# Tutorial 3

## Outline

- Scikit-learn:
  - Data preprocessing: StandardScaler (for continuous featrues), OnehotEncoder (for categorical features)
  - Data splitting
- Artificial Neural Network:
  - Activation function
- RDKit
  - SMILES: Simplified Molecular Input Line Entry System

## 1. Scikit-learn

A package that provides implementation of various machine learning algorithms (including supervised learning and unsupervised learning), as well as tools for data preprocessing and analysis.

Documentations:

- Scikit-learn
- StandardScaler
- OneHotEncoder
- KFold

### StandardScaler

$$X_{\text{scale}} = \frac{X - \text{avg}(X)}{\text{std}(X)}$$

In [38]:
```
import numpy as np
import pandas as pd
from sklearn.preprocessing import StandardScaler
```

In [39]:
```
df = pd.read_csv("Datasets/titanic.csv")
df.head()
# data cleaning
subdf = df[["Pclass", "Sex", "SibSp", "Parch", "Embarked", "Age", "Fare", "Survived

# Categorical features: ["Pclass", "Sex", "Embarked"]
categorical_features = subdf[["Pclass", "Sex", "Embarked"]]
# Continuous features: ["Age", "Fare", "SibSp", "Parch"]
```

```
continuous_features = subdf[["Age", "Fare", "SibSp", "Parch"]]

X_cont = continuous_features.values # n_sample * n_feature
print(X_cont.shape)
```

```
(712, 4)
```

In [40]:
```
# calculate avg. and std.
print("Avg:", np.mean(X_cont, axis=0))
print("Std:", np.std(X_cont, axis=0))
```

```
Avg: [29.6420927  34.5672514   0.51404494  0.43258427]
Std: [14.4827517  52.9014591   0.93003832  0.85358139]
```

In [41]:
```
# scale (or normalize)
scaler = StandardScaler()
X_norm = scaler.fit_transform(X_cont)
```

In [42]:
```
# avg. and std. of scaled data
print("After scaling:")
print("Avg:", np.mean(X_norm, axis=0))
print("Std:", np.std(X_norm, axis=0))
```

```
After scaling:
Avg: [ 2.94396218e-16 -6.73618464e-17 -1.49692992e-17  1.49692992e-17]
Std: [1. 1. 1. 1.]
```

## OnehotEncoder

Good approach to represent categorical features

| Fruits | Label Encoding | One-hot Encoding |
|---|---|---|
| Apple | 1 | [0, 1] |
| Banana | 2 | [1, 0] |

In [43]:
```
from sklearn.preprocessing import OneHotEncoder
```

In [44]:
```
# find three catagorical features as an example
X_cate = categorical_features.values
X_cate
```

Out[44]:
```
array([[3, 'male', 'S'],
       [1, 'female', 'C'],
       [3, 'female', 'S'],
       ...,
       [1, 'female', 'S'],
       [1, 'male', 'C'],
       [3, 'male', 'Q']], dtype=object)
```

In [45]:
```
# OneHotEncoding
encoder = OneHotEncoder()

X_onehot = encoder.fit_transform(X_cate).toarray()
```

```
print(X_onehot.shape)
X_onehot
```

```
(712, 8)
```

Out[45]:
```
array([[0., 0., 1., ..., 0., 0., 1.],
       [1., 0., 0., ..., 1., 0., 0.],
       [0., 0., 1., ..., 0., 0., 1.],
       ...,
       [1., 0., 0., ..., 0., 0., 1.],
       [1., 0., 0., ..., 1., 0., 0.],
       [0., 0., 1., ..., 0., 1., 0.]])
```

In [46]:
```
# access categories
encoder.categories_
```

Out[46]:
```
[array([1, 2, 3], dtype=object),
 array(['female', 'male'], dtype=object),
 array(['C', 'Q', 'S'], dtype=object)]
```

In [47]:
```
# tranform from One-Hot encoding back to original data
X_test = X_onehot[:3]
print(X_test)
encoder.inverse_transform(X_test)
```

```
[[0. 0. 1. 0. 1. 0. 0. 1.]
 [1. 0. 0. 1. 0. 1. 0. 0.]
 [0. 0. 1. 1. 0. 0. 0. 1.]]
```

Out[47]:
```
array([[3, 'male', 'S'],
       [1, 'female', 'C'],
       [3, 'female', 'S']], dtype=object)
```

# Data splitting

## Overfitting

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Split data to Train/Validation/Test set can resolve this issue to some extent:

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Prepare the Titanic data:

In [48]:
```
# combine categorical & continuous features
X = np.hstack((X_norm, X_onehot))

# it is recommended to reshape the outputs
# to (n_samples, 1) in order to avoid unexpected broadcasting
y = subdf['Survived'].values.reshape(-1, 1)
```

```
# print the dimensions
print(X.shape, y.shape)
```

```
(712, 12) (712, 1)
```

## Train-test split

In [49]:
```
from sklearn.model_selection import train_test_split
```

In [50]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2)
```

In [51]:
```
print(X_train.shape, y_train.shape)
print(X_test.shape, y_test.shape)
```

```
(569, 12) (569, 1)
(143, 12) (143, 1)
```

## K-Fold

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In [52]:
```
from sklearn.model_selection import KFold
```

In [53]:
```
# Kfold
kf = KFold(n_splits=5, shuffle=True)

for train_index, test_index in kf.split(X):
    print(train_index, test_index)
```

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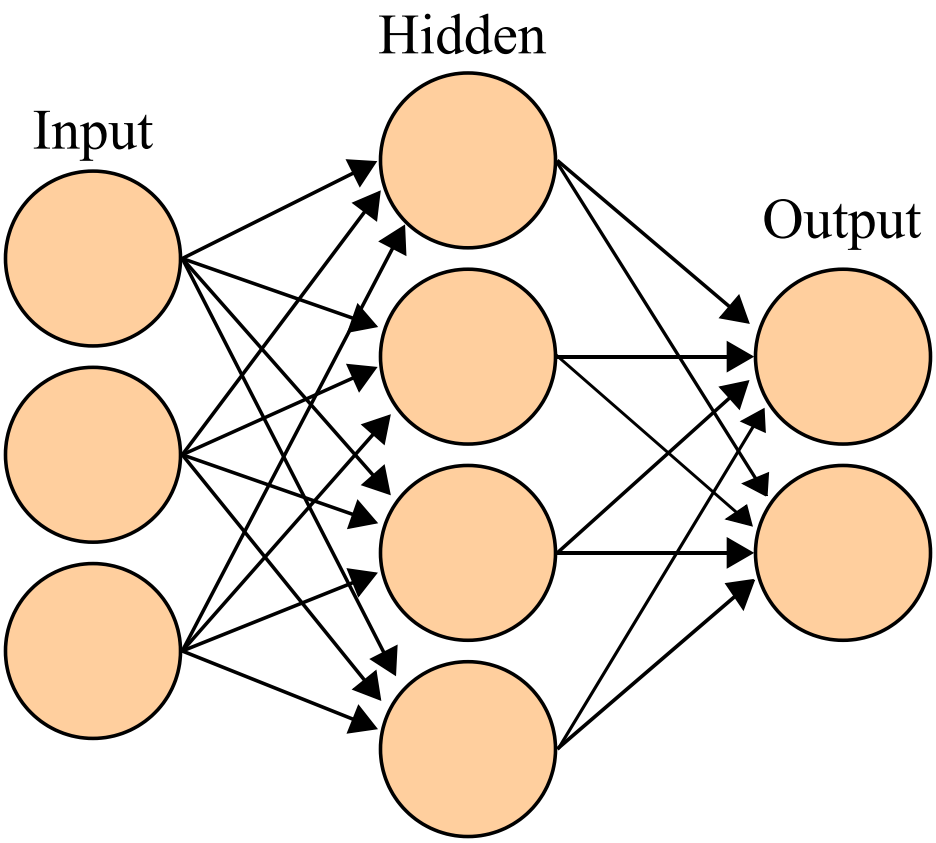
```

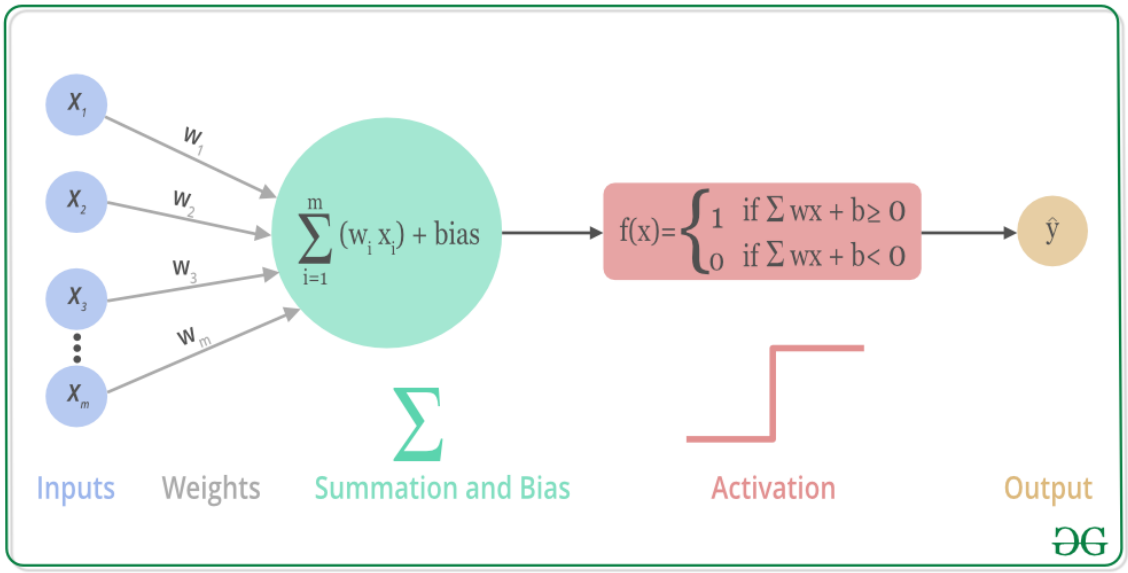
# 2. ANN




In [54]:
```
import matplotlib.pyplot as plt


def plot(func, name):
    x = np.linspace(-5, 5, 200)
    y = func(x)
    fig, ax = plt.subplots(1, 1, figsize=(4, 3))
    ax.plot(x, y)
    ax.grid(True)
    ax.set_title(name)
```

## Activation Function

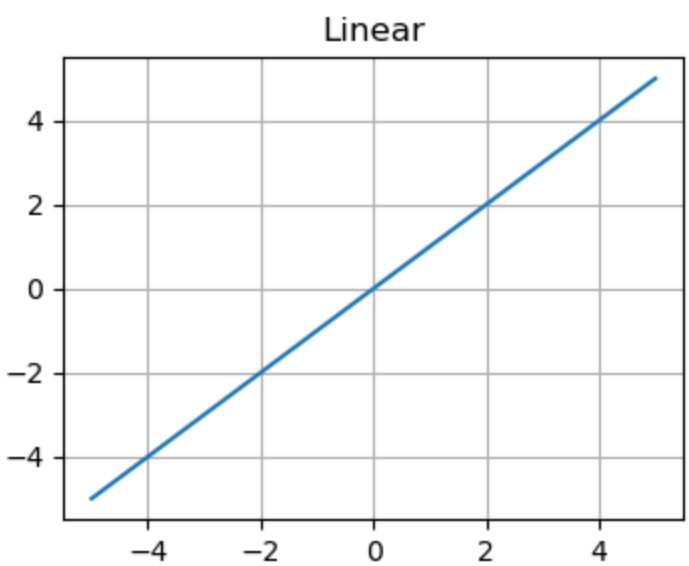



- Linear

$$z(x) = x$$

$$z'(x) = 1$$

In [55]:
```
plot(lambda x: x, "Linear")
```

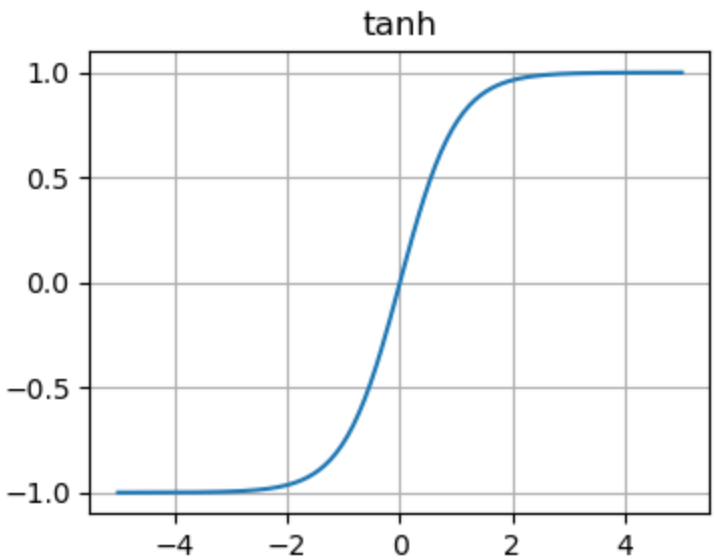



- tanh

$$z(x) = \tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$z'(x) = 1 - \tanh^2 x$$

In [56]:
```
plot(np.tanh, "tanh")
```




- sigmoid

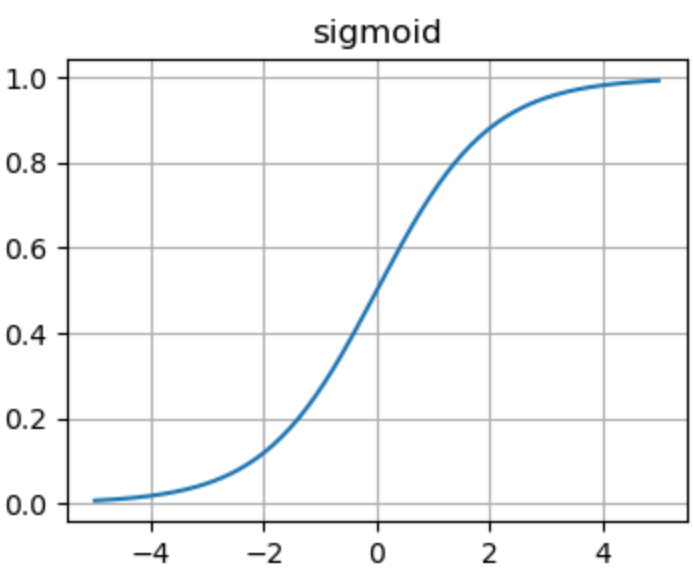
$$z(x) = \frac{1}{1+e^{-x}}$$

$$z'(x) = \frac{e^{-x}}{(1+e^{-x})^2} = z(x)[1-z(x)]$$

*Hint for HW3*: You are going to use this in Logistic Regression

In [57]:
```
def sigmoid(x):
    return 1 / (1 + np.exp(-x))

plot(sigmoid, "sigmoid")
```



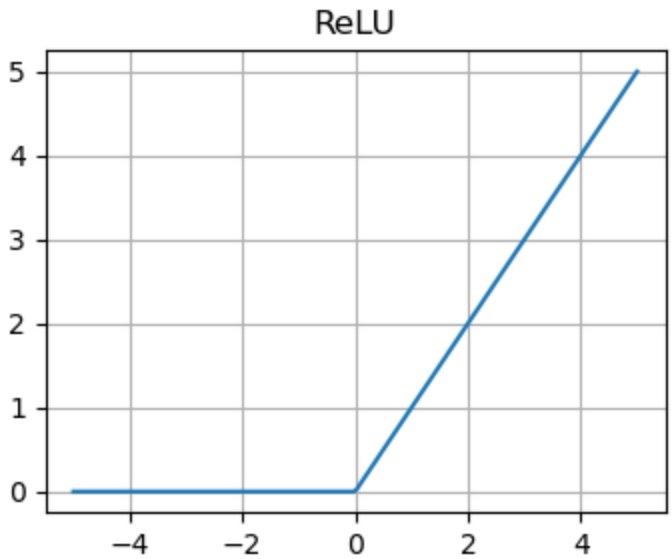

- ReLU

$$z(x) = \max(0, x)$$

$$z'(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

In [58]:
```
def relu(x):
    return x * (x > 0)

plot(relu, "ReLU")
```




- More: https://en.wikipedia.org/wiki/Activation_function

# 3. RDKit

## Introduction

RDKit is open-source toolkit for cheminformatics and it provides API in C++, Python, Java, C# and even JavaScript.

Funtionalities:

- 2D and 3D molecular operations
- Descriptor generation for machine learning
- ...

References:

- RDKit Website
- RDKit Python API

## Installation

`conda activate c142` (replace with your environment name)

`conda install rdkit -c conda-forge -y` (this may take some time)

## SMILES

- Reference
- A website for converting structures to SMILES
- A website for converting SMILES to structures

SMILES (**S**implified **M**olecular **I**nput **L**ine **E**ntry **S**ystem) is a line notation (a typographical method using printable characters) for entering and representing molecules and reactions.

### Examples:

- Methane: C
- Ethene: C=C
- Hydrogen cyanide: C#N
- Neopentane: C(C)(C)(C)C
- Cyclohexane: C1CCCCC1
- Benzene: c1ccccc1

### Basic Rules:

- Atoms are specified by its symbol with square brakets `[]` except for B, C, N, O, P, S, F, Cl, Br, I when they are normal valenced. **Hydrogens are implicitly represented.**
- Bonds are specified with "-" (single), "=" (double) or "#" (triple).
- Branches are specified by enclosing them in parentheses, and can be nested or stacked.
- Cyclic structures are represented by breaking one bond in each ring. The bonds are numbered in any order, designating ring opening (or ring closure) bonds by a digit immediately following the atomic symbol at each ring closure.
- Aromatic systems can be specified with lowercase characters or in Kekule form (in practice the latter may be preferred).
- ...

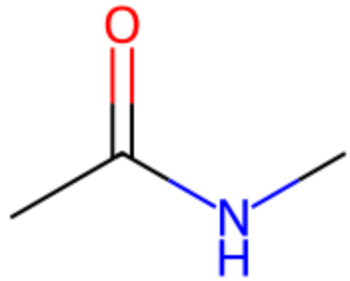
## Basic Usage

In [59]:
```
from rdkit import Chem
from rdkit.Chem import AllChem, Draw
```

Parse a SMILES string to a `Mol` object.

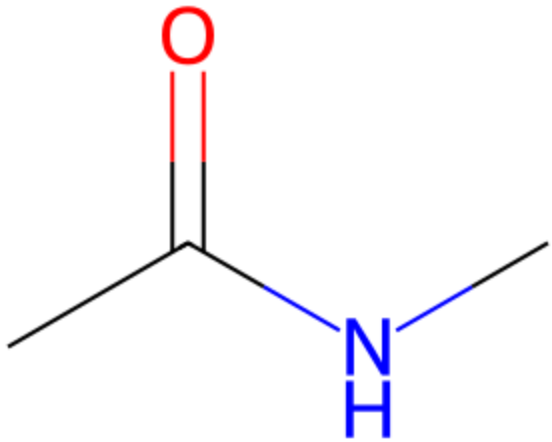
In [60]:
```
mol = Chem.MolFromSmiles("CC(=O)NC")
mol
```

Out[60]:




In [61]:
```
# if not displayed, use the following code
Draw.MolToImage(mol)
```

Out[61]:




Export a molecule to SMILES

In [62]:
```
Chem.MolToSmiles(mol)
```

Out[62]: 'CNC(C)=O'

Looping over atoms

In [63]:
```
for atom in mol.GetAtoms():
    print(type(atom), atom.GetIdx(), atom.GetSymbol())
```

```
<class 'rdkit.Chem.rdchem.Atom'> 0 C
<class 'rdkit.Chem.rdchem.Atom'> 1 C
<class 'rdkit.Chem.rdchem.Atom'> 2 O
<class 'rdkit.Chem.rdchem.Atom'> 3 N
<class 'rdkit.Chem.rdchem.Atom'> 4 C
```

Add hydrogens (make hydrogens explicitly)

In [64]:
```
mol_h = Chem.AddHs(mol)
mol_h
```

Out[64]:

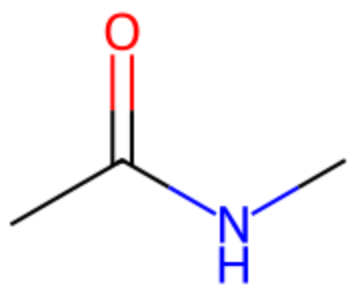

In [65]:
```
for atom in mol_h.GetAtoms():
    print(type(atom), atom.GetIdx(), atom.GetSymbol())
```

```
<class 'rdkit.Chem.rdchem.Atom'> 0 C
<class 'rdkit.Chem.rdchem.Atom'> 1 C
<class 'rdkit.Chem.rdchem.Atom'> 2 O
<class 'rdkit.Chem.rdchem.Atom'> 3 N
<class 'rdkit.Chem.rdchem.Atom'> 4 C
<class 'rdkit.Chem.rdchem.Atom'> 5 H
<class 'rdkit.Chem.rdchem.Atom'> 6 H
<class 'rdkit.Chem.rdchem.Atom'> 7 H
<class 'rdkit.Chem.rdchem.Atom'> 8 H
<class 'rdkit.Chem.rdchem.Atom'> 9 H
<class 'rdkit.Chem.rdchem.Atom'> 10 H
<class 'rdkit.Chem.rdchem.Atom'> 11 H
```

Delete hydrogens

In [66]:
```
mol_no_h = Chem.RemoveHs(mol)
mol_no_h
```

Out[66]:




Generate a 3D structure.

In [67]:
```
AllChem.EmbedMolecule(mol_h)
```

Out[67]: 0

Optimize the structure with MMFF94 force field

In [68]:
```
AllChem.MMFFOptimizeMolecule(mol_h)
```

Out[68]: 0

I/O with .mol or .sdf format

In [69]:
```
Chem.MolToMolFile(mol_h, "molecule.mol")
```

In [70]:
```
writer = Chem.SDWriter("molecule.sdf")
writer.write(mol_h)
writer.close()
```

In [71]:
```
mol_h = Chem.MolFromMolFile("molecule.mol", removeHs=False)
mol_h = Chem.SDMolSupplier("molecule.sdf", removeHs=False)[0]
```

In [ ]: