

Pour l'exigence des cours :

**Technologies de l'information, intelligence artificielle et innovations
pharmaceutiques**

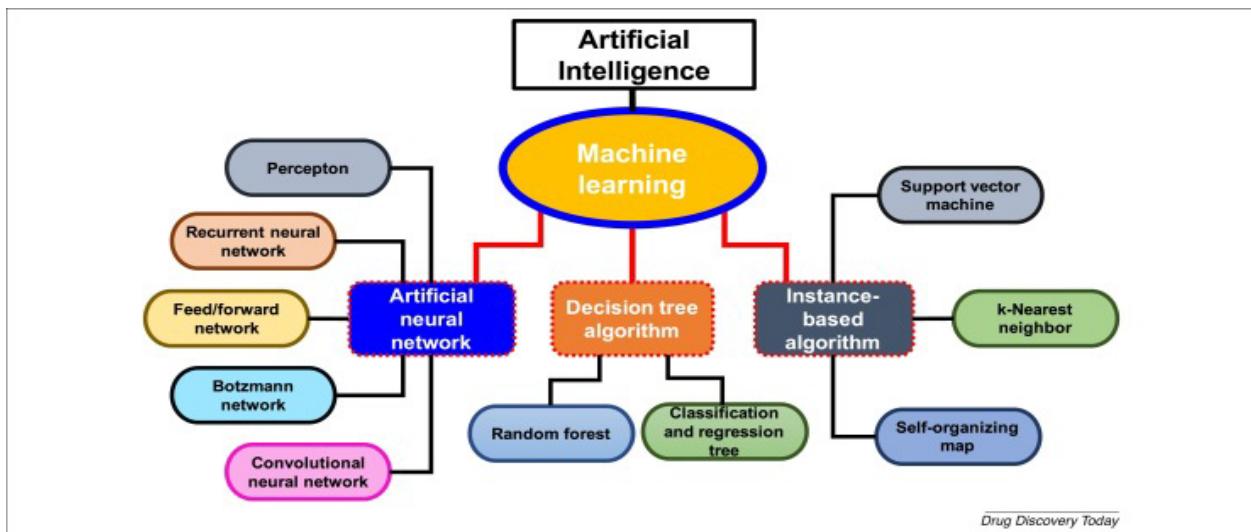
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Par :

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Ce document contient deux sections : La première est un très bref sommaire de l'effet et l'émergence de l'artificial intelligence dans le domaine de biopharmaceutique et la deuxième partie est le code développé en Python qui envisage de faire l'application d'un très riche domaine de l'IA, méthode générative, qui génère et crée la nouvelle médicament et structure moléculaire. Il doit mettre en évidence que la donnée utilisée vient de la méthode quantique en chimie qui clarifie la structure moléculaire point de vue géométrique, thermodynamique et énergétique. Donc la nouvelle molécule qui est générée est créée de la donnée qui désigne la caractéristique chimique obtenue par la méthode qu'il s'appelle Density Méthodes.

L'émergence de l'artificial intelligence est presque et indéniablement conçue comme un bouleversement rapide et omniprésent. Mais la question qui reste et démure comme une exigence scolaire est de trouver la grandeur et l'effet qui peuvent changer la vie humaine dans le domaine pharmaceutique. On peut également mentionner la rapide émergence de l'entreprises biotechnologiques qui ont développé la première plateforme qui peut configurer la structure d'un médicament sans prendre le temps pour recherche clinique.



Supervisée le schéma pour différentes méthodes de l'IA qui se divisent en deux catégories, supervisée et autonome (Paul et al.,2020)

Comme la figure au-dessus démontre, intelligence artificielle se divise en deux catégories, la première division qui s'appelle supervisée, cette catégorie a besoin des données avec le label pour comprendre les règles qui gouverne la génération des données. Dans l'autre cote, il y a la plus grande catégorie qu'il s'appelle non supervisée qui atteint les règles décelées derrière les données obtenus. Dans ces deux catégories notes au-dessus, chacun se divise à plusieurs algorithmes informatiques qui dépende sur la précision qui on veut pour chaque application. Par exemple, on peut décider d'utiliser réseau de neurones artificielle pour classifier les données massives.

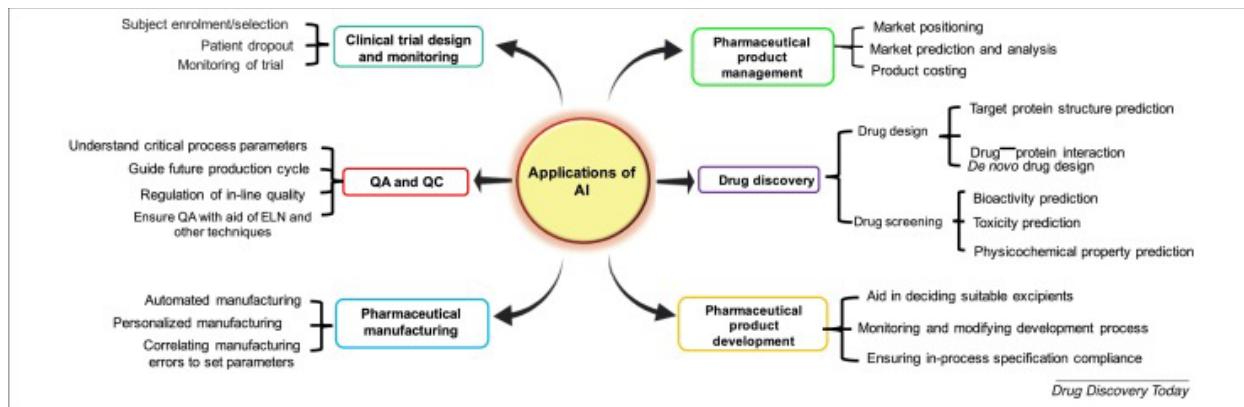


Figure 2 – Plusieurs applications de l'IA pour le domaine de pharmacie et science pharmaceutiques (Paul et al.,2020)

Comme la figure 2 au-dessus la démontre, on peut simplement utiliser l'avancement de l'artificial intelligence pour plusieurs étapes qui peut commencer avec la conception des médicaments et se termine à l'assurance de la qualité du médicament qui est manufacturée.

Notamment, ce qui est plus intéressant est le rôle primordial de l'IA dans l'étape de conception de médicament. Par exemple, on peut l'utiliser pour le prévoir le mode de l'interaction avec le récepteur. Ou également il peut être utilisée en fin de prévoir la dose toxique pour la cellule qui est visée à fin thérapeutique.

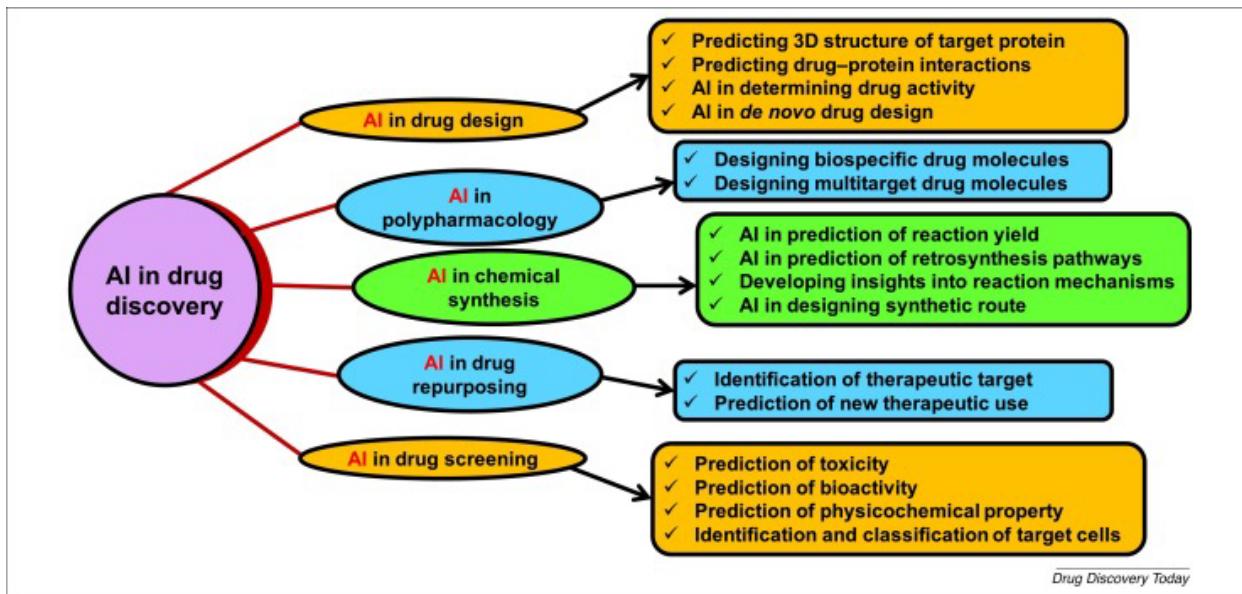


Figure 3- La plusieurs applications de l'intelligence artificielle pour la conception du médicament (Paul et al.,2020)

En commençant par le haut, on peut trouver d'abord l'IA pour déterminer la structure 3D de la protéine visée par le médicament. (Borakoti et al.,2023) Il y avait une étude qui utilisait la méthode de l'IA pour faire prédiction de modèle de l'interaction de protéine visée avec le médicament. (Dhakal et al.,2022)

Plus récemment, la concentration de la méthode scientifique et pharmaceutique a tourné vers la conception de nouveaux médicaments.

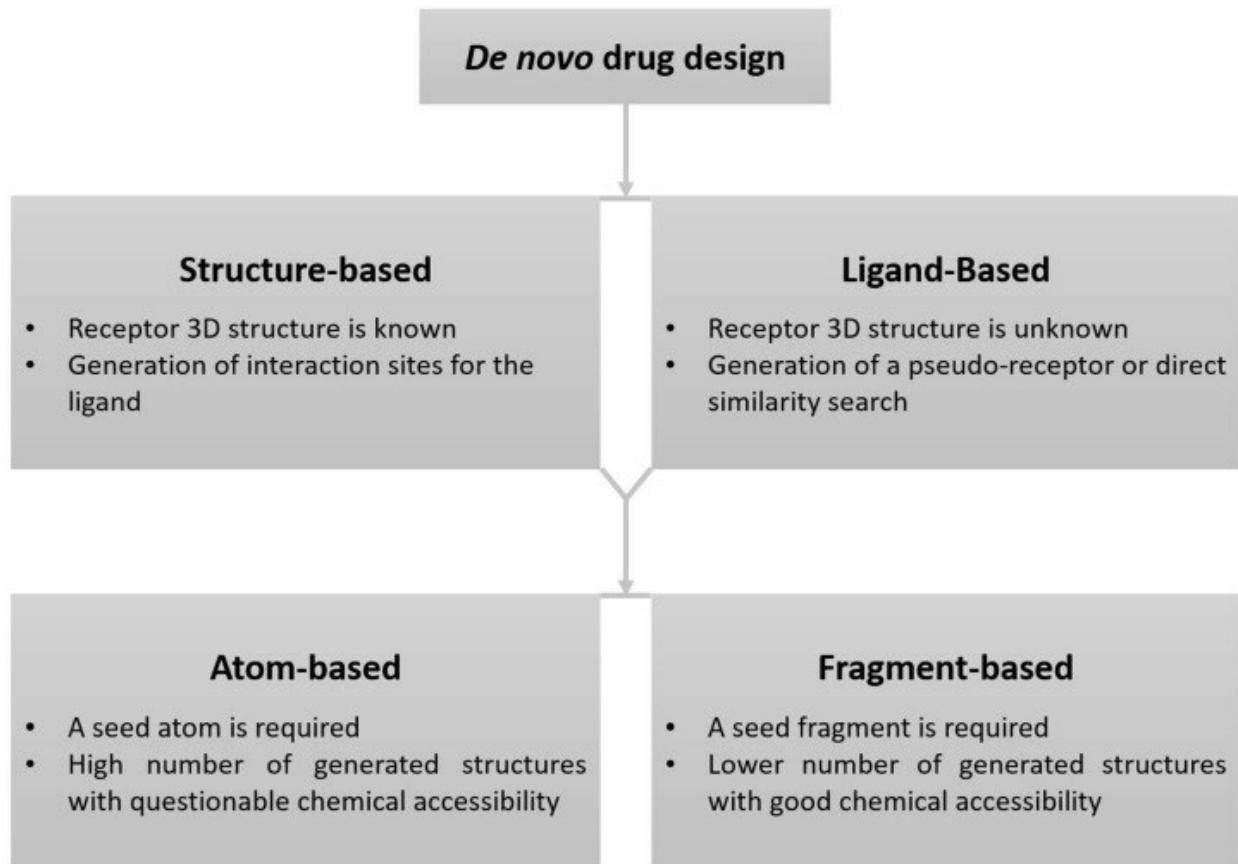


Figure 4 – la méthodologie adaptée pour la conception de nouveaux de médicaments (Mouchlis et al.,2021)

Comme le schéma au-dessus démontre, évidemment pour la conception de nouveaux de médicaments, on doit avant poser la question que si la structure du récepteur visée par le médicament moléculaire est déterminée avant. La réponse à cette question clé va déterminer la méthodologie située et applicable. (Mouchlis et al.,2021)



Figure 4- Les compagnies pharmaceutiques qui visent utiliser l'application de IA et les listes de leurs associés et partenaires qui les aident pour leurs évaluations. (Paul et al.,2020)

Comme la figure 4 au-dessus la démontre, il y a plusieurs plus en plus qui émergent chaque jour visant d'optimiser la découverte pharmaceutique aidée par IA. La majorité et la plupart de cet démarche vise à la secteur oncologie et le maladie de cerveau.

Par exemple, le compagne géante pharmaceutique Bayer et Sanofi, les deux, collaborent avec une nouvelle compagne exemplaire en utilisant IA pour générer le nouveau médicament optimisé par IA pour le maladie oncologique et cardiovasculaire.

Quelques mots sur le projet qui va suivre :

Pour commencer, les données qui spécifient les géométries des molécules de environs de 134,000 avaient été utilisés. Ces donnes est l'une de plus populaires dans ce contexte et il s'appelle QM9.chacun contient informations sur les propriétés géométrique, électronique et surtout thermodynamique. Plus d'information peut être obtenue sur le cite quantum-machine.org

L'une molécule a été choisi et deux méthodes de l'intelligence artificielle a été appliques sur elle a fin de générer une nouvelle molécule.

Il doit être élabore que, cette méthode ne mettre pas en scène la structure d'un récepteur qui va être par la molécule génère, mais ce procès va tenter de démontrer comment génère une nouvelle molécule par l'assistance de l'intelligence artificiel.

Bibliographie

Borkakoti N, Thornton JM. AlphaFold2 protein structure prediction: Implications for drug discovery. *Curr Opin Struct Biol.* 2023 Feb; 78:102526. doi: 10.1016/j.sbi.2022.102526. Epub 2023 Jan 6. PMID: 36621153; PMCID: PMC7614146.

Dhakal A, McKay C, Tanner JJ, Cheng J. Artificial intelligence in the prediction of protein-ligand interactions: recent advances and future directions. *Brief Bioinform.* 2022 Jan 17;23(1):bbab476. doi: 10.1093/bib/bbab476. PMID: 34849575; PMCID: PMC8690157.

Mouchlis VD, Afantitis A, Serra A, Fratello M, Papadiamantis AG, Aidinis V, Lynch I, Greco D, Melagraki G. Advances in de Novo Drug Design: From Conventional to Machine Learning Methods. *Int J Mol Sci.* 2021 Feb 7;22(4):1676. doi: 10.3390/ijms22041676. PMID: 33562347; PMCID: PMC7915729.

Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. *Drug Discov Today.* 2021 Jan;26(1):80-93. doi: 10.1016/j.drudis.2020.10.010. Epub 2020 Oct 21. PMID: 33099022; PMCID: PMC7577280.

Generative Models for Drug Design

Wasserstein Generative Adversarial Network with Gradient Penalty

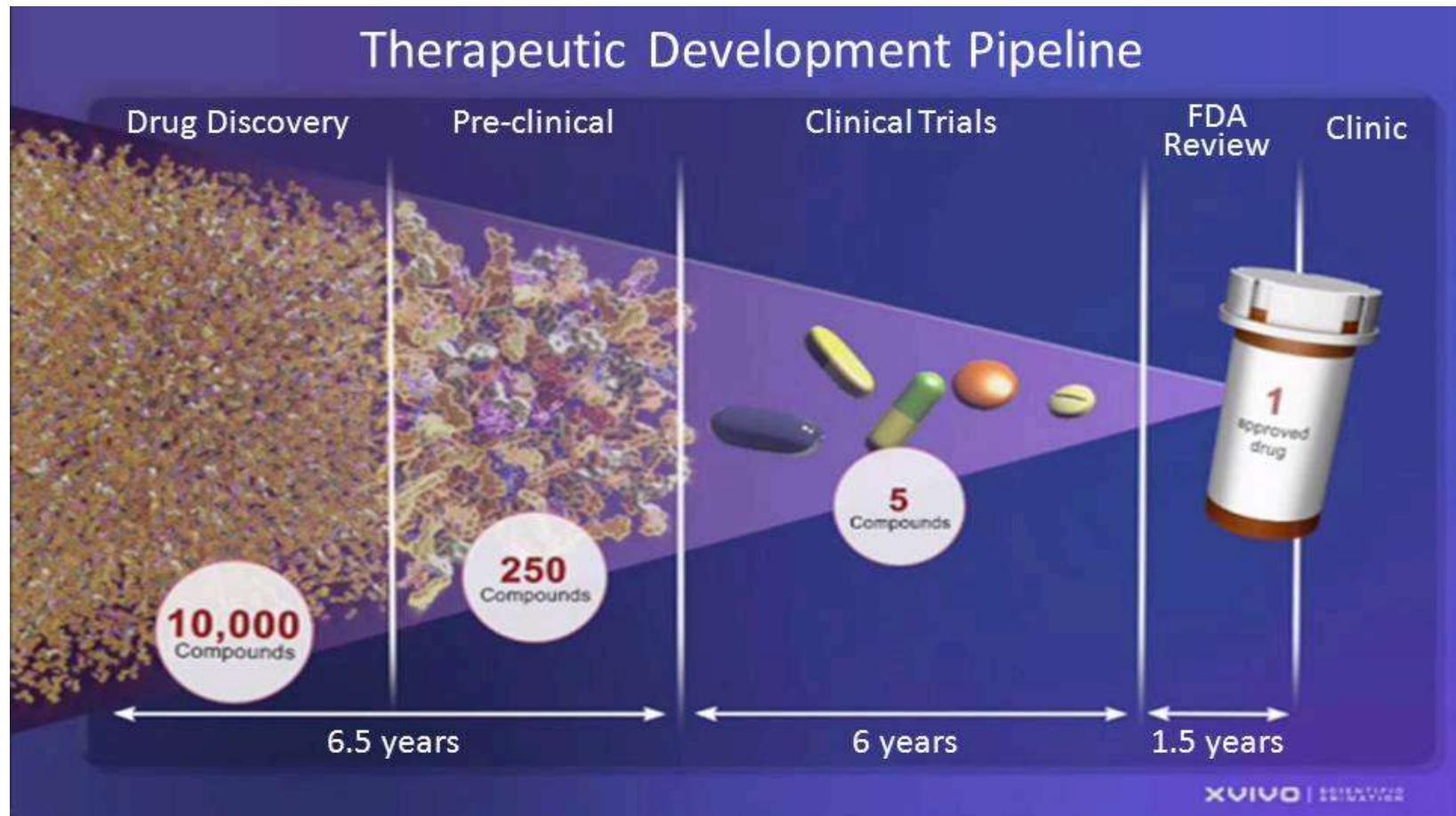


Image Citation: <https://directorsblog.nih.gov/therapeutic-pipeline/>

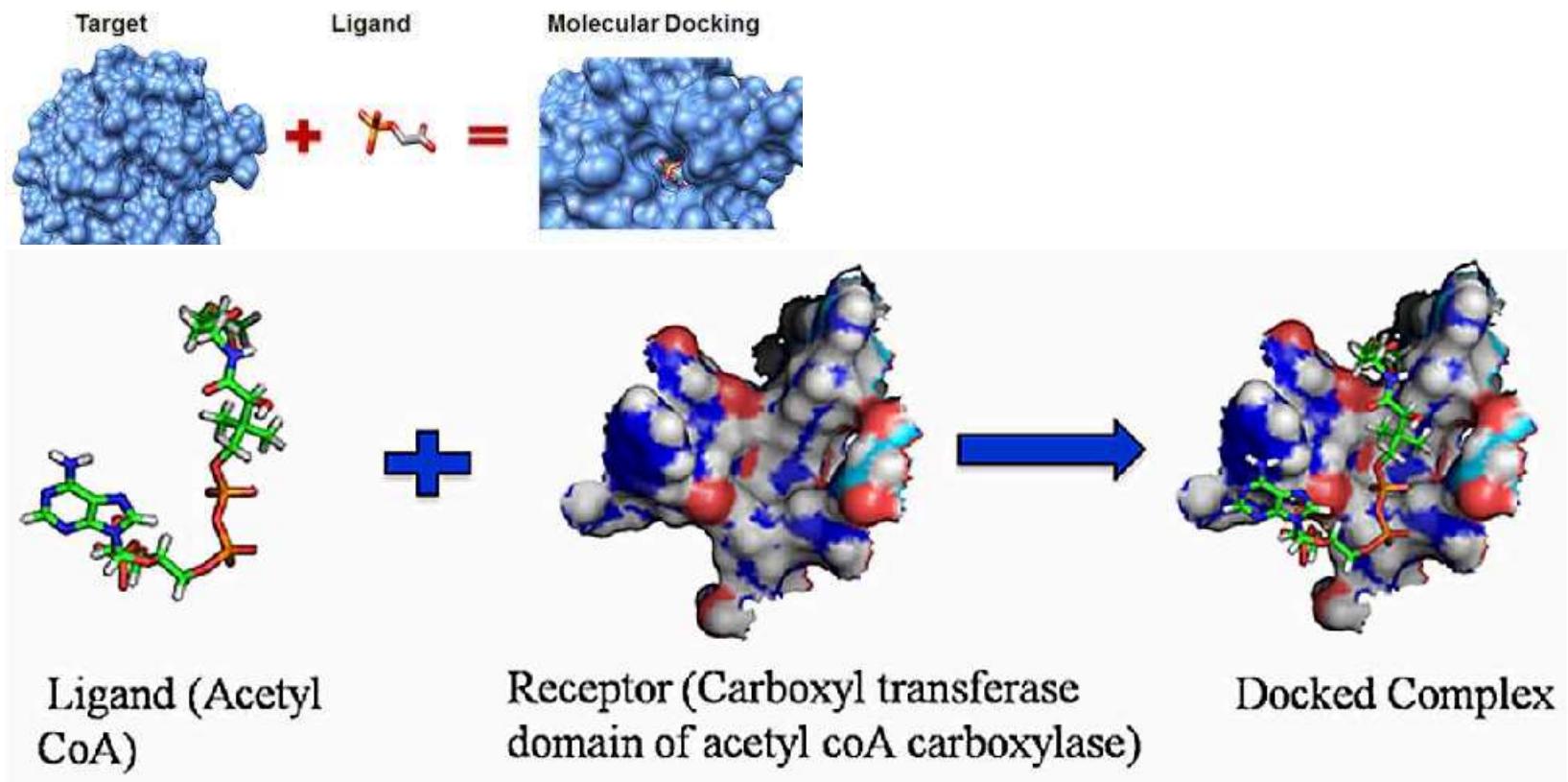
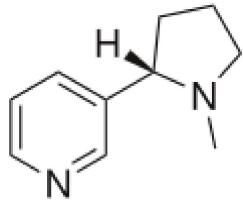


Image Resources : <https://www.semanticscholar.org/paper/Applications-of-Molecular-Docking%3A-Its-Impact-and-Anthony-Rangamaran/01089e715518cc430b7d5d7b1931a201d9f84921>

Generative Models for Drug Design and Molecular Docking

Nicotine to demonstrate the SMILES



CN1CCC[C@H]1c2cccnc2

Simplified molecular-input line-entry system (SMILES)

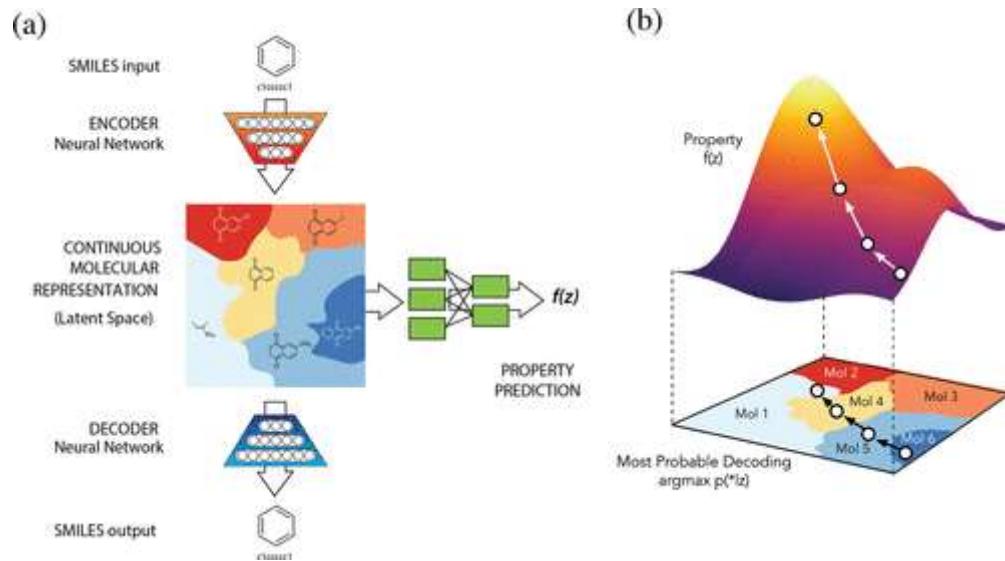


Image Source Citations:<https://arxiv.org/abs/1610.02415>

Step 1: Import Necessary Libraries

```
In [1]: pip -q install rdkit-pypi
```

Note: you may need to restart the kernel to use updated packages.

```
In [2]: pip -q install Pillow
```

Note: you may need to restart the kernel to use updated packages.

```
In [1]: from rdkit import Chem, RDLogger # Creating Molecules , Manipulating Molecules and Molecular Descriptors Like LogP
from rdkit.Chem.Draw import IPythonConsole, MolsToGridImage #to generate a grid image of multiple molecular structures
import numpy as np
import tensorflow as tf
from tensorflow import keras

RDLogger.DisableLog("rdApp.*")
```

Dataset

The QM9 dataset is a collection of molecular data. It includes quantum mechanical calculations for various small organic molecules. Specifically, QM9 contains data for 134,000 unique molecules with up to 9 heavy atoms (C, N, O, F) and up to 29 atoms in total.

Each molecule in the dataset comes with a range of computed properties, including:

- **Geometric properties:** Atomic coordinates, bond lengths, angles.
- **Electronic properties:** Dipole moments, HOMO-LUMO gaps.
- **Thermodynamic properties:** Total energy, entropy,

Citations: <http://quantum-machine.org/> operties.

HOMO-LUMO Gap is important for understanding electronic properties. Dipole Moment and Polarizability provide insights into molecular interactions. Electronic Energy and Total Energy are crucial for understanding stability and reactivity.

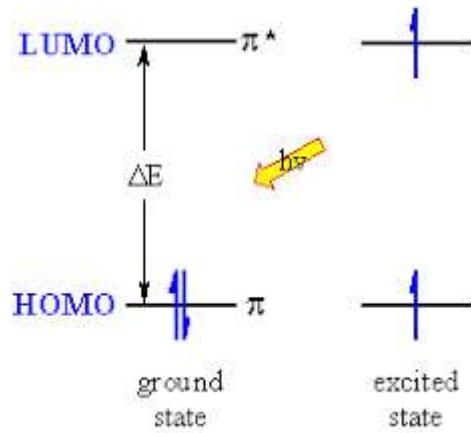


Image Resource : <https://www.chem.ucalgary.ca/courses/351/Carey5th/Ch13/ch13-uvvis.html>

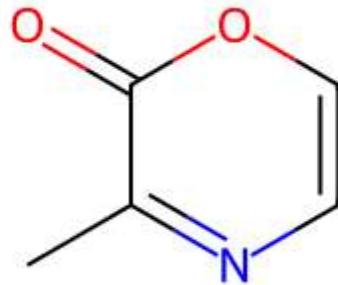
```
In [2]: csv_path = tf.keras.utils.get_file(
    "qm9.csv", "https://deepchemdata.s3-us-west-1.amazonaws.com/datasets/qm9.csv"
)
```

```
In [3]: data = []
with open(csv_path, "r") as f:
    for line in f.readlines()[1:]:
        data.append(line.split(",")[1])
```

```
In [4]: # Let's look at a molecule of the dataset
smiles = data[5000]
print("SMILES:", smiles)
molecule = Chem.MolFromSmiles(smiles)
print("Num heavy atoms:", molecule.GetNumHeavyAtoms())
molecule
```

SMILES: Cc1c(=O)occ1
 Num heavy atoms: 8

Out[4]:



Data Preprocessing Steps

Atom Mapping

```
In [5]: atom_mapping = {
    "C": 0, # Carbon atom represented by index 0
    0: "C", # Index 0 corresponds to Carbon
    "N": 1, # Nitrogen atom represented by index 1
    1: "N", # Index 1 corresponds to Nitrogen
    "O": 2, # Oxygen atom represented by index 2
    2: "O", # Index 2 corresponds to Oxygen
    "F": 3, # Fluorine atom represented by index 3
    3: "F" # Index 3 corresponds to Fluorine
}
```

```
In [6]: # Convert atom type to index
atom_type = "N"
atom_index = atom_mapping[atom_type]
print(f"Index of {atom_type}: {atom_index}")

# Convert index back to atom type
index = 2
atom_type = atom_mapping[index]
print(f"Atom type at index {index}: {atom_type}")
```

Index of N: 1

Atom type at index 2: 0

Bond Mapping

```
In [7]: bond_mapping = {
    "SINGLE": 0,
    0: Chem.BondType.SINGLE,
    "DOUBLE": 1,
    1: Chem.BondType.DOUBLE,
    "TRIPLE": 2,
    2: Chem.BondType.TRIPLE,
    "AROMATIC": 3,
    3: Chem.BondType.AROMATIC
}
```

Bond type "SINGLE" represented by index 0
Index 0 corresponds to Chem.BondType.SINGLE
Bond type "DOUBLE" represented by index 1
Index 1 corresponds to Chem.BondType.DOUBLE
Bond type "TRIPLE" represented by index 2
Index 2 corresponds to Chem.BondType.TRIPLE
Bond type "AROMATIC" represented by index 3
Index 3 corresponds to Chem.BondType.AROMATIC

```
In [8]: from rdkit import Chem

# Convert bond type to index
bond_type = "DOUBLE"
bond_index = bond_mapping[bond_type]
print(f"Index of {bond_type}: {bond_index}")

# Convert index back to RDKit BondType constant
index = 2
bond_type = bond_mapping[index]
print(f"Bond type at index {index}: {bond_type}")
```

Index of DOUBLE: 1
Bond type at index 2: TRIPLE

Parameters Definition

```
In [9]: NUM_ATOMS = 9 # Maximum number of atoms and deciding later the size of the adjacency matrix
ATOM_DIM = 4 + 1 # Number of atom types
BOND_DIM = 4 + 1 # Number of bond types
LATENT_DIM = 64 # Size of the latent space affecting the model's capacity to capture and generalize from input data
```

SMILES transoframtion into a graph representation

```
In [23]: def smiles_to_graph(smiles):
    # Converts SMILES to molecule object
    molecule = Chem.MolFromSmiles(smiles)

    # Initialize adjacency and feature tensor
    adjacency = np.zeros((BOND_DIM, NUM_ATOMS, NUM_ATOMS), "float32")
    features = np.zeros((NUM_ATOMS, ATOM_DIM), "float32")

    # Loop over each atom in molecule
    for atom in molecule.GetAtoms():
        i = atom.GetIdx()
        atom_type = atom_mapping[atom.GetSymbol()]
        features[i] = np.eye(ATOM_DIM)[atom_type]
        # Loop over one-hop neighbors
        for neighbor in atom.GetNeighbors():
            j = neighbor.GetIdx()
            bond = molecule.GetBondBetweenAtoms(i, j)
            bond_type_idx = bond_mapping[bond.GetBondType().name]
            adjacency[bond_type_idx, [i, j], [j, i]] = 1

    # Where no bond, add 1 to last channel (indicating "non-bond")
    # Notice: channels-first
    adjacency[-1, np.sum(adjacency, axis=0) == 0] = 1

    # Where no atom, add 1 to last column (indicating "non-atom")
    features[np.where(np.sum(features, axis=1) == 0)[0], -1] = 1

    return adjacency, features
```

```
In [24]: adjacency
```

```
Out[24]: array([[[0., 1., 0., 0., 0., 1., 0., 0.],
   [1., 0., 1., 0., 0., 0., 0., 1.],
   [0., 1., 0., 1., 0., 0., 0., 1.],
   [0., 0., 1., 0., 1., 0., 1., 0.],
   [0., 0., 0., 1., 0., 1., 0., 1.],
   [0., 0., 0., 0., 1., 0., 1., 0.],
   [1., 0., 0., 1., 0., 1., 0., 1.],
   [0., 0., 0., 0., 1., 0., 1., 0.],
   [0., 1., 0., 0., 0., 0., 1., 0.]],

   [[0., 0., 0., 0., 0., 0., 0., 0.],
   [0., 0., 0., 0., 0., 0., 0., 0.],
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   [[0., 0., 0., 0., 0., 0., 0., 0.],
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   [0., 0., 0., 0., 0., 0., 0., 0.],
   [0., 0., 0., 0., 0., 0., 0., 0.],
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   [0., 0., 0., 0., 0., 0., 0., 0.],
   [0., 0., 0., 0., 0., 0., 0., 0.],
   [0., 0., 0., 0., 0., 0., 0., 0.],
   [0., 0., 0., 0., 0., 0., 0., 0.]],

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

```
[1., 0., 1., 0., 1., 1., 1., 0.],
[1., 1., 0., 1., 0., 1., 1., 1.],
[1., 1., 1., 0., 1., 0., 1., 1.],
[1., 1., 1., 1., 0., 1., 0., 1., 1.],
[0., 1., 1., 0., 1., 0., 1., 0., 1.],
[1., 1., 1., 1., 0., 1., 0., 1., 0.],
[1., 0., 0., 1., 1., 1., 0., 1.]], dtype=float32)
```

Graph representation to Molecules structure

```
In [25]: def graph_to_molecule(graph):
    # Unpack graph
    adjacency, features = graph

    # RWMol is a molecule object intended to be edited
    molecule = Chem.RWMol()

    # Remove "no atoms" & atoms with no bonds
    keep_idx = np.where(
        (np.argmax(features, axis=1) != ATOM_DIM - 1)
        & (np.sum(adjacency[:-1], axis=(0, 1)) != 0)
    )[0]
    features = features[keep_idx]
    adjacency = adjacency[:, keep_idx, :][:, :, keep_idx]

    # Add atoms to molecule
    for atom_type_idx in np.argmax(features, axis=1):
        atom = Chem.Atom(atom_mapping[atom_type_idx])
        _ = molecule.AddAtom(atom)

    # Add bonds between atoms in molecule; based on the upper triangles
    # of the [symmetric] adjacency tensor
    (bonds_ij, atoms_i, atoms_j) = np.where(np.triu(adjacency) == 1)
    for (bond_ij, atom_i, atom_j) in zip(bonds_ij, atoms_i, atoms_j):
        if atom_i == atom_j or bond_ij == BOND_DIM - 1:
            continue
        bond_type = bond_mapping[bond_ij]
        molecule.AddBond(int(atom_i), int(atom_j), bond_type)

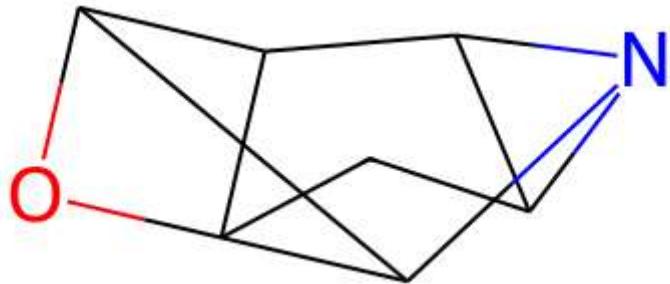
    # Sanitize the molecule; for more information on sanitization, see
```

```
# https://www.rdkit.org/docs/RDKit_Book.html#molecular-sanitization
flag = Chem.SanitizeMol(molecule, catchErrors=True)
# Let's be strict. If sanitization fails, return None
if flag != Chem.SanitizeFlags.SANITIZE_NONE:
    return None

return molecule
```

In [26]: # Test helper functions
graph_to_molecule(smiles_to_graph(smiles))

Out[26]:



In []:

Generate training set

```
In [27]: adjacency_tensor, feature_tensor = [], []

#to iterate through a subset of SMILES strings (data[::10]) and convert each SMILES string into graph representations

for smiles in data[::10]:
    adjacency, features = smiles_to_graph(smiles)
    adjacency_tensor.append(adjacency)
    feature_tensor.append(features)

adjacency_tensor = np.array(adjacency_tensor)
feature_tensor = np.array(feature_tensor)

print("adjacency_tensor.shape =", adjacency_tensor.shape)
print("feature_tensor.shape =", feature_tensor.shape)
```

```
adjacency_tensor.shape = (13389, 5, 9, 9)  
feature_tensor.shape = (13389, 9, 5)
```

To construct adjacency_tensor and feature_tensor for multiple molecules based on SMILES strings, you would typically iterate through each SMILES string, convert them into graph representations (adjacency matrices and feature matrices), and collect them into lists (adjacency_tensor and feature_tensor).

Graph GAN Model

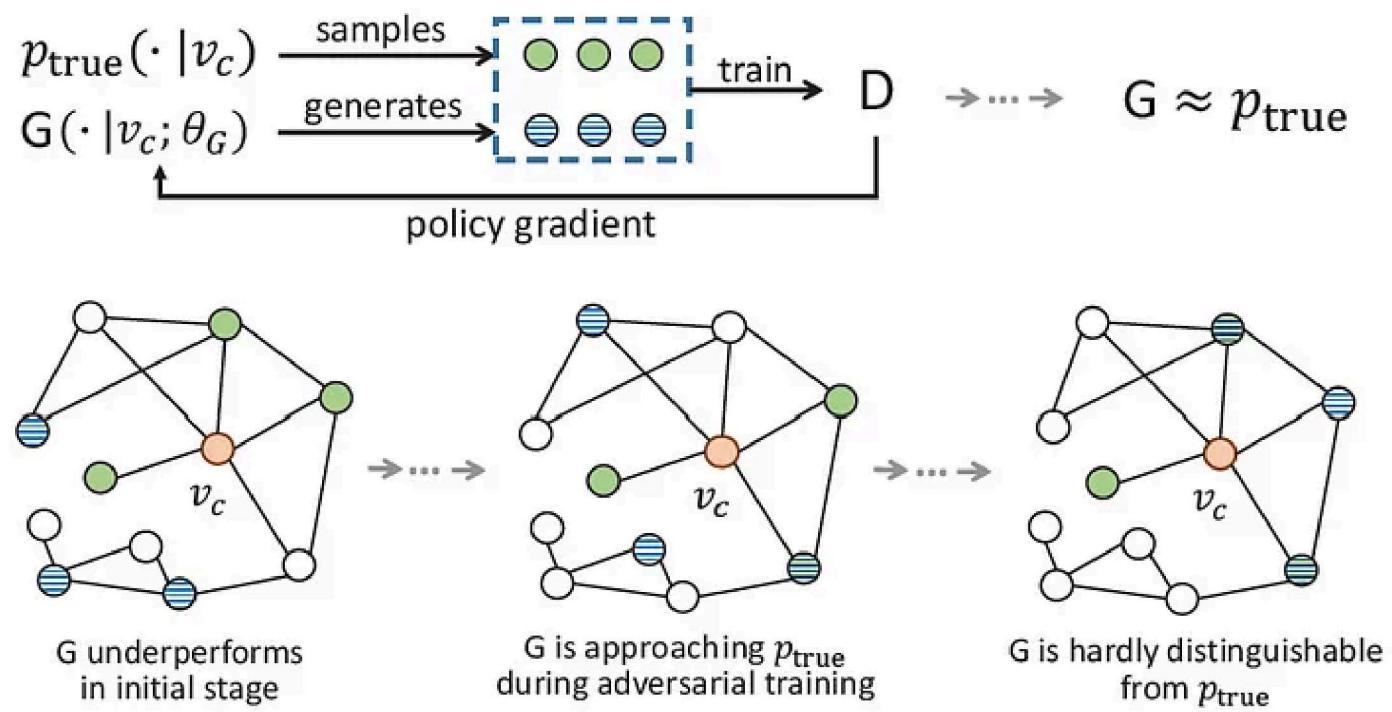


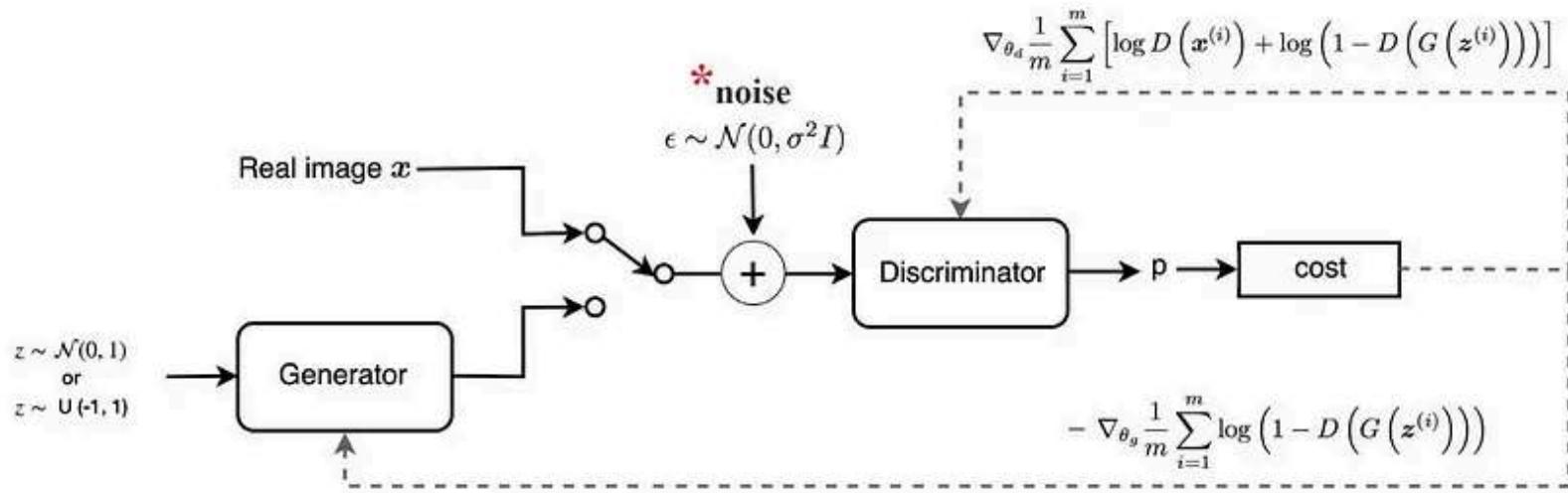
Figure 1: Illustration of GraphGAN framework.

Wasserstein Generative Adversarial Network with Gradient Penalty

$$W(\mathbb{P}_r, \mathbb{P}_g) = \inf_{\gamma \in \Pi(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}_{(x,y) \sim \gamma} [\|x - y\|],$$

$$D_{KL}(P||Q) = \sum_{x=1}^N P(x) \log \frac{P(x)}{Q(x)}$$

$$D_{JS}(p||q) = \frac{1}{2} D_{KL}(p||\frac{p+q}{2}) + \frac{1}{2} D_{KL}(q||\frac{p+q}{2})$$



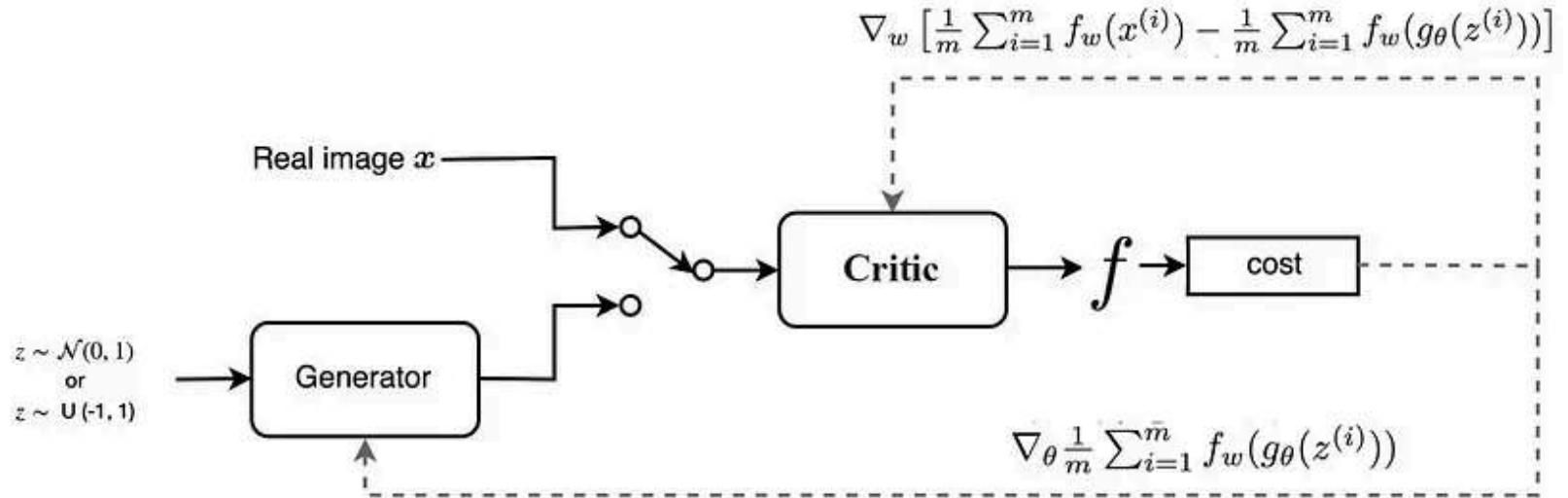


Image Resources: <https://jonathan-hui.medium.com/gan-wasserstein-gan-wgan-gp-6a1a2aa1b490>

Graph Generator

```
In [28]: import tensorflow as tf
from tensorflow import keras
from tensorflow.keras import layers, Model

def build_generator(latent_dim, num_nodes, node_feature_dim, dense_units, dropout_rate):
    """
    Build a generator model for graph data in Keras.

    Parameters:
    - latent_dim: Dimension of the latent space
    - num_nodes: Number of nodes in the generated graph
    - node_feature_dim: Dimension of the node features
    - dense_units: List of integers for the number of units in each dense layer
    - dropout_rate: Dropout rate for the dropout layers

    Returns:
    - generator: A Keras Model representing the generator
    """

    inputs = keras.Input(shape=(latent_dim,))

    x = layers.Dense(dense_units[0])(inputs)
    x = layers.BatchNormalization()(x)
    x = layers.LeakyReLU()(x)

    for units in dense_units[1:]:
        x = layers.Dense(units)(x)
        x = layers.BatchNormalization()(x)
        x = layers.LeakyReLU()(x)

    x = layers.Dense(num_nodes * node_feature_dim)(x)
    x = layers.Reshape((num_nodes, node_feature_dim))(x)

    outputs = layers.Dense(1)(x)

    return Model(inputs, outputs)
```

```

"""
# Define input for the Latent space
z = keras.layers.Input(shape=(latent_dim,))

# Propagate through one or more densely connected Layers
x = z
for units in dense_units:
    x = keras.layers.Dense(units, activation="tanh")(x)
    x = keras.layers.Dropout(dropout_rate)(x)

# Generate node features
node_features = keras.layers.Dense(num_nodes * node_feature_dim, activation='sigmoid', name='node_features')(x)
node_features = keras.layers.Reshape((num_nodes, node_feature_dim))(node_features)

# Generate adjacency matrix
adjacency_shape = (num_nodes, num_nodes)
adjacency_size = num_nodes * num_nodes

# Map outputs of previous layer (x) to continuous adjacency tensors (x_adjacency)
x_adjacency = keras.layers.Dense(adjacency_size)(x)
x_adjacency = keras.layers.Reshape(adjacency_shape)(x_adjacency)

# Combine node features and adjacency matrix
generator = keras.Model(z, [node_features, x_adjacency], name='graph_generator')

return generator

```

```

latent_dim = LATENT_DIM
num_nodes = 10
node_feature_dim = 5
dense_units = [128, 64, 32] # List of dense Layer units
dropout_rate = 0.3
LATENT_DIM
generator = build_generator(latent_dim, num_nodes, node_feature_dim, dense_units, dropout_rate)
generator.summary()

```

Model: "graph_generator"

Layer (type)	Output Shape	Param #	Connected to
input_layer_3 (InputLayer)	(None, 64)	0	-
dense_7 (Dense)	(None, 128)	8,320	input_layer_3[0]...
dropout_5 (Dropout)	(None, 128)	0	dense_7[0][0]
dense_8 (Dense)	(None, 64)	8,256	dropout_5[0][0]
dropout_6 (Dropout)	(None, 64)	0	dense_8[0][0]
dense_9 (Dense)	(None, 32)	2,080	dropout_6[0][0]
dropout_7 (Dropout)	(None, 32)	0	dense_9[0][0]
node_features (Dense)	(None, 50)	1,650	dropout_7[0][0]
dense_10 (Dense)	(None, 100)	3,300	dropout_7[0][0]
reshape_2 (Reshape)	(None, 10, 5)	0	node_features[0]...
reshape_3 (Reshape)	(None, 10, 10)	0	dense_10[0][0]

Total params: 23,606 (92.21 KB)

Trainable params: 23,606 (92.21 KB)

Non-trainable params: 0 (0.00 B)

Graph discriminator & Graph Convolutional Network

```
In [29]: class RelationalGraphConvLayer(keras.layers.Layer):
    def __init__(self,
                 units=128,
                 activation="relu",
                 ...)
```

```
use_bias=False,
kernel_initializer="glorot_uniform",
bias_initializer="zeros",
kernel_regularizer=None,
bias_regularizer=None,
**kwargs
):
    super().__init__(**kwargs)

    self.units = units
    self.activation = keras.activations.get(activation)
    self.use_bias = use_bias
    self.kernel_initializer = keras.initializers.get(kernel_initializer)
    self.bias_initializer = keras.initializers.get(bias_initializer)
    self.kernel_regularizer = keras.regularizers.get(kernel_regularizer)
    self.bias_regularizer = keras.regularizers.get(bias_regularizer)

    def build(self, input_shape):
        bond_dim = input_shape[0][1]
        atom_dim = input_shape[1][2]

        self.kernel = self.add_weight(
            shape=(bond_dim, atom_dim, self.units),
            initializer=self.kernel_initializer,
            regularizer=self.kernel_regularizer,
            trainable=True,
            name="W",
            dtype=tf.float32,
        )

        if self.use_bias:
            self.bias = self.add_weight(
                shape=(bond_dim, 1, self.units),
                initializer=self.bias_initializer,
                regularizer=self.bias_regularizer,
                trainable=True,
                name="b",
                dtype=tf.float32,
            )

        self.built = True
```

```

def call(self, inputs, training=False):
    adjacency, features = inputs
    # Aggregate information from neighbors
    x = tf.matmul(adjacency, features[:, None, :, :])
    # Apply linear transformation
    x = tf.matmul(x, self.kernel)
    if self.use_bias:
        x += self.bias
    # Reduce bond types dim
    x_reduced = tf.reduce_sum(x, axis=1)
    # Apply non-linear transformation
    return self.activation(x_reduced)

def GraphDiscriminator(
    gconv_units, dense_units, dropout_rate, adjacency_shape, feature_shape
):

    adjacency = keras.layers.Input(shape=adjacency_shape)
    features = keras.layers.Input(shape=feature_shape)

    # Propagate through one or more graph convolutional layers
    features_transformed = features
    for units in gconv_units:
        features_transformed = RelationalGraphConvLayer(units)(
            [adjacency, features_transformed]
        )

    # Reduce 2-D representation of molecule to 1-D
    x = keras.layers.GlobalAveragePooling1D()(features_transformed)

    # Propagate through one or more densely connected layers
    for units in dense_units:
        x = keras.layers.Dense(units, activation="relu")(x)
        x = keras.layers.Dropout(dropout_rate)(x)

    # For each molecule, output a single scalar value expressing the
    # "realness" of the inputted molecule
    x_out = keras.layers.Dense(1, dtype="float32")(x)

    return keras.Model(inputs=[adjacency, features], outputs=x_out)

```

```
discriminator = GraphDiscriminator(  
    gconv_units=[128, 128, 128, 128],  
    dense_units=[512, 512],  
    dropout_rate=0.2,  
    adjacency_shape=(BOND_DIM, NUM_ATOMS, NUM_ATOMS),  
    feature_shape=(NUM_ATOMS, ATOM_DIM),  
)  
discriminator.summary()
```

Model: "functional_3"

Layer (type)	Output Shape	Param #	Connected to
input_layer_4 (InputLayer)	(None, 5, 9, 9)	0	-
input_layer_5 (InputLayer)	(None, 9, 5)	0	-
relational_graph_c... (RelationalGraphCo...)	(None, 9, 128)	3,200	input_layer_4[0]... input_layer_5[0]...
relational_graph_c... (RelationalGraphCo...)	(None, 9, 128)	81,920	input_layer_4[0]... relational_graph...
relational_graph_c... (RelationalGraphCo...)	(None, 9, 128)	81,920	input_layer_4[0]... relational_graph...
relational_graph_c... (RelationalGraphCo...)	(None, 9, 128)	81,920	input_layer_4[0]... relational_graph...
global_average_poo... (GlobalAveragePool...)	(None, 128)	0	relational_graph...
dense_11 (Dense)	(None, 512)	66,048	global_average_p...
dropout_8 (Dropout)	(None, 512)	0	dense_11[0][0]
dense_12 (Dense)	(None, 512)	262,656	dropout_8[0][0]
dropout_9 (Dropout)	(None, 512)	0	dense_12[0][0]
dense_13 (Dense)	(None, 1)	513	dropout_9[0][0]

Total params: 578,177 (2.21 MB)

Trainable params: 578,177 (2.21 MB)

Non-trainable params: 0 (0.00 B)

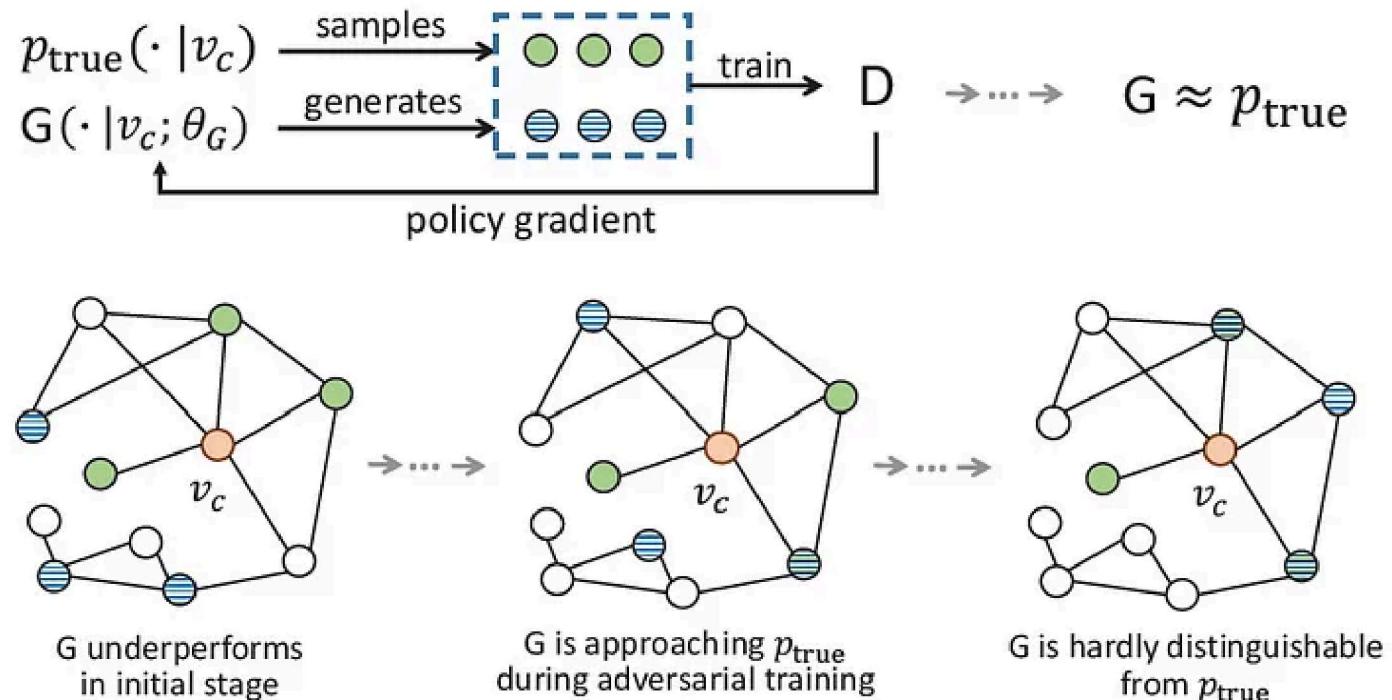


Figure 1: Illustration of GraphGAN framework.

Source Image: https://medium.com/@_psycoplankton/graphgan-generative-adversarial-networks-for-graphs-ff4584375a81

Wasserstein Generative Adverserial Network with Gradient Penalty Model

```
In [30]: class GraphGAN(keras.Model):
    def __init__(self,
                 generator,
```

```
discriminator,
discriminator_steps=1,
generator_steps=1,
gp_weight=10,
**kwargs
):
    super().__init__(**kwargs)
    self.generator = generator
    self.discriminator = discriminator
    self.discriminator_steps = discriminator_steps
    self.generator_steps = generator_steps
    self.gp_weight = gp_weight
    self.latent_dim = self.generator.input_shape[-1]

    def compile(self, optimizer_generator, optimizer_discriminator, **kwargs):
        super().compile(**kwargs)
        self.optimizer_generator = optimizer_generator
        self.optimizer_discriminator = optimizer_discriminator
        self.metric_generator = keras.metrics.Mean(name="loss_gen")
        self.metric_discriminator = keras.metrics.Mean(name="loss_dis")

    def train_step(self, inputs):

        if isinstance(inputs[0], tuple):
            inputs = inputs[0]

        graph_real = inputs

        self.batch_size = tf.shape(inputs[0])[0]

        # Train the discriminator for one or more steps
        for _ in range(self.discriminator_steps):
            z = tf.random.normal((self.batch_size, self.latent_dim))

            with tf.GradientTape() as tape:
                graph_generated = self.generator(z, training=True)
                loss = self._loss_discriminator(graph_real, graph_generated)

            grads = tape.gradient(loss, self.discriminator.trainable_weights)
            self.optimizer_discriminator.apply_gradients(
                zip(grads, self.discriminator.trainable_weights)
            )
```

```

        self.metric_discriminator.update_state(loss)

    # Train the generator for one or more steps
    for _ in range(self.generator_steps):
        z = tf.random.normal((self.batch_size, self.latent_dim))

        with tf.GradientTape() as tape:
            graph_generated = self.generator(z, training=True)
            loss = self._loss_generator(graph_generated)

            grads = tape.gradient(loss, self.generator.trainable_weights)
            self.optimizer_generator.apply_gradients(
                zip(grads, self.generator.trainable_weights)
            )
        self.metric_generator.update_state(loss)

    return {m.name: m.result() for m in self.metrics}

def _loss_discriminator(self, graph_real, graph_generated):
    logits_real = self.discriminator(graph_real, training=True)
    logits_generated = self.discriminator(graph_generated, training=True)
    loss = tf.reduce_mean(logits_generated) - tf.reduce_mean(logits_real)
    loss_gp = self._gradient_penalty(graph_real, graph_generated)
    return loss + loss_gp * self.gp_weight

def _loss_generator(self, graph_generated):
    logits_generated = self.discriminator(graph_generated, training=True)
    return -tf.reduce_mean(logits_generated)

def _gradient_penalty(self, graph_real, graph_generated):
    # Unpack graphs
    adjacency_real, features_real = graph_real
    adjacency_generated, features_generated = graph_generated

    # Generate interpolated graphs (adjacency_interp and features_interp)
    alpha = tf.random.uniform([self.batch_size])
    alpha = tf.reshape(alpha, (self.batch_size, 1, 1, 1))
    adjacency_interp = (adjacency_real * alpha) + (1 - alpha) * adjacency_generated
    alpha = tf.reshape(alpha, (self.batch_size, 1, 1))
    features_interp = (features_real * alpha) + (1 - alpha) * features_generated

    # Compute the Logits of interpolated graphs

```

```
    with tf.GradientTape() as tape:
        tape.watch(adjacency_interp)
        tape.watch(features_interp)
        logits = self.discriminator(
            [adjacency_interp, features_interp], training=True
        )

        # Compute the gradients with respect to the interpolated graphs
        grads = tape.gradient(logits, [adjacency_interp, features_interp])
        # Compute the gradient penalty
        grads_adjacency_penalty = (1 - tf.norm(grads[0], axis=1)) ** 2
        grads_features_penalty = (1 - tf.norm(grads[1], axis=2)) ** 2
        return tf.reduce_mean(
            tf.reduce_mean(grads_adjacency_penalty, axis=(-2, -1))
            + tf.reduce_mean(grads_features_penalty, axis=(-1))
        )
```

```
In [32]: wgan = GraphWGAN(generator, discriminator, discriminator_steps=1)
```

```
In [33]: wgan.compile(
    optimizer_generator=keras.optimizers.Adam(5e-4),
    optimizer_discriminator=keras.optimizers.Adam(5e-4),
)
```

```
In [ ]:
```

```
In [1]: from rdkit import Chem, RDLogger
from rdkit.Chem.Draw import IPythonConsole, MolsToGridImage
import numpy as np
import tensorflow as tf
from tensorflow import keras

RDLogger.DisableLog("rdApp.*")
```

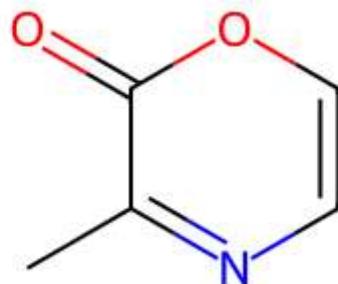
```
In [2]: csv_path = tf.keras.utils.get_file(
    "qm9.csv", "https://deepchemdata.s3-us-west-1.amazonaws.com/datasets/qm9.csv"
)

data = []
with open(csv_path, "r") as f:
    for line in f.readlines()[1:]:
        data.append(line.split(",")[1])

# Let's Look at a molecule of the dataset
smiles = data[5000]
print("SMILES:", smiles)
molecule = Chem.MolFromSmiles(smiles)
print("Num heavy atoms:", molecule.GetNumHeavyAtoms())
molecule
```

SMILES: Cc1c(=O)occn1
Num heavy atoms: 8

Out[2]:



```
In [3]: atom_mapping = {
    "C": 0,
    0: "C",
    "N": 1,
```

```
    1: "N",
    "O": 2,
    2: "O",
    "F": 3,
    3: "F",
}

bond_mapping = {
    "SINGLE": 0,
    0: Chem.BondType.SINGLE,
    "DOUBLE": 1,
    1: Chem.BondType.DOUBLE,
    "TRIPLE": 2,
    2: Chem.BondType.TRIPLE,
    "AROMATIC": 3,
    3: Chem.BondType.AROMATIC,
}

NUM_ATOMS = 9 # Maximum number of atoms
ATOM_DIM = 4 + 1 # Number of atom types
BOND_DIM = 4 + 1 # Number of bond types
LATENT_DIM = 64 # Size of the latent space

def smiles_to_graph(smiles):
    # Converts SMILES to molecule object
    molecule = Chem.MolFromSmiles(smiles)

    # Initialize adjacency and feature tensor
    adjacency = np.zeros((BOND_DIM, NUM_ATOMS, NUM_ATOMS), "float32")
    features = np.zeros((NUM_ATOMS, ATOM_DIM), "float32")

    # Loop over each atom in molecule
    for atom in molecule.GetAtoms():
        i = atom.GetIdx()
        atom_type = atom_mapping[atom.GetSymbol()]
        features[i] = np.eye(ATOM_DIM)[atom_type]
        # Loop over one-hop neighbors
        for neighbor in atom.GetNeighbors():
            j = neighbor.GetIdx()
            bond = molecule.GetBondBetweenAtoms(i, j)
            bond_type_idx = bond_mapping[bond.GetBondType().name]
```

```

adjacency[bond_type_idx, [i, j], [j, i]] = 1

# Where no bond, add 1 to last channel (indicating "non-bond")
# Notice: channels-first
adjacency[-1, np.sum(adjacency, axis=0) == 0] = 1

# Where no atom, add 1 to last column (indicating "non-atom")
features[np.where(np.sum(features, axis=1) == 0)[0], -1] = 1

return adjacency, features

def graph_to_molecule(graph):
    # Unpack graph
    adjacency, features = graph

    # RWMol is a molecule object intended to be edited
    molecule = Chem.RWMol()

    # Remove "no atoms" & atoms with no bonds
    keep_idx = np.where(
        (np.argmax(features, axis=1) != ATOM_DIM - 1)
        & (np.sum(adjacency[:-1], axis=(0, 1)) != 0)
    )[0]
    features = features[keep_idx]
    adjacency = adjacency[:, keep_idx, :][:, :, keep_idx]

    # Add atoms to molecule
    for atom_type_idx in np.argmax(features, axis=1):
        atom = Chem.Atom(atom_mapping[atom_type_idx])
        _ = molecule.AddAtom(atom)

    # Add bonds between atoms in molecule; based on the upper triangles
    # of the [symmetric] adjacency tensor
    (bonds_ij, atoms_i, atoms_j) = np.where(np.triu(adjacency) == 1)
    for (bond_ij, atom_i, atom_j) in zip(bonds_ij, atoms_i, atoms_j):
        if atom_i == atom_j or bond_ij == BOND_DIM - 1:
            continue
        bond_type = bond_mapping[bond_ij]
        molecule.AddBond(int(atom_i), int(atom_j), bond_type)

    # Sanitize the molecule; for more information on sanitization, see

```

```

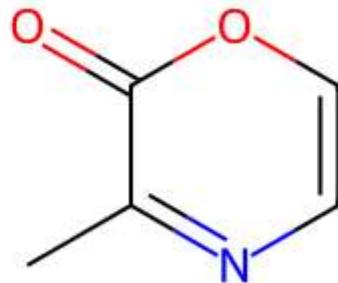
# https://www.rdkit.org/docs/RDKit_Book.html#molecular-sanitization
flag = Chem.SanitizeMol(molecule, catchErrors=True)
# Let's be strict. If sanitization fails, return None
if flag != Chem.SanitizeFlags.SANITIZE_NONE:
    return None

return molecule

# Test helper functions
graph_to_molecule(smiles_to_graph(smiles))

```

Out[3]:



```

In [4]: adjacency_tensor, feature_tensor = [], []
for smiles in data[::10]:
    adjacency, features = smiles_to_graph(smiles)
    adjacency_tensor.append(adjacency)
    feature_tensor.append(features)

adjacency_tensor = np.array(adjacency_tensor)
feature_tensor = np.array(feature_tensor)

print("adjacency_tensor.shape =", adjacency_tensor.shape)
print("feature_tensor.shape =", feature_tensor.shape)

adjacency_tensor.shape = (13389, 5, 9, 9)
feature_tensor.shape = (13389, 9, 5)

```

```

In [5]: import numpy as np
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, LSTM, Reshape, Dropout
from tensorflow.keras.preprocessing.sequence import pad_sequences
from rdkit import Chem

```

```
# Load dataset
csv_path = tf.keras.utils.get_file(
    "qm9.csv", "https://deepchemdata.s3-us-west-1.amazonaws.com/datasets/qm9.csv"
)

# Extract SMILES strings
data = []
with open(csv_path, "r") as f:
    for line in f.readlines()[1:]:
        data.append(line.split(",")[1])

# Create a set of unique characters in the SMILES strings
all_smiles_chars = set(''.join(data))
char_to_int = {c: i for i, c in enumerate(all_smiles_chars)}
int_to_char = {i: c for c, i in char_to_int.items()}

# Convert SMILES strings to integer sequences
def smiles_to_int(smiles):
    return [char_to_int[char] for char in smiles]

# Convert all SMILES strings
data_int = [smiles_to_int(smiles) for smiles in data]

# Pad sequences for consistency
max_length = max(len(seq) for seq in data_int)
num_classes = len(all_smiles_chars)
data_padded = pad_sequences(data_int, maxlen=max_length, padding='post')
data_padded = np.array([tf.keras.utils.to_categorical(seq, num_classes) for seq in data_padded])

# Define GAN components
def build_generator():
    model = Sequential()
    model.add(Dense(256, input_dim=100, activation='relu'))
    model.add(Dense(max_length * num_classes, activation='sigmoid'))
    model.add(Reshape((max_length, num_classes)))
    return model

def build_discriminator():
    model = Sequential()
    model.add(LSTM(128, input_shape=(max_length, num_classes), return_sequences=True))
    model.add(Dropout(0.5))
```

```
model.add(LSTM(128))
model.add(Dense(1, activation='sigmoid'))
return model

def build_gan(generator, discriminator):
    model = Sequential()
    model.add(generator)
    model.add(discriminator)
    return model

# Instantiate models
generator = build_generator()
discriminator = build_discriminator()
discriminator.compile(loss='binary_crossentropy', optimizer='adam', metrics=['accuracy'])

# Freeze discriminator when training GAN
discriminator.trainable = False
gan = build_gan(generator, discriminator)
gan.compile(loss='binary_crossentropy', optimizer='adam')

# Train the GAN
def train_gan(gan, generator, discriminator, data, epochs=1000, batch_size=64):
    for epoch in range(epochs):
        # Train discriminator
        idx = np.random.randint(0, data.shape[0], batch_size)
        real_smiles = data[idx]
        real_labels = np.ones((batch_size, 1))

        noise = np.random.randn(batch_size, 100)
        fake_smiles = generator.predict(noise)
        fake_labels = np.zeros((batch_size, 1))

        d_loss_real = discriminator.train_on_batch(real_smiles, real_labels)
        d_loss_fake = discriminator.train_on_batch(fake_smiles, fake_labels)
        d_loss = 0.5 * np.add(d_loss_real, d_loss_fake)

        # Train generator
        noise = np.random.randn(batch_size, 100)
        valid_labels = np.ones((batch_size, 1))
        g_loss = gan.train_on_batch(noise, valid_labels)

        if epoch % 100 == 0:
```

```

        print(f"epoch) [D loss: {d_loss[0]} | D accuracy: {100 * d_loss[1]}] [G loss: {g_loss}]")

# Call the training function
train_gan(gan, generator, discriminator, data_padded)

# Generate new SMILES strings
def generate_smiles(generator):
    noise = np.random.randn(1, 100)
    generated_sequence = generator.predict(noise)
    generated_smiles = ''.join(int_to_char[np.argmax(char)] for char in generated_sequence[0])
    return generated_smiles.strip()

# Generate and display a new SMILES string
new_smiles = generate_smiles(generator)
print("Generated SMILES:", new_smiles)

# Convert the generated SMILES string to a molecule and check its properties
molecule = Chem.MolFromSmiles(new_smiles)
if molecule:
    print("Num heavy atoms:", molecule.GetNumHeavyAtoms())
else:
    print("Generated SMILES could not be converted to a molecule.")

```

C:\Users\rezan\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

C:\Users\rezan\anaconda3\Lib\site-packages\keras\src\layers\rnn\rnn.py:204: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

super().__init__(**kwargs)

2/2 ————— 0s 4ms/step

C:\Users\rezan\anaconda3\Lib\site-packages\keras\src\backend\tensorflow\trainer.py:71: UserWarning: The model does not have any trainable weights.

warnings.warn("The model does not have any trainable weights.")

```
0 [D loss: 0.6772428154945374 | D accuracy: 80.078125] [G loss: [array(0.66722906, dtype=float32), array(0.66722906, dtype=float32), array(0.8671875, dtype=float32)]]  
2/2 ━━━━━━ 0s 3ms/step  
WARNING:tensorflow:5 out of the last 5 calls to <function TensorFlowTrainer.make_train_function.<locals>.one_step_on_iterator at 0x00000151CC4AD6C0> triggered tf.function retracing. Tracing is expensive and the excessive number of tracings could be due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with different shapes, (3) passing Python objects instead of tensors. For (1), please define your @tf.function outside of the loop. For (2), @tf.function has reduce_retracing=True option that can avoid unnecessary retracing. For (3), please refer to https://www.tensorflow.org/guide/function#controlling_retracing and https://www.tensorflow.org/api_docs/python/tf/function for more details.  
WARNING:tensorflow:6 out of the last 6 calls to <function TensorFlowTrainer.make_train_function.<locals>.one_step_on_iterator at 0x00000151A3017D80> triggered tf.function retracing. Tracing is expensive and the excessive number of tracings could be due to (1) creating @tf.function repeatedly in a loop, (2) passing tensors with different shapes, (3) passing Python objects instead of tensors. For (1), please define your @tf.function outside of the loop. For (2), @tf.function has reduce_retracing=True option that can avoid unnecessary retracing. For (3), please refer to https://www.tensorflow.org/guide/function#controlling_retracing and https://www.tensorflow.org/api_docs/python/tf/function for more details.  
2/2 ━━━━━━ 0s 4ms/step  
2/2 ━━━━━━ 0s 6ms/step  
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2/2 ━━━━━━ 0s 3ms/step
```

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2/2 0s 4ms/step
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2/2 0s 9ms/step
2/2 0s 5ms/step
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2/2 0s 5ms/step
2/2 0s 4ms/step
2/2 0s 3ms/step
2/2 0s 3ms/step
2/2 0s 5ms/step
100 [D loss: 0.7288986444473267 | D accuracy: 45.068514347076416] [G loss: [array(0.7290862, dtype=float32), array(0.7290862, dtype=float32), array(0.44956684, dtype=float32)]]
2/2 0s 4ms/step
2/2 0s 3ms/step
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2/2 0s 4ms/step
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2/2 0s 5ms/step
2/2 0s 4ms/step
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2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 0s/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 4ms/step
200 [D loss: 0.7368451356887817 | D accuracy: 42.56700277328491] [G loss: [array(0.7369362, dtype=float32), array(0.7369362, dtype=float32), array(0.42513993, dtype=float32)]]
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 4ms/step
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2/2 ━━━━━━ 0s 4ms/step
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2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 4ms/step
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2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 5ms/step
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2/2 0s 5ms/step
2/2 0s 3ms/step
2/2 0s 5ms/step
2/2 0s 5ms/step
2/2 0s 4ms/step
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2/2 0s 6ms/step
2/2 0s 9ms/step
2/2 0s 6ms/step
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2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 2ms/step
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2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 2ms/step
300 [D loss: 0.7397814989089966 | D accuracy: 41.83034896850586] [G loss: [array(0.7398302, dtype=float32), array(0.7398302, dtype=float32), array(0.4179558, dtype=float32)]]
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 2ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 3ms/step
2/2 ━━━━━━ 0s 2ms/step
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2/2 0s 4ms/step
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2/2 0s 5ms/step
2/2 0s 8ms/step
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2/2 0s 9ms/step
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2/2 0s 9ms/step
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2/2 0s 4ms/step
2/2 0s 10ms/step
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2/2 0s 6ms/step
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2/2 0s 4ms/step
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2/2 0s 4ms/step
2/2 0s 6ms/step
2/2 0s 7ms/step
2/2 0s 5ms/step
2/2 0s 8ms/step
2/2 0s 18ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 5ms/step
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 6ms/step
2/2 0s 3ms/step
2/2 0s 4ms/step
2/2 0s 11ms/step
2/2 0s 9ms/step
2/2 0s 7ms/step
2/2 0s 6ms/step
2/2 0s 9ms/step
2/2 0s 8ms/step
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2/2 0s 6ms/step
2/2 0s 11ms/step
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2/2 0s 7ms/step
2/2 0s 4ms/step
2/2 0s 8ms/step
2/2 0s 4ms/step
2/2 0s 7ms/step
2/2 0s 4ms/step
2/2 0s 6ms/step
2/2 0s 15ms/step
2/2 0s 11ms/step
2/2 0s 8ms/step

2/2 0s 5ms/step
2/2 0s 7ms/step
400 [D loss: 0.7413629293441772 | D accuracy: 41.45159125328064] [G loss: [array(0.74140316, dtype=float32), array(0.74140316, dtype=float32), array(0.41425732, dtype=float32)]]
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 11ms/step
2/2 0s 9ms/step
2/2 0s 9ms/step
2/2 0s 6ms/step
2/2 0s 7ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 9ms/step
2/2 0s 6ms/step
2/2 0s 8ms/step
2/2 0s 5ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 7ms/step
2/2 0s 12ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 5ms/step
2/2 0s 11ms/step
2/2 0s 7ms/step
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2/2 0s 8ms/step
2/2 0s 10ms/step
2/2 0s 9ms/step
2/2 0s 10ms/step
2/2 0s 8ms/step
2/2 0s 18ms/step
2/2 0s 14ms/step

2/2 0s 8ms/step
2/2 0s 9ms/step
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2/2 0s 9ms/step
2/2 0s 5ms/step
2/2 0s 6ms/step
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2/2 0s 6ms/step
2/2 0s 7ms/step
2/2 0s 6ms/step
2/2 0s 9ms/step
2/2 0s 13ms/step
2/2 0s 18ms/step
2/2 0s 16ms/step
2/2 0s 18ms/step
2/2 0s 12ms/step
2/2 0s 11ms/step
2/2 0s 9ms/step
2/2 0s 12ms/step
2/2 0s 8ms/step
2/2 0s 9ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 9ms/step
2/2 0s 9ms/step
2/2 0s 7ms/step
2/2 0s 7ms/step
2/2 0s 13ms/step
2/2 0s 7ms/step
2/2 0s 10ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 7ms/step
2/2 0s 9ms/step

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2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 6ms/step
500 [D loss: 0.7423701882362366 | D accuracy: 41.13830327987671] [G loss: [array(0.74240303, dtype=float32), array(0.74240303, dtype=float32), array(0.41117764, dtype=float32)]]
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 4ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 0s/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 19ms/step
2/2 ━━━━━━ 0s 8ms/step
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2/2 0s 12ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 10ms/step
2/2 0s 6ms/step
2/2 0s 11ms/step
2/2 0s 11ms/step
2/2 0s 6ms/step
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 8ms/step
2/2 0s 9ms/step
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2/2 0s 8ms/step
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2/2 0s 8ms/step
2/2 0s 6ms/step
2/2 0s 10ms/step
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2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 6ms/step
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2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 5ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 14ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 8ms/step
600 [D loss: 0.7430009841918945 | D accuracy: 40.99563956260681] [G loss: [array(0.7430251, dtype=float32), array(0.7430251, dtype=float32), array(0.40978578, dtype=float32)]]
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 7ms/step
```

2/2 0s 5ms/step
2/2 0s 8ms/step
2/2 0s 8ms/step
2/2 0s 9ms/step
2/2 0s 9ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 10ms/step
2/2 0s 8ms/step
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2/2 0s 10ms/step
2/2 0s 10ms/step
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2/2 0s 9ms/step
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2/2 0s 11ms/step
2/2 0s 19ms/step
2/2 0s 13ms/step
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2/2 0s 12ms/step
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2/2 0s 9ms/step
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 6ms/step
2/2 0s 9ms/step
2/2 0s 12ms/step
2/2 0s 10ms/step
2/2 0s 8ms/step
2/2 0s 10ms/step

```
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 9ms/step
700 [D loss: 0.7434636354446411 | D accuracy: 40.84352254867554] [G loss: [array(0.74348384, dtype=float32), array(0.74348384, dtype=float32), array(0.4082895, dtype=float32)]]
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 6ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 7ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 16ms/step
2/2 ━━━━━━ 0s 12ms/step
```

2/2 0s 9ms/step
2/2 0s 10ms/step
2/2 0s 10ms/step
2/2 0s 8ms/step
2/2 0s 11ms/step
2/2 0s 9ms/step
2/2 0s 12ms/step
2/2 0s 10ms/step
2/2 0s 9ms/step
2/2 0s 14ms/step
2/2 0s 9ms/step
2/2 0s 9ms/step
2/2 0s 10ms/step
2/2 0s 9ms/step
2/2 0s 11ms/step
2/2 0s 8ms/step
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2/2 0s 11ms/step
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2/2 0s 11ms/step
2/2 0s 10ms/step
2/2 0s 16ms/step
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2/2 0s 16ms/step
2/2 0s 9ms/step
2/2 0s 7ms/step
2/2 0s 12ms/step
2/2 0s 13ms/step
2/2 0s 9ms/step
2/2 0s 8ms/step
2/2 0s 9ms/step
2/2 0s 12ms/step
2/2 0s 8ms/step
2/2 0s 12ms/step
2/2 0s 10ms/step
2/2 0s 13ms/step
2/2 0s 16ms/step
2/2 0s 19ms/step
2/2 0s 8ms/step

2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 8ms/step
2/2 ━━━━━━ 0s 9ms/step
2/2 ━━━━━━ 0s 15ms/step
2/2 ━━━━━━ 0s 15ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 18ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 16ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 11ms/step
2/2 ━━━━━━ 0s 16ms/step
2/2 ━━━━━━ 0s 15ms/step
2/2 ━━━━━━ 0s 22ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 17ms/step
2/2 ━━━━━━ 0s 19ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 15ms/step
2/2 ━━━━━━ 0s 20ms/step
2/2 ━━━━━━ 0s 17ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 17ms/step
2/2 ━━━━━━ 0s 16ms/step
2/2 ━━━━━━ 0s 12ms/step
2/2 ━━━━━━ 0s 14ms/step
2/2 ━━━━━━ 0s 16ms/step
2/2 ━━━━━━ 0s 13ms/step

800 [D loss: 0.7438410520553589 | D accuracy: 40.708911418914795] [G loss: [array(0.74386084, dtype=float32), array(0.74386084, dtype=float32), array(0.406962, dtype=float32)]]

2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 13ms/step
2/2 ━━━━━━ 0s 17ms/step
2/2 ━━━━━━ 0s 25ms/step
2/2 ━━━━━━ 0s 10ms/step
2/2 ━━━━━━ 0s 11ms/step
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2/2 0s 21ms/step
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2/2 0s 10ms/step
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2/2 0s 14ms/step
2/2 0s 28ms/step
2/2 0s 18ms/step
2/2 0s 11ms/step
2/2 0s 15ms/step
2/2 0s 13ms/step
2/2 0s 17ms/step
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2/2 0s 14ms/step
2/2 0s 26ms/step
2/2 0s 11ms/step
2/2 0s 11ms/step
2/2 0s 15ms/step
2/2 0s 14ms/step
2/2 0s 31ms/step
2/2 0s 16ms/step
2/2 0s 14ms/step
2/2 0s 13ms/step
2/2 0s 22ms/step
2/2 0s 12ms/step
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2/2 0s 12ms/step
2/2 0s 12ms/step
2/2 0s 23ms/step

2/2 0s 17ms/step
2/2 0s 10ms/step
2/2 0s 11ms/step
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2/2 0s 22ms/step
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2/2 0s 6ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 9ms/step
2/2 0s 5ms/step
900 [D loss: 0.7441505193710327 | D accuracy: 40.632808208465576] [G loss: [array(0.74416655, dtype=float32), array(0.74416655, dtype=float32), array(0.4062153, dtype=float32)]]
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 6ms/step
2/2 0s 6ms/step
2/2 0s 8ms/step
2/2 0s 5ms/step
2/2 0s 8ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 10ms/step
2/2 0s 7ms/step
2/2 0s 5ms/step
2/2 0s 5ms/step
2/2 0s 9ms/step
2/2 0s 7ms/step
2/2 0s 35ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 7ms/step
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2/2 0s 18ms/step
2/2 0s 10ms/step
2/2 0s 10ms/step
2/2 0s 7ms/step
2/2 0s 7ms/step
2/2 0s 8ms/step
2/2 0s 7ms/step
2/2 0s 6ms/step
2/2 0s 5ms/step
2/2 0s 4ms/step
2/2 0s 5ms/step
2/2 0s 7ms/step
2/2 0s 7ms/step
2/2 0s 5ms/step
1/1 0s 145ms/step

Generated SMILES:))[HHNHFHN3HH3F2#F##F#o]N4-]#

Generated SMILES could not be converted to a molecule.

In []: