Import Library

```
!pip install torch
!pip install torch-geometric
```

```
Requirement already satisfied: torch in /usr/local/lib/python3.10/dist-packages (2.3.1+cu121)
Requirement already satisfied: filelock in /usr/local/lib/python3.10/dist-packages (from torch) (3.15.4)
Requirement already satisfied: typing-extensions>=4.8.0 in /usr/local/lib/python3.10/dist-packages (from torch) (4.12.2)
Requirement already satisfied: sympy in /usr/local/lib/python3.10/dist-packages (from torch) (1.13.1)
Requirement already satisfied: networkx in /usr/local/lib/python3.10/dist-packages (from torch) (3.3)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.10/dist-packages (from torch) (3.1.4)
Requirement already satisfied: fsspec in /usr/local/lib/python3.10/dist-packages (from torch) (2024.6.1)
Collecting nvidia-cuda-nvrtc-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_nvrtc_cu12-12.1.105-py3-none-manylinux1_x86_64.whl.metadata (1.5 kB)
Collecting nvidia-cuda-runtime-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_runtime_cu12-12.1.105-py3-none-manylinux1_x86_64.whl.metadata (1.5 kB)
Collecting nvidia-cuda-cupti-cu12==12.1.105 (from torch)
  Using cached nvidia_cuda_cupti_cu12-12.1.105-py3-none-manylinux1_x86_64.whl.metadata (1.6 kB)
Collecting nvidia-cudnn-cu12==8.9.2.26 (from torch)
  Using cached nvidia_cudnn_cu12-8.9.2.26-py3-none-manylinux1_x86_64.whl.metadata (1.6 kB)
Collecting nvidia-cublas-cu12==12.1.3.1 (from torch)
  Using cached nvidia_cublas_cu12-12.1.3.1-py3-none-manylinux1_x86_64.whl.metadata (1.5 kB)
Collecting nvidia-cufft-cu12==11.0.2.54 (from torch)
  Using cached nvidia_cufft_cu12-11.0.2.54-py3-none-manylinux1_x86_64.whl.metadata (1.5 kB)
Collecting nvidia-curand-cu12==10.3.2.106 (from torch)
  Using cached nvidia_curand_cu12-10.3.2.106-py3-none-manylinux1_x86_64.whl.metadata (1.5 kB)
Collecting nvidia-cusolver-cu12==11.4.5.107 (from torch)
  Using cached nvidia_cusolver_cu12-11.4.5.107-py3-none-manylinux1_x86_64.whl.metadata (1.6 kB)
Collecting nvidia-cusparse-cu12==12.1.0.106 (from torch)
  Using cached nvidia_cusparse_cu12-12.1.0.106-py3-none-manylinux1_x86_64.whl.metadata (1.6 kB)
Collecting nvidia-nccl-cu12==2.20.5 (from torch)
  Using cached nvidia_nccl_cu12-2.20.5-py3-none-manylinux2014_x86_64.whl.metadata (1.8 kB)
Collecting nvidia-nvtx-cu12==12.1.105 (from torch)
  Using cached nvidia_nvtx_cu12-12.1.105-py3-none-manylinux1_x86_64.whl.metadata (1.7 kB)
Requirement already satisfied: triton==2.3.1 in /usr/local/lib/python3.10/dist-packages (from torch) (2.3.1)
Collecting nvidia-nvjitlink-cu12 (from nvidia-cusolver-cu12==11.4.5.107->torch)
  Using cached nvidia_nvjitlink_cu12-12.6.20-py3-none-manylinux2014_x86_64.whl.metadata (1.5 kB)
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.10/dist-packages (from jinja2->torch) (2.1.5)
Requirement already satisfied: mpmath<1.4,>=1.1.0 in /usr/local/lib/python3.10/dist-packages (from sympy->torch) (1.3.0)
Using cached nvidia_cublas_cu12-12.1.3.1-py3-none-manylinux1_x86_64.whl (410.6 MB)
Using cached nvidia_cuda_cupti_cu12-12.1.105-py3-none-manylinux1_x86_64.whl (14.1 MB)
Using cached nvidia_cuda_nvrtc_cu12-12.1.105-py3-none-manylinux1_x86_64.whl (23.7 MB)
Using cached nvidia_cuda_runtime_cu12-12.1.105-py3-none-manylinux1_x86_64.whl (823 kB)
Using cached nvidia_cudnn_cu12-8.9.2.26-py3-none-manylinux1_x86_64.whl (731.7 MB)
Using cached nvidia_cufft_cu12-11.0.2.54-py3-none-manylinux1_x86_64.whl (121.6 MB)
Using cached nvidia_curand_cu12-10.3.2.106-py3-none-manylinux1_x86_64.whl (56.5 MB)
Using cached nvidia_cusolver_cu12-11.4.5.107-py3-none-manylinux1_x86_64.whl (124.2 MB)
Using cached nvidia_cusparse_cu12-12.1.0.106-py3-none-manylinux1_x86_64.whl (196.0 MB)
Using cached nvidia_nccl_cu12-2.20.5-py3-none-manylinux2014_x86_64.whl (176.2 MB)
Using cached nvidia_nvtx_cu12-12.1.105-py3-none-manylinux1_x86_64.whl (99 kB)
Using cached nvidia_nvjitlink_cu12-12.6.20-py3-none-manylinux2014_x86_64.whl (19.7 MB)
Installing collected packages: nvidia-nvtx-cu12, nvidia-nvjitlink-cu12, nvidia-nccl-cu12, nvidia-curand-cu12, nvidia-cufft-cu12, nvidia-cuda-runtime-cu12, nvidia-cuda-nvrtc-cu12, nvidia-cuda-cupti-cu12, nvidia-cublas-cu12, nvidia-cusparse-cu12, nvidia-cudnn-cu12, nvidia-cusolver-cu
Successfully installed nvidia-cublas-cu12-12.1.3.1 nvidia-cuda-cupti-cu12-12.1.105 nvidia-cuda-nvrtc-cu12-12.1.105 nvidia-cuda-runtime-cu12-12.1.105 nvidia-cudnn-cu12-8.9.2.26 nvidia-cufft-cu12-11.0.2.54 nvidia-curand-cu12-10.3.2.106 nvidia-cusolver-cu12-11.4.5.107 nvidia-cusparse-
Collecting torch-geometric
  Downloading torch_geometric-2.5.3-py3-none-any.whl.metadata (64 kB)
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Requirement already satisfied: tqdm in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (4.66.5)
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (1.26.4)
Requirement already satisfied: scipy in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (1.13.1)
Requirement already satisfied: fsspec in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (2024.6.1)
Requirement already satisfied: jinja2 in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (3.1.4)
Requirement already satisfied: aiohttp in /usr/local/lib/python3.10/dist-packages (from torch-geometric) (3.10.1)
```

```
import scipy.io
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.preprocessing import OneHotEncoder
import xgboost as xgb
from sklearn.model_selection import train_test_split, KFold, cross_val_score
from sklearn.preprocessing import StandardScaler
from sklearn.svm import SVR
from sklearn.linear_model import LinearRegression
from xgboost import XGBRegressor
from sklearn.metrics import mean_squared_error, r2_score

from sklearn.model_selection import StratifiedKFold, GridSearchCV
from sklearn.kernel_ridge import KernelRidge
from sklearn.metrics import mean_absolute_error
from sklearn.preprocessing import KBinsDiscretizer

import torch
from scipy.sparse import csr_matrix
from torch_geometric.utils import dense_to_sparse
import torch.nn.functional as F
from torch_geometric.nn import GCNConv
```

Read Data

```
# Load the .mat file
mat = scipy.io.loadmat('qm7.mat')
mat.keys()
```

```
dict_keys(['__header__', '__version__', '__globals__', 'X', 'R', 'Z', 'T', 'P'])
```

```
# Extract the variables
X = mat['X']  # Feature matrix
R = mat['R']  # Cartesian coordinates
Z = mat['Z']  # Atomic numbers
T = mat['T']  # Atomization energies (label)
P = mat['P']  # Other properties
```

Change Shape

```
R_flattened = R.reshape(R.shape[0], -1)
X_flattened = X.reshape(X.shape[0], -1)
```

```
Z
```

```
array([[6., 1., 1., ..., 0., 0., 0.],
       [6., 6., 1., ..., 0., 0., 0.],
       [6., 6., 1., ..., 0., 0., 0.],
       ...,
       [6., 6., 6., ..., 0., 0., 0.],
       [6., 6., 6., ..., 0., 0., 0.],
       [6., 6., 6., ..., 0., 0., 0.]], dtype=float32)
```

```
def one_hot_encode_Z(Z):
    num_samples, num_atoms = Z.shape
    max_atom_type = int(np.max(Z)) + 1
    encoder = OneHotEncoder(categories=[range(max_atom_type)], sparse=False)
    Z_reshaped = Z.reshape(-1, 1)
    Z_encoded = encoder.fit_transform(Z_reshaped).reshape(num_samples, num_atoms * max_atom_type)
    return Z_encoded

Z_encoded = one_hot_encode_Z(Z)
```

```
/usr/local/lib/python3.10/dist-packages/sklearn/preprocessing/_encoders.py:975: FutureWarning: `sparse` was renamed to `sparse_output` in version 1.2 and will be removed in 1.4. `sparse_output` is ignored unless you leave `sparse` to its default value.
  warnings.warn(
```

```
print(X_flattened.shape)
print(R_flattened.shape)
print(Z_encoded.shape)
print(P.shape)
```

```
(7165, 529)
(7165, 69)
(7165, 391)
(5, 1433)
```

```
P_reshape = P.reshape(7165, -1)
print(P_reshape.shape)
```

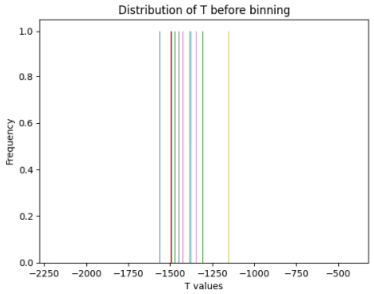
```
(7165, 1)
```

```
all_features = np.hstack((X_flattened, R_flattened, Z_encoded, P_reshape))
print(f"All features shape after trimming: {all_features.shape}")
```

```
All features shape after trimming: (7165, 990)
```

Convert to csv file

```
plt.hist(T, bins=50)
plt.title('Distribution of T before binning')
plt.xlabel('T values')
plt.ylabel('Frequency')
plt.show()
```




```
df = pd.DataFrame(data)

# Save to CSV
df.to_csv('Features.csv', index=False)
```

```
df2=pd.read_csv('Features.csv')
df2.head()
```

	0	1	2	3	4	5	6	7	8	9	...	981	982	983	984	985	986	987	988	989	Label
0	36.858105	2.907633	2.907612	2.907564	2.905349	0.000000	0.000000	0.000000	0.000000	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5578.0	-417.96
1	36.858105	12.599944	2.902000	1.473118	1.473101	2.901973	2.901886	1.473102	0.000000	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2504.0	-712.42
2	36.858105	14.261827	1.503703	2.924997	2.924732	1.503680	0.000000	0.000000	0.000000	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	4851.0	-564.21
3	36.858105	15.871878	2.979434	1.401225	0.000000	0.000000	0.000000	0.000000	0.000000	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3130.0	-404.88
4	73.516693	17.885317	10.561490	4.355064	2.062530	2.069614	1.581991	1.590780	1.261482	0.0	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6670.0	-808.87

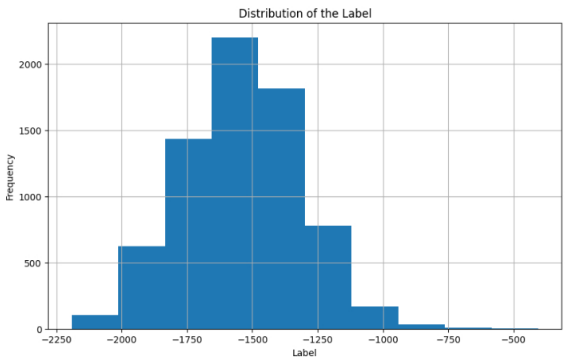
5 rows × 991 columns

```
df2.describe()
```

	0	1	2	3	4	5	6	7	8	9	...	981	982	983	984	985	986	987	988	989	Label
count	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	7165.000000	...	7165.0	7165.0	7165.0	7165.0	7165.0	7165.0	7165.0	7165.0	7165.000000	7165.000000
mean	78.447518	13.247392	13.651229	12.761609	11.313269	9.741235	7.374219	1.992688	1.709067	1.595967	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3582.000000	-1538.037630
std	65.448339	6.134428	6.168350	5.406752	4.984658	4.785995	4.318243	0.912114	0.721890	0.698753	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2068.501672	223.934546
min	36.858105	2.907633	1.503703	1.172837	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000000	-2192.000000
25%	53.358707	9.065171	9.293125	9.019773	7.737596	6.671409	4.668823	1.421404	1.297994	1.192658	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1791.000000	-1704.230000
50%	73.516693	12.434812	12.495984	10.668070	10.247300	8.685217	6.669063	1.717358	1.562530	1.470488	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3582.000000	-1544.380000
75%	73.516693	15.262316	17.618086	17.504143	14.998941	10.677979	9.189721	2.049483	1.957705	1.774468	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5373.000000	-1385.890000
max	388.023438	47.143398	47.179157	47.015327	29.794344	29.790239	29.617144	4.379876	4.373618	4.364484	...	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	7164.000000	-404.880000

8 rows × 991 columns

```
plt.figure(figsize=(10, 6))
df2['Label'].hist()
plt.title('Distribution of the Label')
plt.xlabel('Label')
plt.ylabel('Frequency')
plt.show()
```



Run on Machine Learning Models

```
# Check the shape of the concatenated data
print(df2.shape)

# Define the feature matrix X and target vector y
X = df2.iloc[:, :-1].values
y = df2.iloc[:, -1].values

# Check the distribution of y
print(np.unique(y, return_counts=True))

X=np.array(X)
y=np.array(y)
```

```
(7165, 991)
(array([-2192.  , -2191.85, -2191.74, ...,  -564.21,  -417.96,  -404.88]), array([1, 1, 1, ..., 1, 1, 1]))
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
# Standardize the features
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

```
models = {
    'KernelRidge': KernelRidge(alpha=1e-3),
    'SVR': SVR(),
    'LinearRegression': LinearRegression(),
    'XGBRegressor': xgb.XGBRegressor(n_estimators=200)
}

kf = KFold(n_splits=10, shuffle=True, random_state=1)
kernels = ['poly', 'rbf', 'sigmoid']
```

```
def evaluate_model(model, X, y, cv):
```

```
    # Tính toán MSE và lưu lại tất cả các điểm số
    mse_scores = -cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv)
    mse_mean = mse_scores.mean()
    mse_std = mse_scores.std()

    # Tính toán R2 và lưu lại tất cả các điểm số
    r2_scores = cross_val_score(model, X, y, scoring='r2', cv=cv)
    r2_mean = r2_scores.mean()
    r2_std = r2_scores.std()

    return mse_mean, mse_std, r2_mean, r2_std
```

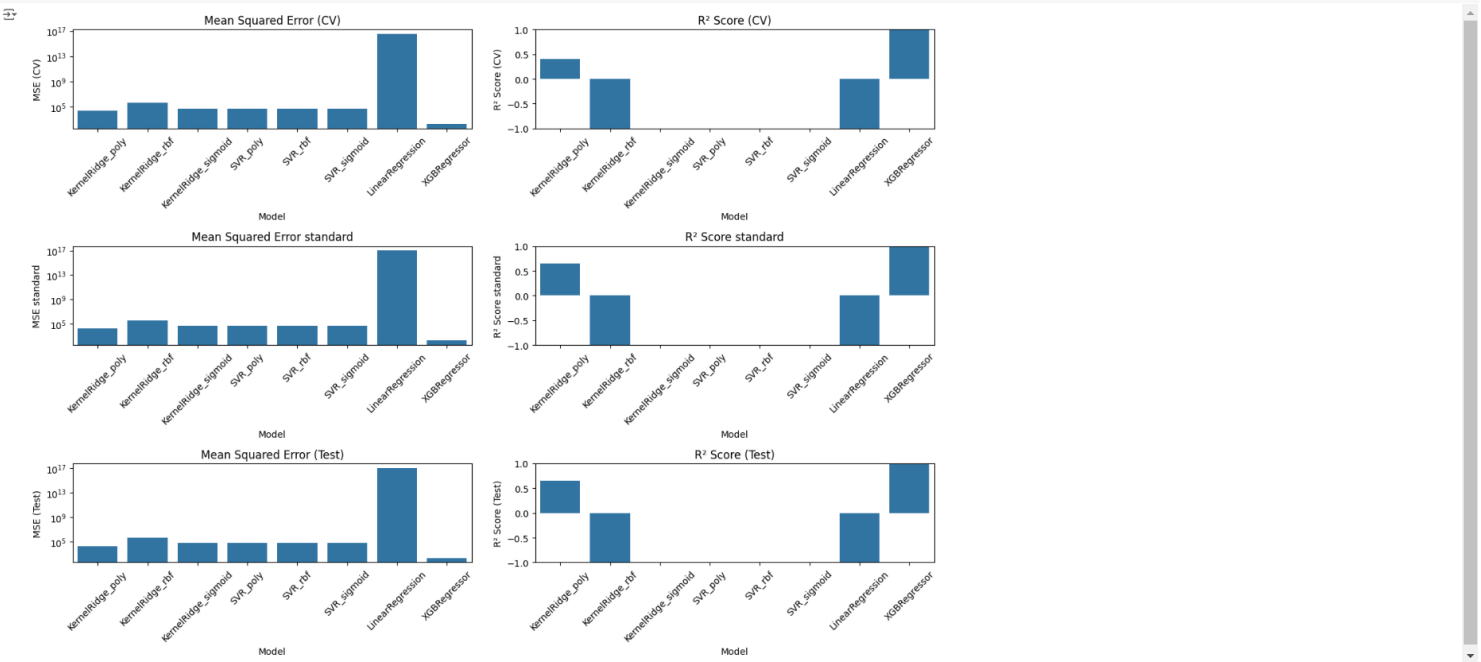
```
results = {}

for model_name, model in models.items():
    if model_name in ['KernelRidge', 'SVR']:
        for kernel in kernels:
            model.set_params(kernel=kernel)

            # Cross-validation scores
            mse_cv, mse_std, r2_cv, r2_std = evaluate_model(model, X_train, y_train, kf)

            # Train the model
            model.fit(X_train, y_train)

            # Predict on the test set
            y_pred = model.predict(X_test)

            # Calculate metrics
            mse_test = mean_squared_error(y_test, y_pred)
            r2_test = r2_score(y_test, y_pred)

            # Store results
            results[f"{model_name}_{kernel}"] = {
                'MSE (CV)': mse_cv,
                'MSE Std (CV)': mse_std,
                'R2 Score (CV)': r2_cv,
                'R2 Std (CV)': r2_std,
                'MSE (Test)': mse_test,
                'R2 Score (Test)': r2_test
            }
    else:
        # Cross-validation scores
        mse_cv, mse_std, r2_cv, r2_std = evaluate_model(model, X_train, y_train, kf)

        # Train the model
        model.fit(X_train, y_train)

        # Predict on the test set
        y_pred = model.predict(X_test)

        # Calculate metrics
        mse_test = mean_squared_error(y_test, y_pred)
        r2_test = r2_score(y_test, y_pred)

        # Store results
        results[model_name] = {
            'MSE (CV)': mse_cv,
            'MSE Std (CV)': mse_std,
            'R2 Score (CV)': r2_cv,
            'R2 Std (CV)': r2_std,
            'MSE (Test)': mse_test,
            'R2 Score (Test)': r2_test
        }

# Convert results to DataFrame
results_df = pd.DataFrame(results).T
print(results_df)
```

```
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.38174e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.74014e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.44152e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.54641e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.89509e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.26118e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.58482e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.35888e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.62235e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.48786e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.38174e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.74014e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.44152e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.54641e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.89509e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.26118e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.58482e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.35888e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=1.62235e-17): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=9.48786e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:237: LinAlgWarning: Ill-conditioned matrix (rcond=6.76203e-18): result may not be accurate.
  dual_coef = linalg.solve(K, y, assume_a="pos", overwrite_a=False)
                     MSE (CV)  MSE Std (CV)  R2 Score (CV)   R2 Std (CV)  \
KernelRidge_poly   2.855964e+04  1.884581e+04   4.065057e-01  4.403843e-01
KernelRidge_rbf    4.246292e+05  2.489542e+04  -7.527440e+00  3.680041e-01
KernelRidge_sigmoid  5.000993e+04  3.426761e+03  -2.686898e-03  3.967614e-03
SVR_poly           4.988002e+04  3.401032e+03  -9.245291e-05  3.021174e-03
SVR_rbf            4.996648e+04  3.388323e+03  -1.855336e-03  2.954795e-03
SVR_sigmoid        5.000534e+04  3.363868e+03  -2.682985e-03  3.509209e-03
LinearRegression   3.323062e+16  9.133213e+16  -6.463397e+11  1.765149e+12
XGBRegressor       2.129528e+02  3.908760e+01   9.957225e-01  7.761498e-04

                    MSE (Test)  R2 Score (Test)
KernelRidge_poly   1.789371e+04     6.481075e-01
KernelRidge_rbf    3.942758e+05    -6.753714e+00
KernelRidge_sigmoid  5.095103e+04    -1.988278e-03
SVR_poly           5.074120e+04     2.138204e-03
SVR_rbf            5.083689e+04     2.564354e-04
```

Visualize Result

```
plt.figure(figsize=(14, 10))

# MSE (CV)
plt.subplot(3, 2, 1)
sns.barplot(x=results_df.index, y=results_df['MSE (CV)'])
plt.title('Mean Squared Error (CV)')
plt.xlabel('Model')
plt.ylabel('MSE (CV)')
plt.yscale('log')
plt.xticks(rotation=45)

# R² Score (CV)
plt.subplot(3, 2, 2)
sns.barplot(x=results_df.index, y=results_df['R2 Score (CV)'])
plt.title('R² Score (CV)')
plt.xlabel('Model')
plt.ylabel('R² Score (CV)')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

# MSE std
plt.subplot(3, 2, 3)
sns.barplot(x=results_df.index, y=results_df['MSE (Test)'])
plt.title('Mean Squared Error standard')
plt.xlabel('Model')
plt.ylabel('MSE standard')
plt.yscale('log')
plt.xticks(rotation=45)

# R² std
plt.subplot(3, 2, 4)
```

```
sns.barplot(x=results_df.index, y=results_df['R2 Score (Test)'])
plt.title('R² Score standard')
plt.xlabel('Model')
plt.ylabel('R² Score standard')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

# MSE (Test)
plt.subplot(3, 2, 5)
sns.barplot(x=results_df.index, y=results_df['MSE (Test)'])
plt.title('Mean Squared Error (Test)')
plt.xlabel('Model')
plt.ylabel('MSE (Test)')
plt.yscale('log')
plt.xticks(rotation=45)

# R² Score (Test)
plt.subplot(3, 2, 6)
sns.barplot(x=results_df.index, y=results_df['R2 Score (Test)'])
plt.title('R² Score (Test)')
plt.xlabel('Model')
plt.ylabel('R² Score (Test)')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

plt.tight_layout()
plt.show()
```



GNN

```
# Convert train and test data into sparse matrix
sparse_matrix_train = csr_matrix(X_train)
sparse_matrix_test = csr_matrix(X_test)

# Convert sparse matrix into dense matrix
node_features_train = torch.tensor(sparse_matrix_train.toarray(), dtype=torch.float)
node_features_test = torch.tensor(sparse_matrix_test.toarray(), dtype=torch.float)

# Convert dense matrix into sparse representation
edge_index_train, edge_attr_train = dense_to_sparse(node_features_train)
edge_index_test, edge_attr_test = dense_to_sparse(node_features_test)

# Convert labels into tensor
labels_train = torch.tensor(y_train, dtype=torch.float)
labels_test = torch.tensor(y_test, dtype=torch.float)

print(f"Train Edge Index:\n{edge_index_train}")
print(f"Train Node Features Shape: {node_features_train.shape}")
print(f"Train Labels Shape: {labels_train.shape}")
```

```
Train Edge Index:
tensor([[   0,    0,    0, ..., 5731, 5731, 5731],
        [   0,    1,    2, ...,  955,  972,  989]])
Train Node Features Shape: torch.Size([5732, 990])
Train Labels Shape: torch.Size([5732])
```

```
class GCNRegression(torch.nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim):
        super(GCNRegression, self).__init__()
        self.conv1 = GCNConv(input_dim, hidden_dim)
        self.conv2 = GCNConv(hidden_dim, output_dim)

    def forward(self, node_features, edge_index):
        x = self.conv1(node_features, edge_index)
        x = F.relu(x)
        x = self.conv2(x, edge_index)
        return x
```

```
model = GCNRegression(input_dim=node_features_train.shape[1], hidden_dim=64, output_dim=1)

# Use Adam optimizer and Mean Squared Error loss
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
criterion = torch.nn.MSELoss()
```

```
# List to store loss values
train_losses = []

# Training loop with loss storage
model.train()
for epoch in range(100):
    optimizer.zero_grad()
    out = model(node_features_train, edge_index_train).squeeze()
    loss = criterion(out, labels_train)
    loss.backward()
    optimizer.step()

    train_losses.append(loss.item())

    if epoch % 5 == 0:
        print(f'Epoch {epoch}, Loss: {loss.item()}')
```

```
Epoch 0, Loss: 4562712.0
Epoch 5, Loss: 5468117.0
Epoch 10, Loss: 3582781.25
Epoch 15, Loss: 3096413.0
Epoch 20, Loss: 2744736.0
Epoch 25, Loss: 2443654.5
Epoch 30, Loss: 2252135.5
Epoch 35, Loss: 2162911.0
Epoch 40, Loss: 2133029.5
Epoch 45, Loss: 2125043.25
Epoch 50, Loss: 2122809.0
Epoch 55, Loss: 2121201.0
```

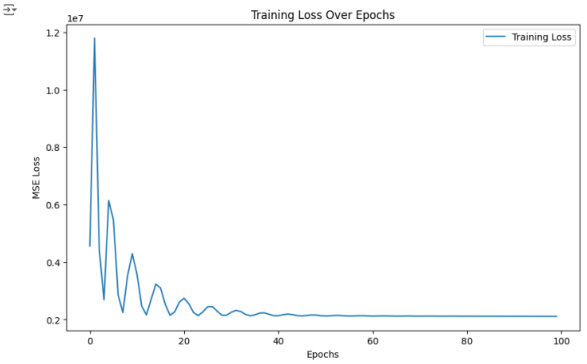
```
Epoch 60, Loss: 2119464.5
Epoch 65, Loss: 2117790.5
Epoch 70, Loss: 2116322.0
Epoch 75, Loss: 2115062.75
Epoch 80, Loss: 2113924.75
Epoch 85, Loss: 2112798.75
Epoch 90, Loss: 2111627.75
Epoch 95, Loss: 2110426.5
```

```
# After training, evaluate and visualize the predictions
model.eval()
with torch.no_grad():
    output_test = model(node_features_test, edge_index_test).squeeze()
    mse_test = criterion(output_test, labels_test).item()
    print(f'Test Mean Squared Error: {mse_test}')

    # Convert tensors to numpy for plotting
    output_test_np = output_test.cpu().numpy()
    labels_test_np = labels_test.cpu().numpy()
```

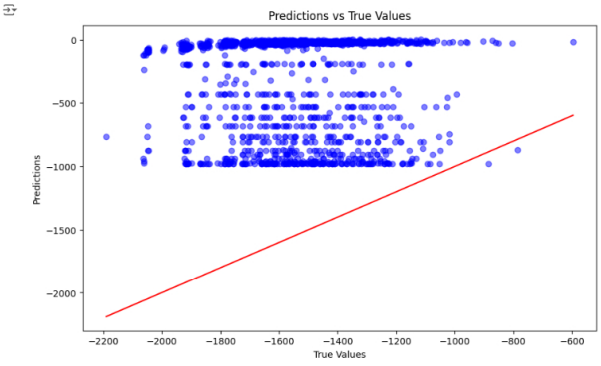
```
Test Mean Squared Error: 1697099.625
```

Visualize Result

```
# Plot the training loss over epochs
plt.figure(figsize=(10, 6))
plt.plot(train_losses, label='Training Loss')
plt.xlabel('Epochs')
plt.ylabel('MSE Loss')
plt.title('Training Loss Over Epochs')
plt.legend()
plt.show()
```




```
# Plot predictions vs true values
plt.figure(figsize=(10, 6))
plt.scatter(labels_test_np, output_test_np, color='blue', alpha=0.5)
plt.plot([min(labels_test_np), max(labels_test_np)], [min(labels_test_np), max(labels_test_np)], color='red')
plt.xlabel('True Values')
plt.ylabel('Predictions')
plt.title('Predictions vs True Values')
plt.show()
```



Features Extraction

```
all_features = np.hstack((X_flattened, R_flattened, P_reshape))
print(f"All features shape after trimming: {all_features.shape}")
```

```
All features shape after trimming: (7165, 599)
```

```
# Check the shape of the concatenated data
print(all_features.shape)

# Define the feature matrix X and target vector y
X = all_features[:, :-1]
y = all_features[:, -1]

# Check the distribution of y
print(np.unique(y, return_counts=True))

X=np.array(X)
y=np.array(y)
```

```
(7165, 599)
(array([0.000e+00, 1.000e+00, 2.000e+00, ..., 7.162e+03, 7.163e+03,
       7.164e+03]), array([1, 1, 1, ..., 1, 1, 1]))
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
# Standardize the features
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

```
models = {
    'KernelRidge': KernelRidge(alpha=1e-3),
    'SVR': SVR(),
    'LinearRegression': LinearRegression(),
    'XGBRegressor': xgb.XGBRegressor(n_estimators=200)
}

kf = KFold(n_splits=10, shuffle=True, random_state=1)
kernels = ['poly', 'rbf', 'sigmoid']
```

```
def evaluate_model(model, X, y, cv):
    # Tính toán MSE và lưu lại tất cả các điểm số
    mse_scores = -cross_val_score(model, X, y, scoring='neg_mean_squared_error', cv=cv)
    mse_mean = mse_scores.mean()
    mse_std = mse_scores.std()

    # Tính toán R2 và lưu lại tất cả các điểm số
    r2_scores = cross_val_score(model, X, y, scoring='r2', cv=cv)
    r2_mean = r2_scores.mean()
```

```python
    r2_std = r2_scores.std()

    return mse_mean, mse_std, r2_mean, r2_std
```

```python
results = {}

for model_name, model in models.items():
    if model_name in ['KernelRidge', 'SVR']:
        for kernel in kernels:
            model.set_params(kernel=kernel)

            # Cross-validation scores
            mse_cv, mse_std, r2_cv, r2_std = evaluate_model(model, X_train, y_train, kf)

            # Train the model
            model.fit(X_train, y_train)

            # Predict on the test set
            y_pred = model.predict(X_test)

            # Calculate metrics
            mse_test = mean_squared_error(y_test, y_pred)
            r2_test = r2_score(y_test, y_pred)

            # Store results
            results[f"{model_name}_{kernel}"] = {
                'MSE (CV)': mse_cv,
                'MSE Std (CV)': mse_std,
                'R2 Score (CV)': r2_cv,
                'R2 Std (CV)': r2_std,
                'MSE (Test)': mse_test,
                'R2 Score (Test)': r2_test
            }
    else:
        # Cross-validation scores
        mse_cv, mse_std, r2_cv, r2_std = evaluate_model(model, X_train, y_train, kf)

        # Train the model
        model.fit(X_train, y_train)

        # Predict on the test set
        y_pred = model.predict(X_test)

        # Calculate metrics
        mse_test = mean_squared_error(y_test, y_pred)
        r2_test = r2_score(y_test, y_pred)

        # Store results
        results[model_name] = {
            'MSE (CV)': mse_cv,
            'MSE Std (CV)': mse_std,
            'R2 Score (CV)': r2_cv,
            'R2 Std (CV)': r2_std,
            'MSE (Test)': mse_test,
            'R2 Score (Test)': r2_test
        }

# Convert results to DataFrame
results_df = pd.DataFrame(results).T
print(results_df)
```

```
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
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/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
/usr/local/lib/python3.10/dist-packages/sklearn/linear_model/_ridge.py:239: UserWarning: Singular matrix in solving dual problem. Using least-squares solution instead.
  warnings.warn(
                        MSE (CV)  MSE Std (CV)  R2 Score (CV)  R2 Std (CV)  \
KernelRidge_poly     2.058873e+07  4.262519e+06      -3.856747     1.001932
KernelRidge_rbf      5.341503e+06  2.450530e+05      -0.259211     0.047398
KernelRidge_sigmoid  4.817034e+06  1.696370e+06      -0.135385     0.400261
SVR_poly             4.255618e+06  1.982779e+05      -0.002514     0.002950
SVR_rbf              4.254027e+06  1.985850e+05      -0.002134     0.002776
SVR_sigmoid          4.253990e+06  1.987521e+05      -0.002124     0.002821
LinearRegression     5.063501e+07  1.252421e+08     -10.937504    29.540165
XGBRegressor         5.218638e+06  2.349284e+05      -0.230309     0.045336

                       MSE (Test)  R2 Score (Test)
KernelRidge_poly     2.214123e+07        -4.048684
KernelRidge_rbf      5.454509e+06        -0.243747
KernelRidge_sigmoid  4.382663e+06         0.000657
SVR_poly             4.383017e+06         0.000576
SVR_rbf              4.385370e+06         0.000040
SVR_sigmoid          4.385622e+06        -0.000017
LinearRegression     8.868284e+06        -1.022162
XGBRegressor         5.247707e+06        -0.196592
```
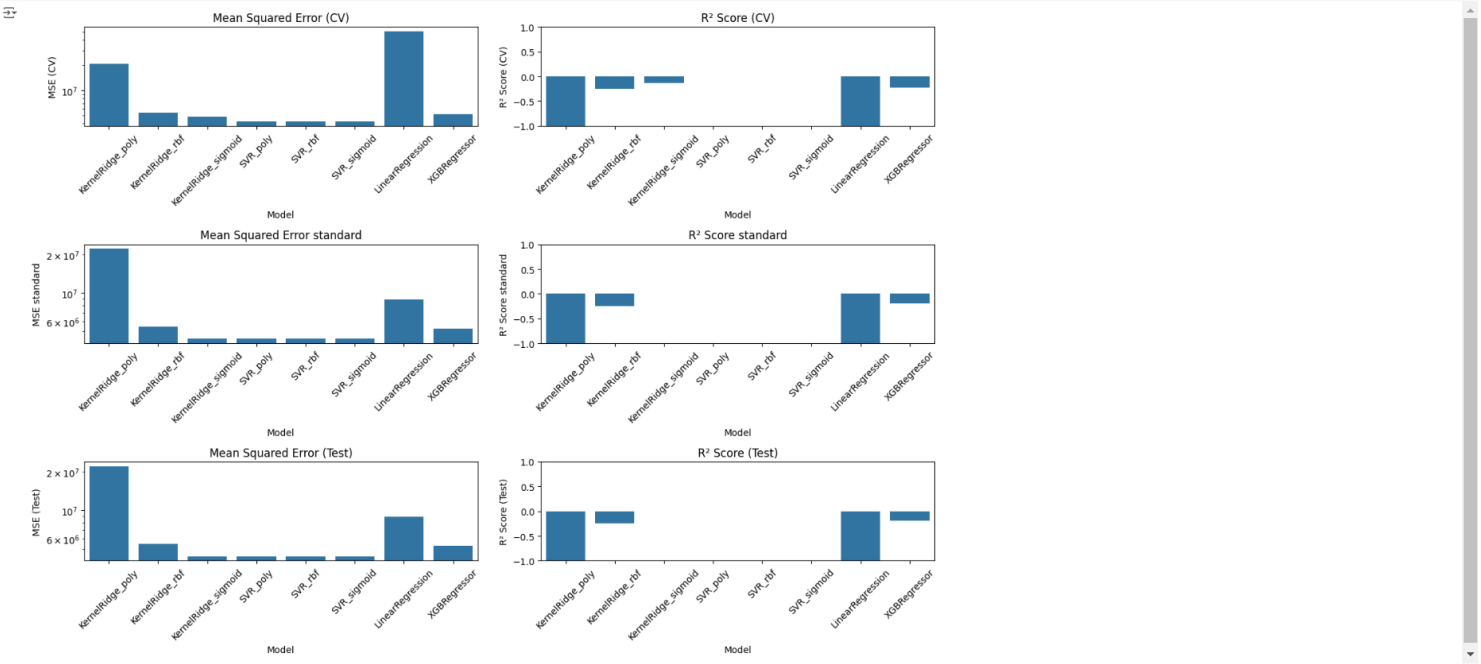

```python
plt.figure(figsize=(14, 10))

# MSE (CV)
plt.subplot(3, 2, 1)
sns.barplot(x=results_df.index, y=results_df['MSE (CV)'])
plt.title('Mean Squared Error (CV)')
plt.xlabel('Model')
plt.ylabel('MSE (CV)')
plt.yscale('log')
plt.xticks(rotation=45)

# R² Score (CV)
plt.subplot(3, 2, 2)
sns.barplot(x=results_df.index, y=results_df['R2 Score (CV)'])
plt.title('R² Score (CV)')
plt.xlabel('Model')
plt.ylabel('R² Score (CV)')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

# MSE std
plt.subplot(3, 2, 3)
sns.barplot(x=results_df.index, y=results_df['MSE (Test)'])
plt.title('Mean Squared Error standard')
plt.xlabel('Model')
plt.ylabel('MSE standard')
plt.yscale('log')
plt.xticks(rotation=45)

# R² std
plt.subplot(3, 2, 4)
sns.barplot(x=results_df.index, y=results_df['R2 Score (Test)'])
plt.title('R² Score standard')
plt.xlabel('Model')
plt.ylabel('R² Score standard')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

# MSE (Test)
plt.subplot(3, 2, 5)
sns.barplot(x=results_df.index, y=results_df['MSE (Test)'])
plt.title('Mean Squared Error (Test)')
plt.xlabel('Model')
plt.ylabel('MSE (Test)')
```

```
plt.yscale('log')
plt.xticks(rotation=45)

# R² Score (Test)
plt.subplot(3, 2, 6)
sns.barplot(x=results_df.index, y=results_df['R2 Score (Test)'])
plt.title('R² Score (Test)')
plt.xlabel('Model')
plt.ylabel('R² Score (Test)')
plt.ylim(-1, 1)
plt.xticks(rotation=45)

plt.tight_layout()
plt.show()
```



GNN For Features Extraction

```
# Convert train and test data into sparse matrix
sparse_matrix_train = csr_matrix(X_train)
sparse_matrix_test = csr_matrix(X_test)

# Convert sparse matrix into dense matrix
node_features_train = torch.tensor(sparse_matrix_train.toarray(), dtype=torch.float)
node_features_test = torch.tensor(sparse_matrix_test.toarray(), dtype=torch.float)

# Convert dense matrix into sparse representation
edge_index_train, edge_attr_train = dense_to_sparse(node_features_train)
edge_index_test, edge_attr_test = dense_to_sparse(node_features_test)

# Convert labels into tensor
labels_train = torch.tensor(y_train, dtype=torch.float)
labels_test = torch.tensor(y_test, dtype=torch.float)

print(f"Train Edge Index:\n{edge_index_train}")
print(f"Train Node Features Shape: {node_features_train.shape}")
print(f"Train Labels Shape: {labels_train.shape}")
```

```
Train Edge Index:
tensor([[   0,    0,    0,  ..., 5731, 5731, 5731],
        [   0,    1,    2,  ...,  568,  569,  570]])
Train Node Features Shape: torch.Size([5732, 598])
Train Labels Shape: torch.Size([5732])
```

```
class GCNRegression(torch.nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim):
        super(GCNRegression, self).__init__()
        self.conv1 = GCNConv(input_dim, hidden_dim)
        self.conv2 = GCNConv(hidden_dim, output_dim)

    def forward(self, node_features, edge_index):
        x = self.conv1(node_features, edge_index)
        x = F.relu(x)
        x = self.conv2(x, edge_index)
        return x
```

```
model = GCNRegression(input_dim=node_features_train.shape[1], hidden_dim=64, output_dim=1)

# Use Adam optimizer and Mean Squared Error loss
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
criterion = torch.nn.MSELoss()
```

```
# List to store loss values
train_losses = []

# Training loop with loss storage
model.train()
for epoch in range(100):
    optimizer.zero_grad()
    out = model(node_features_train, edge_index_train).squeeze()
    loss = criterion(out, labels_train)
    loss.backward()
    optimizer.step()

    train_losses.append(loss.item())

    if epoch % 5 == 0:
        print(f'Epoch {epoch}, Loss: {loss.item()}')
```

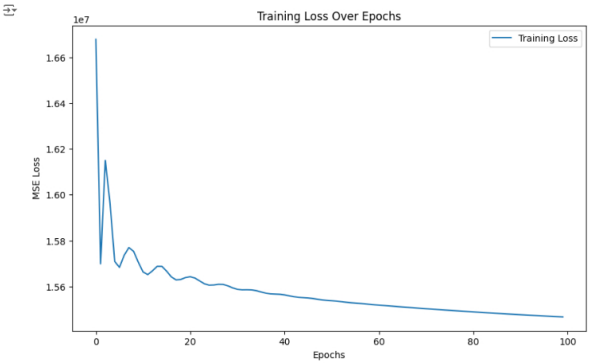
```
Epoch 0, Loss: 16677674.0
Epoch 5, Loss: 15684064.0
Epoch 10, Loss: 15664284.0
Epoch 15, Loss: 15667583.0
Epoch 20, Loss: 15643379.0
Epoch 25, Loss: 15607472.0
Epoch 30, Loss: 15588737.0
Epoch 35, Loss: 15577462.0
Epoch 40, Loss: 15564567.0
Epoch 45, Loss: 15551147.0
Epoch 50, Loss: 15539169.0
Epoch 55, Loss: 15528964.0
Epoch 60, Loss: 15520058.0
Epoch 65, Loss: 15511996.0
Epoch 70, Loss: 15504469.0
Epoch 75, Loss: 15497388.0
Epoch 80, Loss: 15490698.0
Epoch 85, Loss: 15484376.0
Epoch 90, Loss: 15478455.0
Epoch 95, Loss: 15472950.0
```

```
# After training, evaluate and visualize the predictions
model.eval()
with torch.no_grad():
    output_test = model(node_features_test, edge_index_test).squeeze()
```

```
        mse_test = criterion(output_test, labels_test).item()
        print(f'Test Mean Squared Error: {mse_test}')

        # Convert tensors to numpy for plotting
        output_test_np = output_test.cpu().numpy()
        labels_test_np = labels_test.cpu().numpy()
```

```
Test Mean Squared Error: 13136575.0
```

```
[ ] # Plot the training loss over epochs
    plt.figure(figsize=(10, 6))
    plt.plot(train_losses, label='Training Loss')
    plt.xlabel('Epochs')
    plt.ylabel('MSE Loss')
    plt.title('Training Loss Over Epochs')
    plt.legend()
    plt.show()
```



Các sản phẩm có tính phí của Colab - Huỷ hợp đồng tại đây