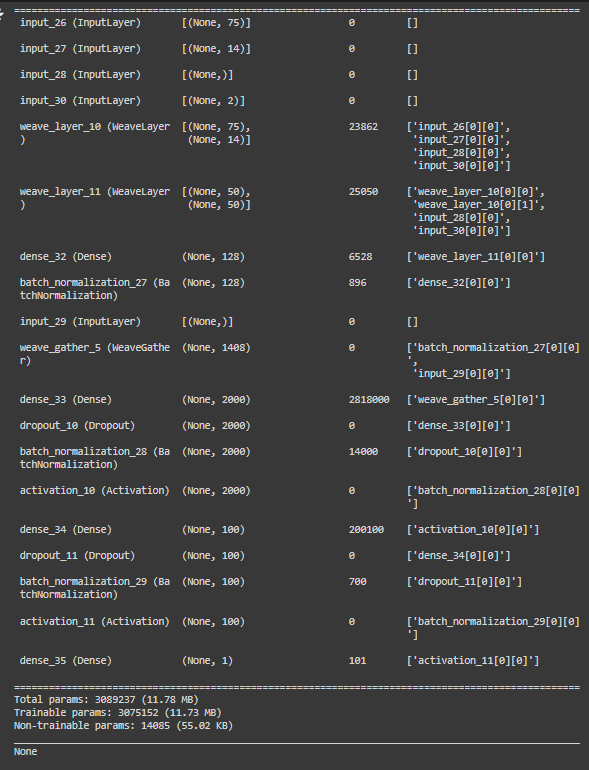
1. **MPNN from rdkit:**

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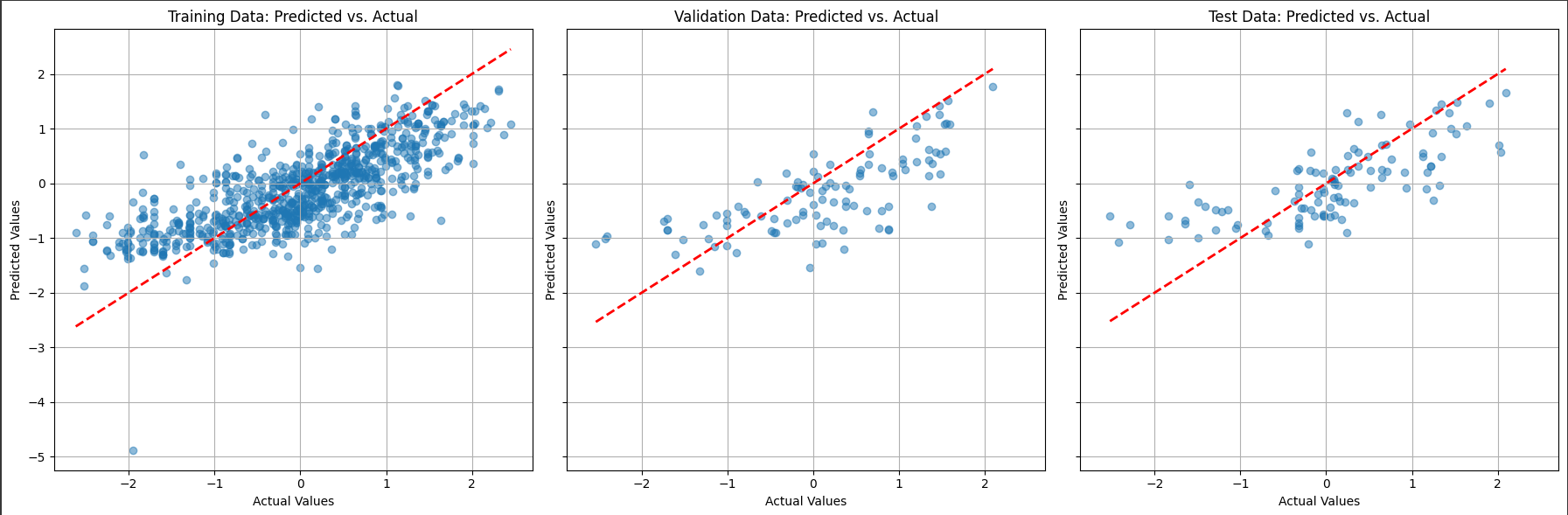
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1. **WeaveModel from deepchem:**

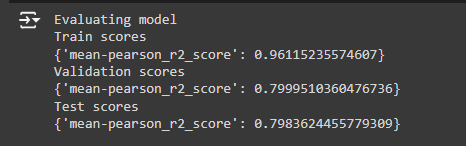
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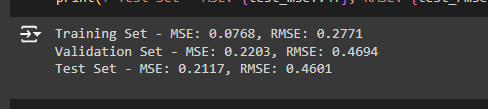
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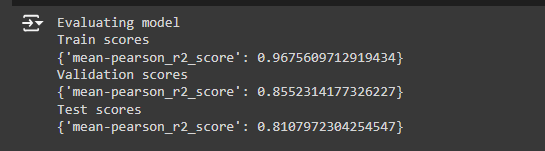
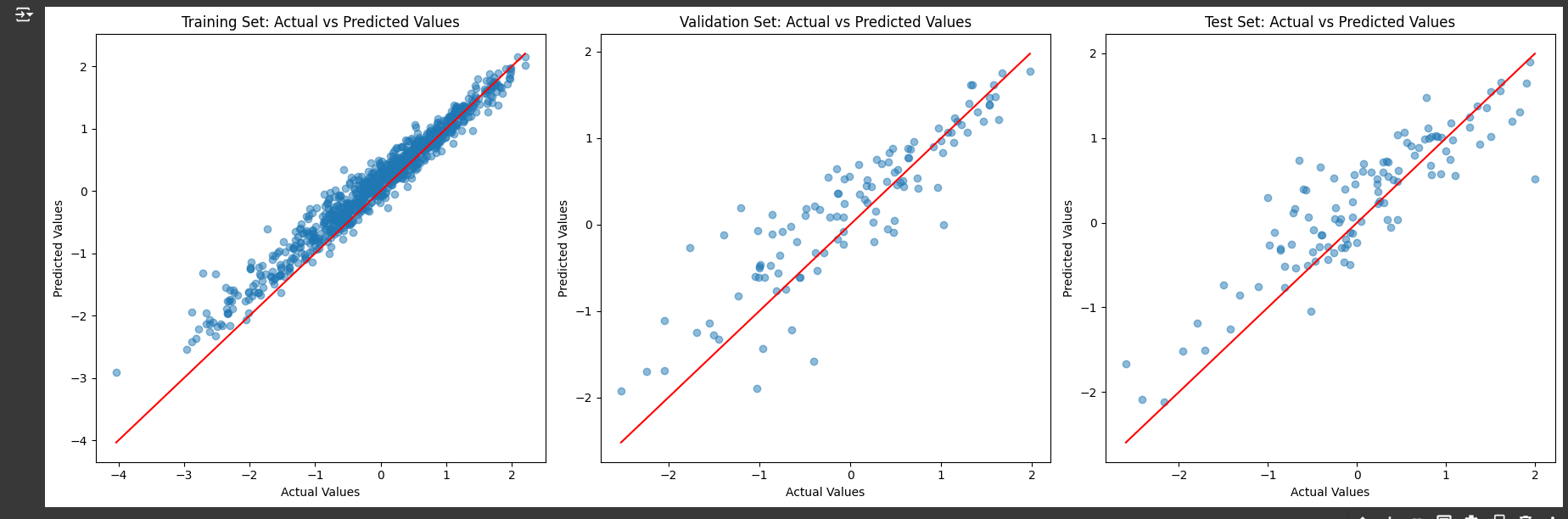
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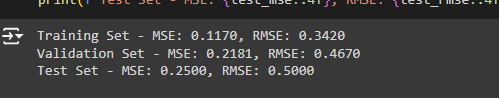
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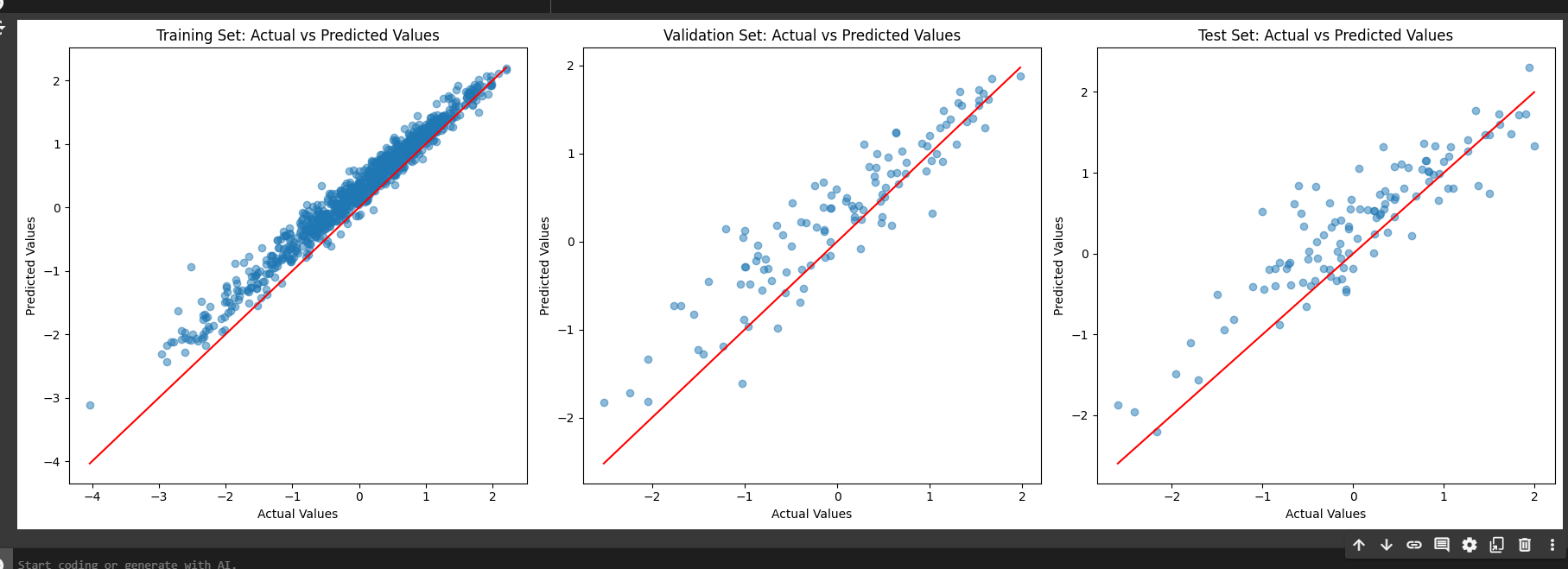
**graph convmodel:**

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