TFM_Exp1_Local

June 20, 2025

1 Experimento 1

Basado en los notebooks proporcionados en los siguientes enlaces:

- pykan/…/tutorials/Example/Example_1_function_fitting
- pykan/hellokan.ipynb

El teorema de representación de Kolmogorov-Arnold establece que si f es una función continua multivariada en un dominio acotado, entonces se puede escribir como una composición finita de funciones continuas de una sola variable y la operación binaria de suma.

Por lo tanto, dada $f : [0,1]^n \to \mathbb{R}$ cumpliendo ciertas condiciones,

$$f(x) = f(x_1, ..., x_n) = \sum_{q=1}^{2n+1} \Phi_q(\sum_{p=1}^{n} \phi_{q,p}(x_p))$$

donde $\phi_{q,p} : [0,1] \to \mathbb{R}$ y $\Phi_q : \mathbb{R} \to \mathbb{R}$.

En cierto sentido, el KART indica que la única operación multivariada verdadera es la operación suma, ya que cualquier otra función puede escribirse usando funciones univariadas y la suma.

Sin embargo, esta representación de Kolmogorov-Arnold de 2 capas de ancho $(2n+1)$ puede no ser suave debido a su limitada capacidad expresiva.

En liu et al. (2024) se aumenta su capacidad expresiva generalizándola a profundidades y anchos arbitrarios.

1.1 Instalación de pykan

[1]:
```
!pip install pykan
```

```
Collecting pykan
  Using cached pykan-0.2.8-py3-none-any.whl.metadata (11 kB)
Using cached pykan-0.2.8-py3-none-any.whl (78 kB)
Installing collected packages: pykan
Successfully installed pykan-0.2.8
```

[5]:
```
!pip install tqdm
```

```
Collecting tqdm
  Using cached tqdm-4.67.1-py3-none-any.whl.metadata (57 kB)
```

```
Requirement already satisfied: colorama in
c:\users\jorge\anaconda3\envs\kan_pytorch\lib\site-packages (from tqdm) (0.4.6)
Using cached tqdm-4.67.1-py3-none-any.whl (78 kB)
Installing collected packages: tqdm
Successfully installed tqdm-4.67.1
```

1.2 Configuración de torch, device y generación de modelo base

[7]:
```
from kan import *
torch.set_default_dtype(torch.float64)

device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)

# create a KAN: 2D inputs, 1D output, and 5 hidden neurons. cubic spline (k=3),␣
↪5 grid intervals (grid=5).
model = KAN(width=[2,5,1], grid=3, k=3, seed=42, device=device)
```

```
cuda
checkpoint directory created: ./model
saving model version 0.0
```

1.3 Creación del dataset

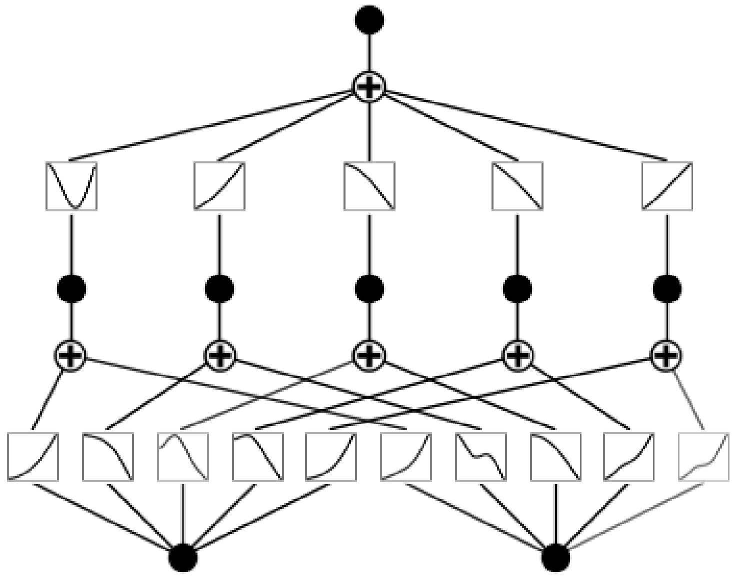
Se genera un conjunto de datos conformado con las evaluaciones de una función en una serie de valores de sus variables de entrada. La función create_dataset nos genera un conjunto de 1000 valores de entrenamiento y de etiquetas de entrenamiento asociadas.

[8]:
```
from kan.utils import create_dataset
# create dataset f(x,y) = exp(sin(pi*x)+y^2)
f = lambda x: torch.exp(torch.sin(torch.pi*x[:,[0]]) + x[:,[1]]**2)
dataset = create_dataset(f, n_var=2, device=device)
dataset['train_input'].shape, dataset['train_label'].shape
```

[8]:
```
(torch.Size([1000, 2]), torch.Size([1000, 1]))
```

1.4 Inicialización del modelo

[9]:
```
# plot KAN at initialization
model(dataset['train_input']);
model.plot()
```



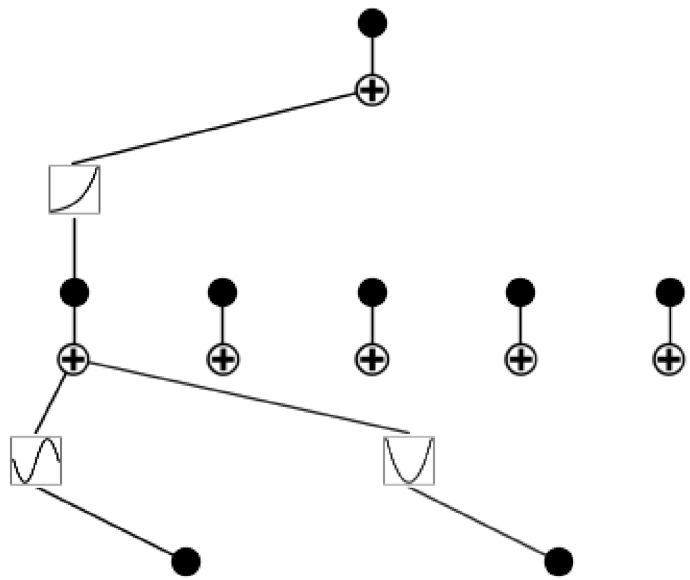
1.5 Entrenamiento inicial

[10]:
```
# train the model
model.fit(dataset, opt="LBFGS", steps=50, lamb=0.001);
```

```
| train_loss: 1.91e-02 | test_loss: 1.88e-02 | reg: 5.74e+00 | : 100%| | 50/50
[00:18<00:00,  2.77it
```

```
saving model version 0.1
```

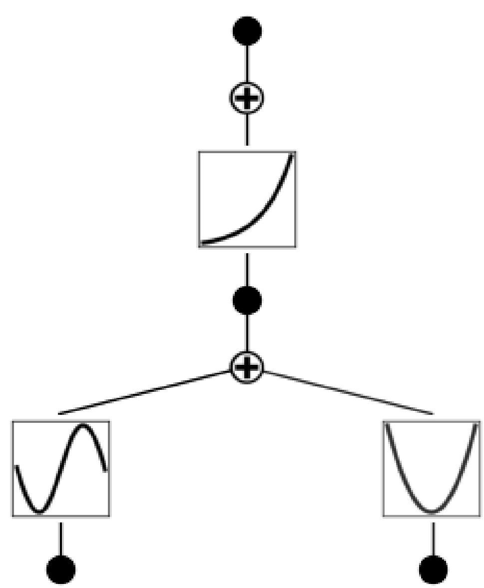
[11]:
```
model.plot()
```



1.6 Poda del modelo

[12]:
```
model = model.prune()
model.plot()
```

```
saving model version 0.2
```



1.7 Entrenamiento modelo podado

[13]:
```
model.fit(dataset, opt="LBFGS", steps=50);
```

```
| train_loss: 1.78e-02 | test_loss: 1.70e-02 | reg: 8.13e+00 | : 100%| | 50/50
[00:12<00:00,  3.97it
```

```
saving model version 0.3
```

1.8 Refinamos el grid del modelo

[14]:
```
model = model.refine(10)
```

```
saving model version 0.4
```

1.9 Entrenamiento modelo refinado

[15]:
```
model.fit(dataset, opt="LBFGS", steps=50);
```

```
| train_loss: 4.65e-04 | test_loss: 4.71e-04 | reg: 8.13e+00 | : 100%| | 50/50
[00:12<00:00,  4.12it
```

```
saving model version 0.5
```

1.10 Obtención de la expresión simbólica

[16]:
```
mode = "auto" # "manual"

if mode == "manual":
    # manual mode
    model.fix_symbolic(0,0,0,'sin');
    model.fix_symbolic(0,1,0,'x^2');
    model.fix_symbolic(1,0,0,'exp');
elif mode == "auto":
    # automatic mode
    lib = ['x','x^2','x^3','x^4','exp','log','sqrt','tanh','sin','abs']
    model.auto_symbolic(lib=lib)
```

```
fixing (0,0,0) with sin, r2=0.9999999193565677, c=2
fixing (0,1,0) with x^2, r2=0.9999999823307842, c=2
fixing (1,0,0) with exp, r2=0.9999999908846936, c=2
saving model version 0.6
```

1.11 Último entrenamiento para conseguir precisión máquina

[17]:
```
model.fit(dataset, opt="LBFGS", steps=50);
```

```
| train_loss: 9.41e-12 | test_loss: 3.70e-12 | reg: 0.00e+00 | : 100%| | 50/50
[00:04<00:00, 11.42it
```

```
saving model version 0.7
```

1.12 Expresión final redondeada

[18]:
```
from kan.utils import ex_round

ex_round(model.symbolic_formula()[0][0],4)
```

[18]: $1.0e^{1.0x_2^2+1.0\sin(3.1416x_1)}$

2 Ejemplo nuevo

[55]:
```
# create a KAN: 2D inputs, 1D output, and 5 hidden neurons. cubic spline (k=3),␣
↪5 grid intervals (grid=5).
model = KAN(width=[4,2,1,1], grid=3, k=3, seed=1, device=device)
f = lambda x: torch.exp((torch.cos(torch.pi*(x[:,[0]]**2+x[:,[1]]**2))+torch.
↪cos(torch.pi*(x[:,[2]]**2+x[:,[3]]**2)))/2)
dataset = create_dataset(f, n_var=4, train_num=3000, device=device)

# train the model
model.fit(dataset, opt="LBFGS", steps=20, lamb=0.002, lamb_entropy=2.);
```

```
checkpoint directory created: ./model
saving model version 0.0
```

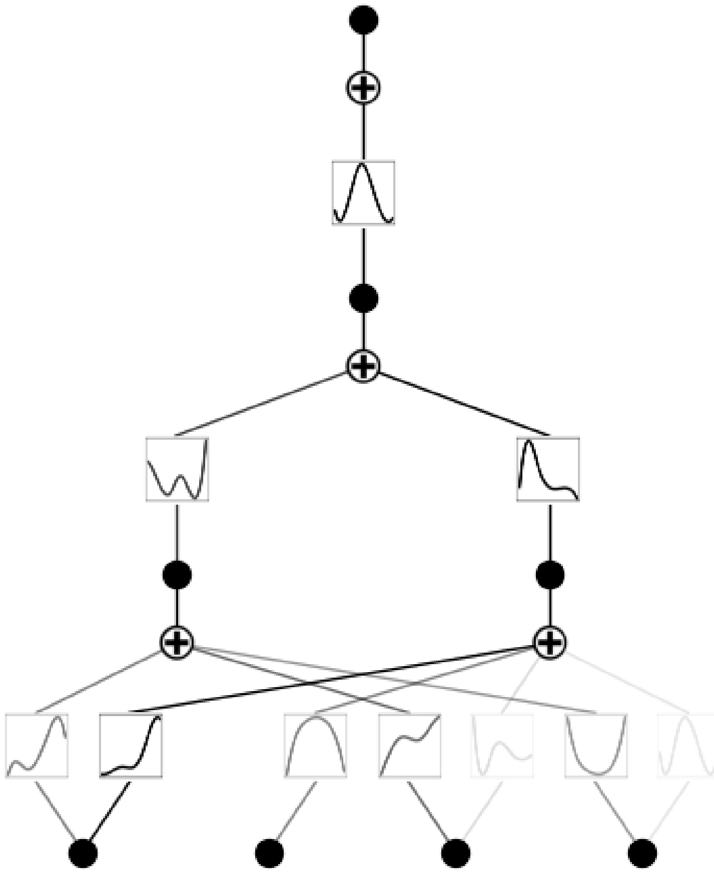
```
| train_loss: 3.36e-01 | test_loss: 3.43e-01 | reg: 1.00e+01 | : 100%| | 20/20
[00:45<00:00,  2.26s/
```

```
saving model version 0.1
```

[56]:
```
model = model.prune(edge_th=1e-2)
```

```
saving model version 0.2
```

[57]:
```
model.plot()
```



```
[58]: #grids = [3,5,10,20,50]
grids = [3,5,10,15]

train_rmse = []
test_rmse = []

for i in range(len(grids)):
    #model = KAN(width=[4,2,1,1], grid=grids[i], k=3, seed=0, device=device).
 ↪initialize_from_another_model(model, dataset['train_input'])
    model = model.refine(grids[i])
    results = model.fit(dataset, opt="LBFGS", steps=50,␣
 ↪stop_grid_update_step=20);
    train_rmse.append(results['train_loss'][-1].item())
    test_rmse.append(results['test_loss'][-1].item())
```

```
saving model version 0.3

| train_loss: 3.35e-01 | test_loss: 3.41e-01 | reg: 1.05e+01 | : 100%| | 50/50
[01:25<00:00,  1.71s/
```

```
saving model version 0.4
saving model version 0.5
```

```
| train_loss: 3.12e-01 | test_loss: 3.33e-01 | reg: 1.05e+01 | : 100%| | 50/50
[01:24<00:00,  1.69s/
```

```
saving model version 0.6
saving model version 0.7
```

```
| train_loss: 2.47e-01 | test_loss: 2.83e-01 | reg: 1.07e+01 | : 100%| | 50/50
[01:24<00:00,  1.69s/
```

```
saving model version 0.8
saving model version 0.9
```

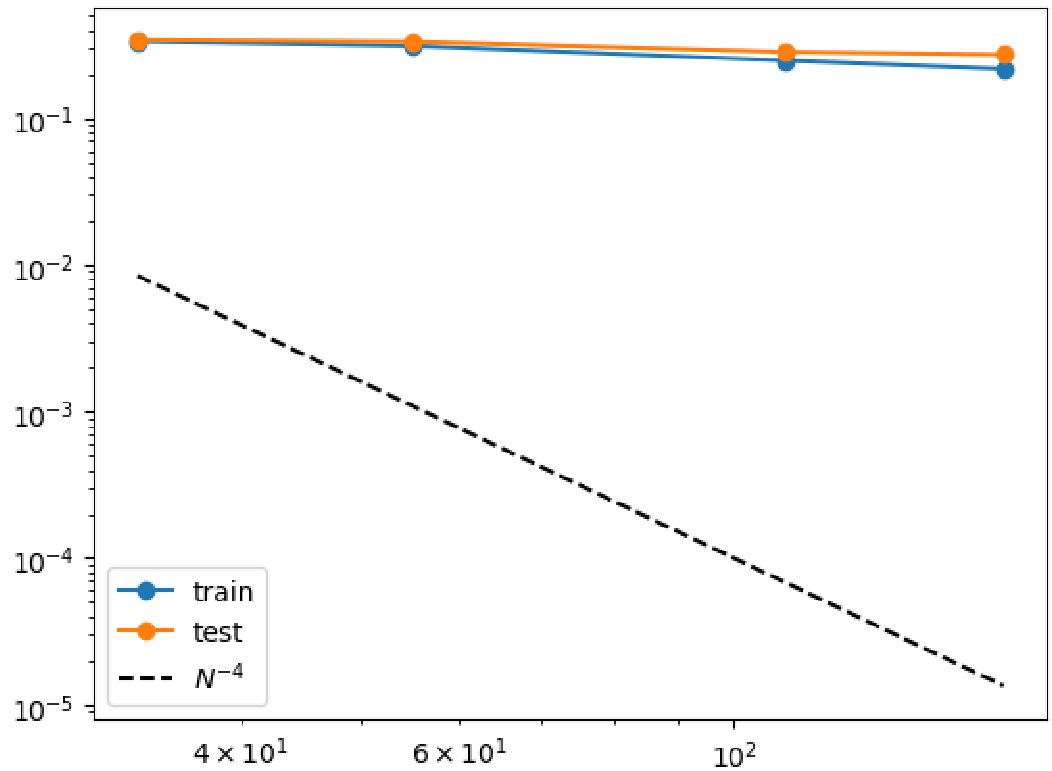
```
| train_loss: 2.17e-01 | test_loss: 2.72e-01 | reg: 1.08e+01 | : 100%| | 50/50
[01:24<00:00,  1.68s/
```

```
saving model version 0.10
```

[59]:

```
import numpy as np
import matplotlib.pyplot as plt

n_params = np.array(grids) * (4*2+2*1+1*1)
plt.plot(n_params, train_rmse, marker="o")
plt.plot(n_params, test_rmse, marker="o")
plt.plot(n_params, 10000*n_params**(-4.), color="black", ls="--")
plt.legend(['train', 'test', r'$N^{-4}$'], loc="lower left")
plt.xscale('log')
plt.yscale('log')
print(train_rmse)
print(test_rmse)
```

```
[0.33491458047828593, 0.3116140012454979, 0.24746186911760043,
0.21699923177666086]
[0.3414907763028715, 0.33281905966089087, 0.2830321329057478,
0.2716074918380671]
```



[60]:
```python
mode = "auto" # "manual"

if mode == "manual":
    # manual mode
    model.fix_symbolic(0,0,0,'sin');
    model.fix_symbolic(0,1,0,'x^2');
    model.fix_symbolic(1,0,0,'exp');
elif mode == "auto":
    # automatic mode
    lib = ['x','x^2','x^3','x^4','exp','log','sqrt','tanh','sin','abs','cos']
    model.auto_symbolic(lib=lib)
```

```
fixing (0,0,0) with x, r2=0.6891954583003471, c=1
fixing (0,0,1) with x, r2=0.7672119687592164, c=1
fixing (0,1,0) with 0
fixing (0,1,1) with x, r2=0.0006527763190471485, c=1
fixing (0,2,0) with x, r2=0.6124331171113655, c=1
fixing (0,2,1) with x, r2=0.015671232694491295, c=1
fixing (0,3,0) with cos, r2=0.9832471704704203, c=2
fixing (0,3,1) with x, r2=0.0013693399691198577, c=1
fixing (1,0,0) with cos, r2=0.9603408213760777, c=2
fixing (1,1,0) with x, r2=0.868049689484838, c=1
```

```
fixing (2,0,0) with x, r2=0.008799896389810453, c=1
saving model version 0.11
```

[61]:
```python
from kan.utils import ex_round

ex_round(model.symbolic_formula()[0][0],4)
```

[61]: $0.0613x_1 - 0.0005x_2 + 0.0003x_3 - 0.0204\cos(2.0762x_1 + 2.1578x_3 - 57.4923\cos(0.348x_4 - 0.0036) + 61.6549) + 1.0277$

3 Ejemplo original

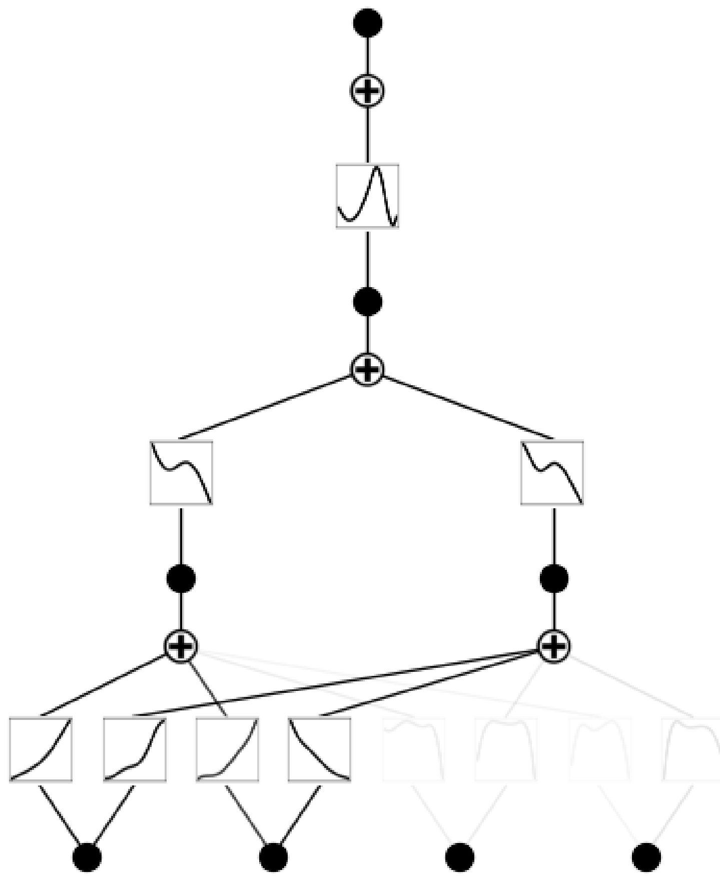
[69]:
```python
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')
print(device)

# create a KAN: 2D inputs, 1D output, and 5 hidden neurons. cubic spline (k=3),␣
↪5 grid intervals (grid=5).
model = KAN(width=[4,2,1,1], grid=3, k=3, seed=1, device=device)
f = lambda x: torch.exp((torch.sin(torch.pi*(x[:,[0]]**2+x[:,[1]]**2))+torch.
↪sin(torch.pi*(x[:,[2]]**2+x[:,[3]]**2)))/2)
dataset = create_dataset(f, n_var=4, train_num=3000, device=device)

# train the model
model.fit(dataset, opt="LBFGS", steps=20, lamb=0.002, lamb_entropy=2.);
```

```
cuda
checkpoint directory created: ./model
saving model version 0.0

| train_loss: 4.26e-01 | test_loss: 4.27e-01 | reg: 8.74e+00 | : 100%| | 20/20
[00:43<00:00,  2.20s/

saving model version 0.1
```

[70]:
```python
model = model.prune(edge_th=1e-2)
```

```
saving model version 0.2
```

[71]:
```python
model.plot()
```



[72]:
```
#grids = [3,5,10,20,50]
grids = [3,5,10]
#grids = [5]

train_rmse = []
test_rmse = []

for i in range(len(grids)):
    #model = KAN(width=[4,2,1,1], grid=grids[i], k=3, seed=0, device=device).
↪initialize_from_another_model(model, dataset['train_input'])
    model = model.refine(grids[i])
    results = model.fit(dataset, opt="LBFGS", steps=50,␣
↪stop_grid_update_step=20);
    train_rmse.append(results['train_loss'][-1].item())
    test_rmse.append(results['test_loss'][-1].item())
```

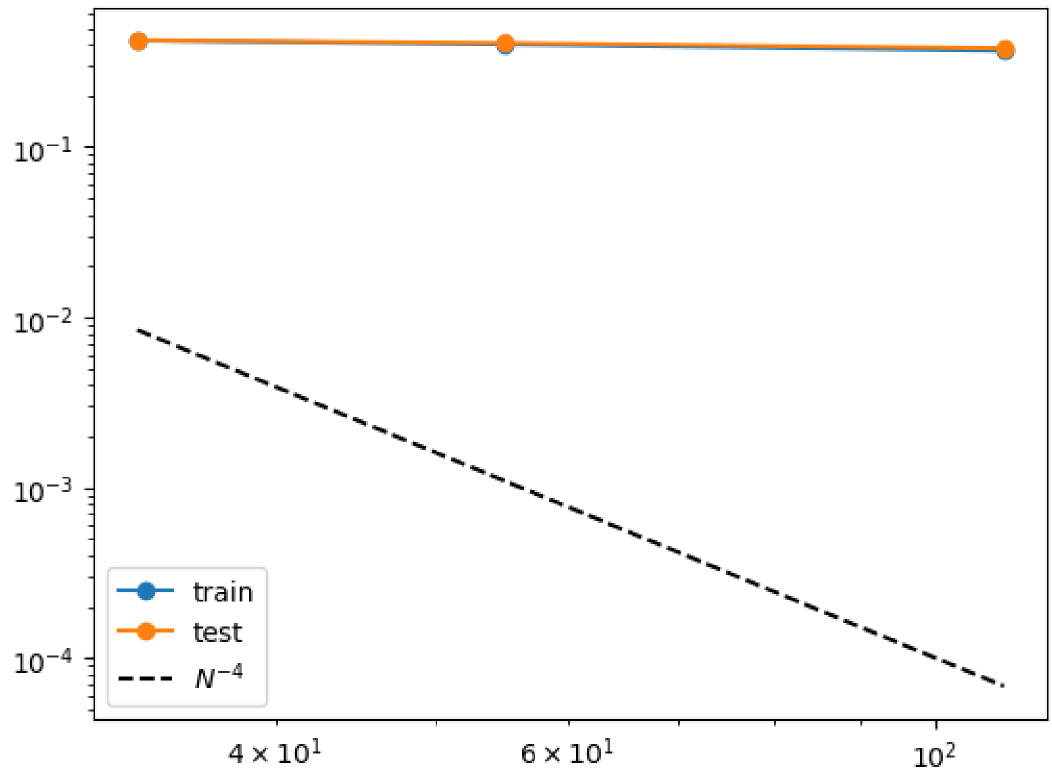
```
saving model version 0.3

| train_loss: 4.23e-01 | test_loss: 4.24e-01 | reg: 8.22e+00 | : 100%| | 50/50
```

```
[01:25<00:00,  1.71s/

saving model version 0.4
saving model version 0.5

| train_loss: 4.01e-01 | test_loss: 4.08e-01 | reg: 8.33e+00 | : 100%| | 50/50
[01:24<00:00,  1.70s/

saving model version 0.6
saving model version 0.7

| train_loss: 3.68e-01 | test_loss: 3.80e-01 | reg: 8.45e+00 | : 100%| | 50/50
[01:26<00:00,  1.73s/

saving model version 0.8
```

[73]:

```python
import numpy as np
import matplotlib.pyplot as plt

n_params = np.array(grids) * (4*2+2*1+1*1)
plt.plot(n_params, train_rmse, marker="o")
plt.plot(n_params, test_rmse, marker="o")
plt.plot(n_params, 10000*n_params**(-4.), color="black", ls="--")
plt.legend(['train', 'test', r'$N^{-4}$'], loc="lower left")
plt.xscale('log')
plt.yscale('log')
print(train_rmse)
print(test_rmse)
```

```
[0.42297619651864254, 0.4005417137509311, 0.3684852027100266]
[0.4237151088255174, 0.4075801067759189, 0.379715286736203]
```



[74]:
```
mode = "auto" # "manual"

if mode == "manual":
    # manual mode
    model.fix_symbolic(0,0,0,'sin');
    model.fix_symbolic(0,1,0,'x^2');
    model.fix_symbolic(1,0,0,'exp');
elif mode == "auto":
    # automatic mode
    lib = ['x','x^2','x^3','x^4','exp','log','sqrt','tanh','sin','abs','cos']
    model.auto_symbolic(lib=lib)
```

```
fixing (0,0,0) with x, r2=0.8741667131630695, c=1
fixing (0,0,1) with x, r2=0.7515288706329102, c=1
fixing (0,1,0) with exp, r2=0.9716346801112927, c=2
fixing (0,1,1) with x, r2=0.9799595525231799, c=1
fixing (0,2,0) with x^2, r2=0.9518431525017247, c=2
fixing (0,2,1) with x, r2=0.003343921618588383, c=1
fixing (0,3,0) with x, r2=0.00032781481554648647, c=1
fixing (0,3,1) with x, r2=0.029609760608970522, c=1
fixing (1,0,0) with x, r2=0.35353241247922423, c=1
fixing (1,1,0) with x, r2=0.40144748124366864, c=1
```

```
fixing (2,0,0) with x, r2=0.0034035748291901505, c=1
saving model version 0.9
```

[75]:
```python
from kan.utils import ex_round

ex_round(model.symbolic_formula()[0][0],4)
```

[75]:

$$-0.0262x_1 + 0.0184x_2 + 0.0001x_4 + 0.0008\left(-x_3 - 0.0303\right)^2 - 0.0001e^{4.0236x_2} + 1.5496$$