AI and Optimization Approaches for Inverse Kinematics in a 7-DOF Robotic Arm

Overview

In this notebook we tackle the inverse kinematics issue for 7-DOF robotic arms by developing and analysing several AI models and optimisation strategies. The study specifically examines the following

- AI models
  - Decision Tree Regressor (DTR)
  - Multi-layer Perceptron regressor (MLP)
- Optimisation strategies
  - Simulated Annealing (SA)
  - Particle Swarm Optimisation (PSO)
  - Genetic Algorithms (GA)
  - Differential Evolution (DE)

We investigate how well these approaches map end-effector postures to joint configurations. This was done by

- Modelling the forward kinematics of a given 7-DOF robotic arm.
- Generation of dataset for training generated based on forward kinematics to obtain the position (in cartesian, polar and spherical coordinates system) that corresponded to various joint angles configurations.
- Iteratively selecting the best hyperparameter values for each approach
- Cross-comparison of the best estimator from each category based on the error between the actual position and the predicted positions.

Environment setup

This note book was run in python 3.9.6 environment. Run the below command to install the dependencies required to successfully run the notebook

`pip install jupyter==1.0.0 numpy==1.26.4 pandas==2.2.1 scikit-learn==1.4.1.post1 scikit-opt==0.6.6 matplotlib==3.8.3`

In [1]:
```
# import required libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

In [2]:
```
# Define robot's DH parameters
alpha = [np.deg2rad(90), 0, 0, 0, 0, 0, 0]  # List of link twist angles in 
a = [0, 1, 1, 1, 1, 1, 1]  # List of link lengths along the common normal
d = [1, 0, 0, 0, 0, 0, 0]  # List of link offsets along the previous z-axis

# Define joint constraints for the robot
```

```
joint_constraints = [
    [2*np.pi, 0],  # Joint 1: [max_angle, min_angle] in radians
    [np.pi/2, 0],  # Joint 2: [max_angle, min_angle] in radians
    [np.pi/2, 0],  # Joint 3: [max_angle, min_angle] in radians
    [np.pi/2, 0],  # Joint 4: [max_angle, min_angle] in radians
    [np.pi/2, 0],  # Joint 5: [max_angle, min_angle] in radians
    [np.pi/2, 0],  # Joint 6: [max_angle, min_angle] in radians
    [np.pi/2, 0]   # Joint 7: [max_angle, min_angle] in radians
]
```

In [3]:

```
import numpy as np


def forward_kinematics(theta):
    '''
    Function to perform forward kinematics on a given set of joint angles.

    Parameters:
    - theta (list): List of joint angles for the robot arm.

    Returns:
    - position (numpy array): Final position of the end effector.
    - transformations_steps (numpy array): Individual transformation steps 
    '''
    # Define Denavit-Hartenberg (DH) parameters (alpha, a, d)
    # Note: These parameters should be defined somewhere in the code before
    dh_params = list(zip(alpha, a, d, theta))

    # Define function to compute Denavit-Hartenberg transformation matrix
    def dh_matrix(alpha, a, d, theta):
        return np.array([
            [np.cos(theta), -np.sin(theta)*np.cos(alpha),
             np.sin(theta)*np.sin(alpha), a*np.cos(theta)],
            [np.sin(theta), np.cos(theta)*np.cos(alpha), -
             np.cos(theta)*np.sin(alpha), a*np.sin(theta)],
            [0, np.sin(alpha), np.cos(alpha), d],
            [0, 0, 0, 1]
        ])

    # Compute transformation matrices for each joint
    T_matrices = [dh_matrix(alpha, a, d, theta)
                  for alpha, a, d, theta in dh_params]

    # Initialize transformation steps with identity matrix for the base fra
    T_prev = np.eye(4)
    transformations_steps = [T_prev[:3, 3]]

    # Compute transformation steps for each joint
    for T in T_matrices:
        T_prev = np.dot(T_prev, T)
        transformations_steps.append(T_prev[:3, 3])

    # Round the transformation steps and final position for better readabil
    transformations_steps = np.round(np.asarray(transformations_steps), 4)
    position = np.round(np.array(T_prev[:3, 3]), 4)

    return position, transformations_steps
```

In [4]:

```
def cylindrical_to_cartesian(r, theta, z):
    '''
    Function to convert cylindrical cordinates to cartesian cordinates
    '''
    x = r * np.cos(theta)
```

```
    y = r * np.sin(theta)
    return x, y, z

def cartesian_to_cylindrical(x, y, z):
    '''
    Function to convert cartesian cordinates to cylindrical cordinates
    '''
    # Compute radial distance
    rho = np.sqrt(x**2 + y**2)

    # Compute polar angle (theta)
    theta = np.arctan2(y, x)

    return rho, theta, z

def cartesian_to_spherical(x, y, z):
    '''
    Function to convert cartesian cordinates to spherical cordinates
    '''
    # Compute radial distance
    r = np.sqrt(x**2 + y**2 + z**2)

    # Compute polar angle (theta)
    theta = np.arctan2(y, x)

    # Compute azimuthal angle (phi)
    phi = np.arccos(z / r)

    return r, theta, phi
```

In [5]:
```
def expand_features(x, y, z) -> dict:
    """
    Expands Cartesian coordinates (x, y, z) to include additional coordinate

    Parameters:
    - x (float): x-coordinate
    - y (float): y-coordinate
    - z (float): z-coordinate

    Returns:
    - dict: Dictionary containing expanded features including Cartesian, sph
    """

    # Convert Cartesian coordinates to spherical coordinates
    r, theta, phi = cartesian_to_spherical(x, y, z)

    # Convert Cartesian coordinates to cylindrical coordinates
    rho, theta, z = cartesian_to_cylindrical(x, y, z)

    # Return dictionary containing expanded features
    return {
        'x': x,          # Original x-coordinate
        'y': y,          # Original y-coordinate
        'z': z,          # Original z-coordinate
        'r': r,          # Radius in spherical coordinates
        'rho': rho,      # Radius in cylindrical coordinates
        'theta': theta,  # Angle theta in spherical and cylindrical coordina
        'phi': phi,      # Angle phi in spherical coordinates
    }
```

In [6]:
```
def set_axes_equal_2d(ax):
    """
    Make axes of 2D plot have equal scale so that squares appear as squares,
```

```
    Input
      ax: a matplotlib axis, e.g., as output from plt.gca().
    """
    x_limits = ax.get_xlim()
    y_limits = ax.get_ylim()

    x_range = abs(x_limits[1] - x_limits[0])
    x_middle = np.mean(x_limits)
    y_range = abs(y_limits[1] - y_limits[0])
    y_middle = np.mean(y_limits)

    # The plot bounding box is a sphere in the sense of the infinity
    # norm, hence I call half the max range the plot radius.
    plot_radius = 0.5*max([x_range, y_range,])

    ax.set_xlim([x_middle - plot_radius, x_middle + plot_radius])
    ax.set_ylim([y_middle - plot_radius, y_middle + plot_radius])

def set_axes_equal_3d(ax):
    """
    Make axes of 3D plot have equal scale so that spheres appear as spheres,
    cubes as cubes, etc.

    Input
      ax: a matplotlib axis, e.g., as output from plt.gca().
    """

    x_limits = ax.get_xlim3d()
    y_limits = ax.get_ylim3d()
    z_limits = ax.get_zlim3d()

    x_range = abs(x_limits[1] - x_limits[0])
    x_middle = np.mean(x_limits)
    y_range = abs(y_limits[1] - y_limits[0])
    y_middle = np.mean(y_limits)
    z_range = abs(z_limits[1] - z_limits[0])
    z_middle = np.mean(z_limits)

    # The plot bounding box is a sphere in the sense of the infinity
    # norm, hence I call half the max range the plot radius.
    plot_radius = 0.5*max([x_range, y_range, z_range])

    ax.set_xlim3d([x_middle - plot_radius, x_middle + plot_radius])
    ax.set_ylim3d([y_middle - plot_radius, y_middle + plot_radius])
    ax.set_zlim3d([z_middle - plot_radius, z_middle + plot_radius])
```

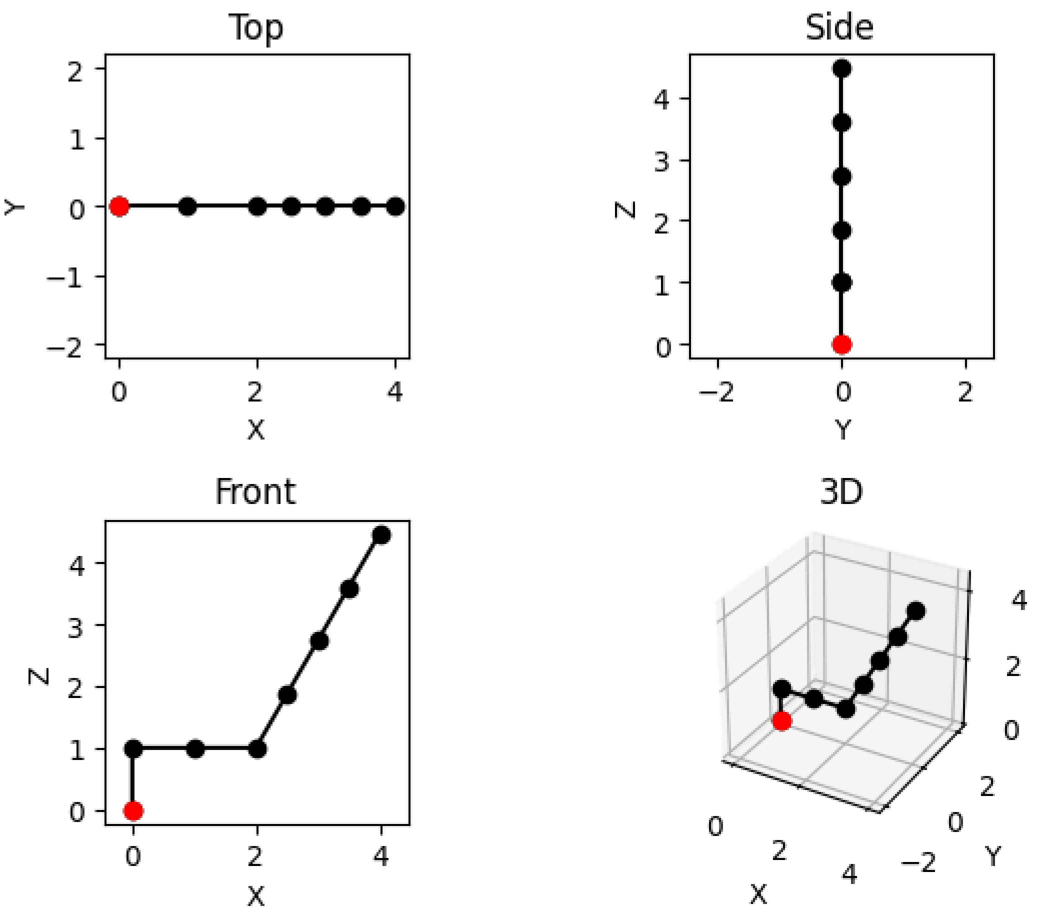
In [7]:

```
def plot_robot(joint_angles, actual=[0,0,0]):
    """
    Plots the robot arm in various perspectives based on the given joint ang

    Parameters:
    - joint_angles (list): List of joint angles for the robot arm.
    - actual (list, optional): Actual end effector position. Defaults to [0,

    Returns:
    - None
    """

    # Create a new figure
    fig = plt.figure()

    # Perform forward kinematics to get the points of the robot arm
    _, points = forward_kinematics(joint_angles)
```

```
    # Add subplots for each perspective
    xy = fig.add_subplot(221)
    xy.set_title("Top")
    xy.set_xlabel('X')
    xy.set_ylabel('Y')

    yz = fig.add_subplot(222)
    yz.set_title("Side")
    yz.set_xlabel('Y')
    yz.set_ylabel('Z')

    xz = fig.add_subplot(223)
    xz.set_title("Front")
    xz.set_xlabel('X')
    xz.set_ylabel('Z')

    xyz = fig.add_subplot(224, projection="3d")
    xyz.set_title("3D")
    xyz.set_xlabel('X')
    xyz.set_ylabel('Y')
    xyz.set_zlabel('Z')

    # Extract x, y, z coordinates from points
    x_coords = points[:,0]
    y_coords = points[:,1]
    z_coords = points[:,2]

    # Plot the robot arm in each perspective
    c = 'black'  # Color of the robot arm
    xy.plot(x_coords, y_coords, c=c, marker='o')
    yz.plot(y_coords, z_coords, c=c, marker='o')
    xz.plot(x_coords, z_coords, c=c, marker='o')
    xyz.plot(x_coords, y_coords, z_coords, c=c, marker='o')

    # Plot the actual end effector position
    xy.plot(actual[0], actual[1], c='r', marker='o')
    yz.plot(actual[1], actual[2], c='r', marker='o')
    xz.plot(actual[0], actual[2], c='r', marker='o')
    xyz.plot(*actual, c='r', marker='o')

    # Set the aspect ratio of 2D subplots to be equal
    for ax in [xy, xz, yz]:
        ax.set_box_aspect(1)
        set_axes_equal_2d(ax)

    # Set the aspect ratio of 3D subplot to be equal
    xyz.set_box_aspect((1, 1, 1))
    set_axes_equal_3d(xyz)

    # Adjust layout and display the plot
    plt.tight_layout()
    plt.show()
```

In [8]:

```
joint_angles = [np.deg2rad(x) for x in [
    0,0,0,60,0,0,0
]]

plot_robot(joint_angles,)
```



In [9]:
```
def plot_positions(positions):
    '''
    Function to plot positions in 2D space.

    Parameters:
    - positions (numpy array): Array containing x, y, z positions of the enc

    Returns:
    - None
    '''
    # Extract x, y, z coordinates from positions array
    x = positions[:, 0]
    y = positions[:, 1]
    z = positions[:, 2]

    # Create a new figure
    fig = plt.figure()

    # Loop through different 2D projections (XY, XZ, YZ)
    i = 0
    for xx, yy, xlabel, ylabel in [(x, y, 'X', 'Y'), (x, z, 'X', 'Z'), (y, z
        i += 1
        # Add subplot for each projection
        ax = fig.add_subplot(int(f'13{i}'))
        # Scatter plot of positions in the current projection
        ax.scatter(xx, yy)
        # Set labels and aspect ratio
        ax.set_xlabel(xlabel)
        ax.set_ylabel(ylabel)
        ax.set_box_aspect(1)
        set_axes_equal_2d(ax)

    # Adjust layout and display the plot
```

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

Dataset Generation

In [10]:
```
import pandas as pd

# Define joint names using list comprehension
joint_names = [f'j{i}' for i in range(1, 8)]  # List of joint names 'j1' to

# Define column names for the DataFrame
columns = ['x', 'y', 'z', 'r', 'rho', 'theta', 'phi', *joint_names]
# Columns: x, y, z represent Cartesian coordinates, r, rho, theta, phi repre
# and joint_names represent joint angles

# Create an empty DataFrame with specified columns
df = pd.DataFrame(columns=columns)

# Display the first few rows of the DataFrame
df.head()
```

Out[10]:

x	y	z	r	rho	theta	phi	j1	j2	j3	j4	j5	j6	j7

In [11]:
```
import pandas as pd
import numpy as np

# Create an empty DataFrame with specified columns
df = pd.DataFrame(columns=columns)

# Set seed for reproducibility
np.random.seed(10)

# Loop until DataFrame has 1000 entries
while len(df.index) < 1000:
    # Generate random joint angles within the specified constraints
    angles = [np.random.uniform(*value) for value in joint_constraints]

    # Perform forward kinematics to get end effector position
    position, _ = forward_kinematics(angles)
    x, y, z = position

    # Skip if the position is at the origin
    if x == 0 and y == 0 and z == 0:
        continue

    # Expand features based on end effector position
    extra_features = expand_features(x, y, z)

    # Skip if phi is greater than pi/2
    if extra_features['phi'] > np.pi/2:
        continue

    # Create entry for DataFrame with expanded features and joint angles
    entry = {
        **extra_features,
        **{name: ang for name, ang in zip(joint_names, angles)},
    }

    # Add entry to DataFrame
    df.loc[len(df.index)] = entry
```

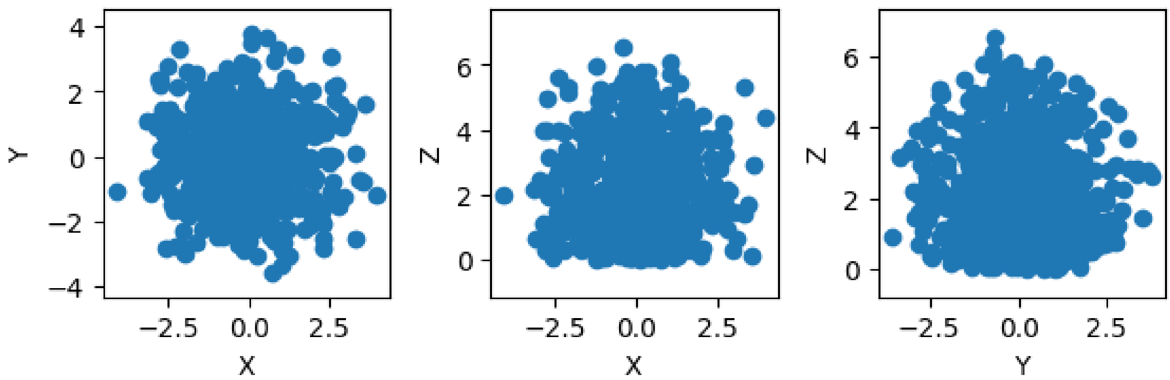
```python
# Round values in DataFrame to 3 decimal places
df = df.round(3)

# Print shape of DataFrame and display the first few rows
print(df.shape)
df.head()
```

(1000, 14)

Out[11]:

	x	y	z	r	rho	theta	phi	j1	j2	j3	j4	j5	
0	-0.214	-1.588	1.825	2.429	1.603	-1.705	0.721	1.437	1.538	0.575	0.395	0.788	1.:
1	-0.112	-1.682	0.515	1.763	1.686	-1.637	1.274	1.505	1.305	1.432	0.494	0.073	1.5
2	-0.674	-1.625	4.111	4.472	1.759	-1.964	0.404	1.177	0.609	0.437	1.112	0.129	0.4
3	-1.204	1.496	1.749	2.597	1.920	2.248	0.832	5.390	0.984	0.512	0.877	0.889	0.6
4	0.181	-0.250	3.667	3.680	0.309	-0.945	0.084	2.197	0.627	0.306	0.751	0.143	1.0

In [12]:
```python
plot_positions(df[['x','y','z']].values)
```



In [13]:
```python
from sklearn.metrics import make_scorer


def evaluate_prediction(positions: list, angles: list):
    '''
    Function to evaluate the prediction error between actual and predicted e

    Parameters:
    - positions (list): List of actual end effector positions.
    - angles (list): List of predicted joint angles.

    Returns:
    - error (float): Mean absolute error between actual and predicted positi
    '''
    distance_errors = []

    # Calculate distance error for each pair of actual and predicted positio
    for position, angle in list(zip(positions, angles)):
        end_effector_position, _ = forward_kinematics(angle)
        error = np.linalg.norm(end_effector_position - position)
        distance_errors.append(error)

    # Calculate mean absolute error
    error = np.round(np.mean(np.absolute(distance_errors)), 3)

    return error


def optimization_scorer():
```

```
    '''
    Function to create a custom optimization scorer for evaluating predicti

    Returns:
    - scorer (callable): Custom scorer function.
    '''
    def scorer(y_true, y_pred):
        '''
        Custom scoring function for optimization.

        Parameters:
        - y_true (array-like): True end effector positions.
        - y_pred (array-like): Predicted joint angles.

        Returns:
        - score (float): Optimization score based on mean absolute distance
        '''
        distance_errors = []

        # Calculate distance error for each pair of true and predicted posi
        for actual, predicted in list(zip(y_true, y_pred)):
            pos_true, _ = forward_kinematics(actual)
            pos_pred, _ = forward_kinematics(predicted)
            d = np.linalg.norm(pos_true - pos_pred)
            distance_errors.append(d)

        # Calculate optimization score
        score = -np.mean(np.abs(distance_errors))
        return score

    # Return custom scorer using make_scorer
    return make_scorer(scorer)
```

In [14]:

```
# Define columns representing Cartesian coordinates
cart_columns = [
    'x',
    'y',
    'z',
]

# Set seed for reproducibility
np.random.seed(10)

# Randomly choose 7 indices from the DataFrame
index_choices = np.random.randint(0, len(df), 7)

# Select Cartesian positions and corresponding joint angles based on chosen
pos_choices = df[cart_columns].iloc[index_choices].values  # Cartesian posi
angle_choices = df[joint_names].iloc[index_choices].values  # Joint angles
```

In [15]:

```
from sklearn.model_selection import GridSearchCV
import warnings
from sklearn.exceptions import ConvergenceWarning


def do_grid_search(estimator, params, X, y, x_plot=None, stringify_xplot=Fal
    '''
    Function to perform grid search with cross-validation and visualize resu

    Parameters:
    - estimator (object): Estimator object implementing 'fit' and 'predict'
    - params (dict): Dictionary with parameters names (str) as keys and list
    - X (array-like): Input features for training.
```

```
    - y (array-like): Target variable for training.
    - x_plot (str or None): Parameter to plot on x-axis (optional).
    - stringify_xplot (bool): Whether to convert x_plot values to strings fo
    - bar_plot (bool): Whether to plot a bar plot instead of a line plot (op
    - xticks_rotation (int): Rotation angle for x-axis tick labels (optiona

    Returns:
    - results (DataFrame): DataFrame containing grid search results sorted b
    '''

    # Filter out convergence warnings
    warnings.filterwarnings("ignore", category=ConvergenceWarning)

    # Perform grid search with cross-validation
    gs = GridSearchCV(
        estimator=estimator,
        param_grid=params,
        cv=len(pos_choices),  # Number of folds for cross-validation
        scoring=optimization_scorer(),  # Scoring metric
        verbose=1,
    )

    gs.fit(X, y)

    # Extract grid search results
    results = pd.DataFrame(gs.cv_results_)

    # Rename columns for readability
    result_columns = {
        **{f'param_{key}': key for key in params.keys()},  # Rename param_*
        'mean_test_score': "MAE",  # Rename mean_test_score column to MAE (M
    }
    for key, value in result_columns.items():
        results = results.rename(columns={key: value})

    # Invert MAE values to represent optimization score
    results['MAE'] = results['MAE'] * -1

    # Visualize results if x_plot is specified
    if x_plot is not None:
        key = f'{x_plot}'
        graph = results.sort_values(key)

        # Plotting
        if stringify_xplot:
            x_plot_str = [str(x) for x in graph[key]]
            plt.plot(x_plot_str, graph["MAE"], marker='o') if not bar_plot e
                x_plot_str, graph["MAE"])
            plt.xticks(x_plot_str)
        else:
            plt.plot(graph[key], graph["MAE"], marker='o') if not bar_plot e
                graph[key], graph["MAE"])
            plt.xticks(list(graph[key].values))

        plt.ylabel('MAE')  # Set y-axis label
        plt.xlabel(x_plot)  # Set x-axis label
        plt.xticks(rotation=xticks_rotation)  # Rotate x-axis tick labels
        plt.show()  # Display plot

    # Return results DataFrame sorted by MAE
    return results[result_columns.values()].sort_values('MAE')
```

Optimization Algorithms Implementation

In [16]:
```
from sklearn.base import BaseEstimator, RegressorMixin
from sko.GA import GA


class GA_Optimizer(BaseEstimator, RegressorMixin):
    '''
    Genetic Algorithm (GA) Optimizer for joint angle prediction.

    Parameters:
    - pop_size (int): Population size for genetic algorithm.
    - max_iteration (int): Maximum number of iterations for genetic algorit
    - mutation (float): Mutation probability for genetic algorithm.

    Attributes:
    - pop_size (int): Population size for genetic algorithm.
    - max_iteration (int): Maximum number of iterations for genetic algorit
    - mutation (float): Mutation probability for genetic algorithm.
    '''

    def __init__(self, pop_size=None, max_iteration=None, mutation=None):
        self.pop_size = pop_size
        self.max_iteration = max_iteration
        self.mutation = mutation

    def fit(self, X, y=None):
        '''
        Fit method for the genetic algorithm optimizer.

        Parameters:
        - X (array-like): Input features (not used in fitting).
        - y (array-like): Target variable (not used in fitting).

        Returns:
        - self (object): Instance of the estimator.
        '''
        return self

    def predict(self, X):
        '''
        Predict method to predict joint angles using genetic algorithm optir

        Parameters:
        - X (array-like): Input features containing end effector positions.

        Returns:
        - predictions (list): Predicted joint angles for each input positior
        '''
        predictions: list = []  # Initialize list to store predictions

        # Iterate over each end effector position
        for position in X:
            np.random.seed(1)  # Set seed for reproducibility

            # Initialize genetic algorithm with specified parameters
            ga = GA(
                func=lambda y: evaluate_prediction([position], [y]),
                n_dim=7,
                size_pop=self.pop_size,
                max_iter=self.max_iteration,
                prob_mut=self.mutation,
                lb=[x[1] for x in joint_constraints],
                ub=[x[0] for x in joint_constraints],
                precision=1e-7,
```

```
            )

            # Run genetic algorithm to find optimal joint angles
            y_pred, _ = ga.run()
            predictions.append(y_pred)  # Append predicted joint angles to l

        return predictions  # Return list of predicted joint angles
```

In [17]:
```
from sklearn.base import BaseEstimator, RegressorMixin
from sko.DE import DE


class DE_Optimizer(BaseEstimator, RegressorMixin):
    '''
    Differential Evolution (DE) Optimizer for joint angle prediction.

    Parameters:
    - pop_size (int): Population size for differential evolution.
    - max_iteration (int): Maximum number of iterations for differential evo
    - mutation (float): Mutation probability for differential evolution.

    Attributes:
    - pop_size (int): Population size for differential evolution.
    - max_iteration (int): Maximum number of iterations for differential evo
    - mutation (float): Mutation probability for differential evolution.
    '''

    def __init__(self, pop_size=None, max_iteration=None, mutation=None):
        self.pop_size = pop_size
        self.max_iteration = max_iteration
        self.mutation = mutation

    def fit(self, X, y=None):
        '''
        Fit method for the differential evolution optimizer.

        Parameters:
        - X (array-like): Input features (not used in fitting).
        - y (array-like): Target variable (not used in fitting).

        Returns:
        - self (object): Instance of the estimator.
        '''
        return self

    def predict(self, X):
        '''
        Predict method to predict joint angles using differential evolution

        Parameters:
        - X (array-like): Input features containing end effector positions.

        Returns:
        - predictions (list): Predicted joint angles for each input position
        '''
        predictions: list = []  # Initialize list to store predictions

        # Iterate over each end effector position
        for position in X:
            np.random.seed(1)  # Set seed for reproducibility

            # Initialize differential evolution with specified parameters
            de = DE(
                func=lambda y: evaluate_prediction([position], [y]),
```

```
                n_dim=7,
                size_pop=self.pop_size,
                max_iter=self.max_iteration,
                prob_mut=self.mutation,
                lb=[x[1] for x in joint_constraints],
                ub=[x[0] for x in joint_constraints],
            )

            # Run differential evolution to find optimal joint angles
            y_pred, _ = de.run()
            predictions.append(y_pred)  # Append predicted joint angles to 

        return predictions  # Return list of predicted joint angles
```

In [18]:
```
from sklearn.base import BaseEstimator, RegressorMixin
from sko.PSO import PSO


class PSO_Optimizer(BaseEstimator, RegressorMixin):
    '''
    Particle Swarm Optimization (PSO) Optimizer for joint angle prediction.

    Parameters:
    - pop_size (int): Population size for particle swarm optimization.
    - max_iteration (int): Maximum number of iterations for particle swarm o
    - inertia (float): Inertia weight for particle swarm optimization.
    - cognitive_param (float): Cognitive parameter for particle swarm optimi
    - social_param (float): Social parameter for particle swarm optimizatio

    Attributes:
    - pop_size (int): Population size for particle swarm optimization.
    - max_iteration (int): Maximum number of iterations for particle swarm o
    - inertia (float): Inertia weight for particle swarm optimization.
    - cognitive_param (float): Cognitive parameter for particle swarm optimi
    - social_param (float): Social parameter for particle swarm optimizatio
    '''

    def __init__(
            self,
            pop_size=None,
            max_iteration=None,
            inertia=None,
            cognitive_param=None,
            social_param=None
    ):
        self.pop_size = pop_size
        self.max_iteration = max_iteration
        self.inertia = inertia
        self.cognitive_param = cognitive_param
        self.social_param = social_param

    def fit(self, X, y=None):
        '''
        Fit method for the particle swarm optimization optimizer.

        Parameters:
        - X (array-like): Input features (not used in fitting).
        - y (array-like): Target variable (not used in fitting).

        Returns:
        - self (object): Instance of the estimator.
        '''
        return self
```

```
    def predict(self, X):
        '''
        Predict method to predict joint angles using particle swarm optimiza

        Parameters:
        - X (array-like): Input features containing end effector positions.

        Returns:
        - predictions (list): Predicted joint angles for each input position
        '''
        predictions: list = []  # Initialize list to store predictions

        # Iterate over each end effector position
        for position in X:
            np.random.seed(1)  # Set seed for reproducibility

            # Initialize particle swarm optimization with specified paramete
            pso = PSO(
                func=lambda y: evaluate_prediction([position], [y]),
                n_dim=7,
                pop=self.pop_size,
                max_iter=self.max_iteration,
                w=self.social_param,
                c1=self.cognitive_param,
                c2=self.social_param,
                lb=[x[1] for x in joint_constraints],
                ub=[x[0] for x in joint_constraints],
            )

            # Run particle swarm optimization to find optimal joint angles
            y_pred, _ = pso.run()
            predictions.append(y_pred)  # Append predicted joint angles to 

        return predictions  # Return list of predicted joint angles
```

In [19]:

```
from sklearn.base import BaseEstimator, RegressorMixin
from sko.SA import SAFast


class SA_Optimizer(BaseEstimator, RegressorMixin):
    '''
    Simulated Annealing (SA) Optimizer for joint angle prediction.

    Parameters:
    - iteration_count (int): Number of iterations for simulated annealing.
    - T_min (float): Minimum temperature for simulated annealing.
    - T_max (float): Maximum temperature for simulated annealing.

    Attributes:
    - iteration_count (int): Number of iterations for simulated annealing.
    - T_min (float): Minimum temperature for simulated annealing.
    - T_max (float): Maximum temperature for simulated annealing.
    '''

    def __init__(
            self,
            iteration_count=None,
            T_min=None,
            T_max=None
    ):
        self.iteration_count = iteration_count
        self.T_min = T_min
        self.T_max = T_max
```

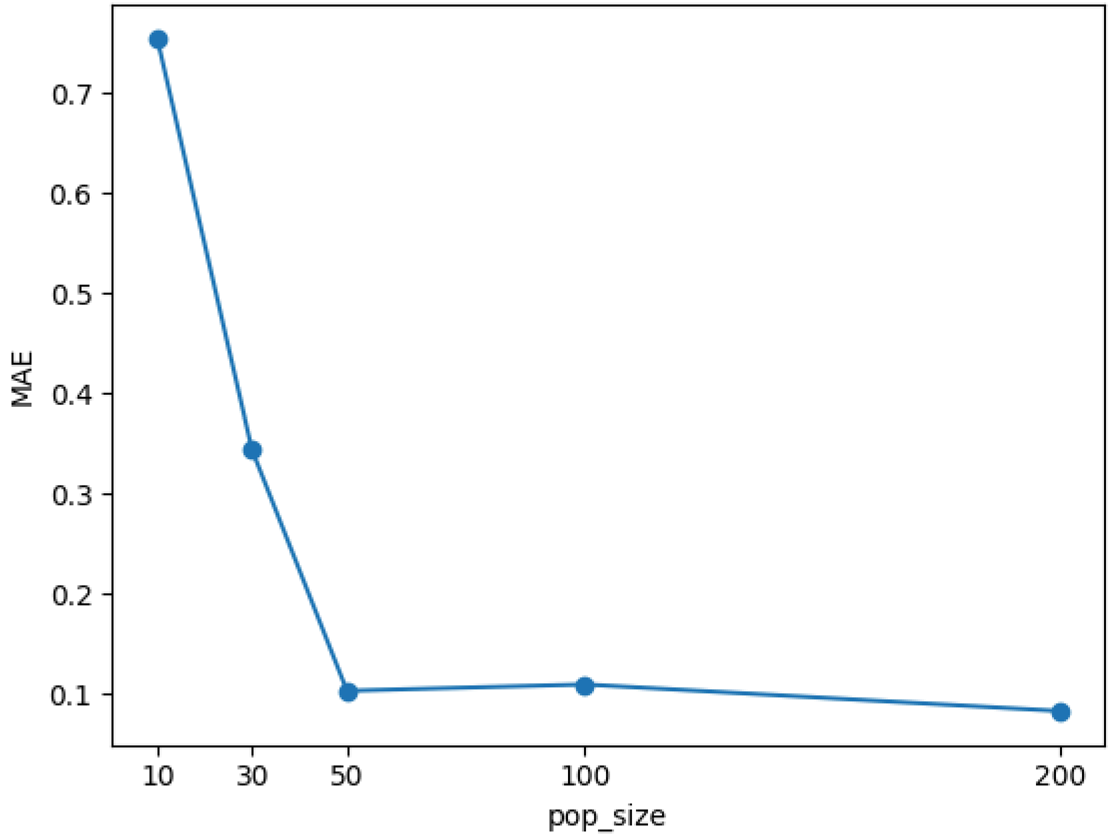
```
    def fit(self, X, y=None):
        '''
        Fit method for the simulated annealing optimizer.

        Parameters:
        - X (array-like): Input features (not used in fitting).
        - y (array-like): Target variable (not used in fitting).

        Returns:
        - self (object): Instance of the estimator.
        '''
        return self

    def predict(self, X):
        '''
        Predict method to predict joint angles using simulated annealing.

        Parameters:
        - X (array-like): Input features containing end effector positions.

        Returns:
        - predictions (list): Predicted joint angles for each input positio
        '''
        predictions: list = []  # Initialize list to store predictions

        # Iterate over each end effector position
        for position in X:
            np.random.seed(1)  # Set seed for reproducibility

            # Initialize simulated annealing with specified parameters
            sa = SAFast(
                func=lambda y: evaluate_prediction([position], [y]),
                x0=[0, 0, 0, 0, 0, 0, 0],  # Initial guess for joint angles
                T_max=self.T_max,
                T_min=self.T_min,
                L=self.iteration_count,
            )

            # Run simulated annealing to find optimal joint angles
            y_pred, _ = sa.run()
            predictions.append(y_pred)  # Append predicted joint angles to 

        return predictions  # Return list of predicted joint angles
```

GA Hyperparameters Selection

In [20]:

```
# varing the population size
params = {
    'pop_size': [10, 30, 50, 100, 200],
    'max_iteration': [10],
    'mutation': [0.0],
}

result=do_grid_search(
    estimator=GA_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='pop_size'
    )
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



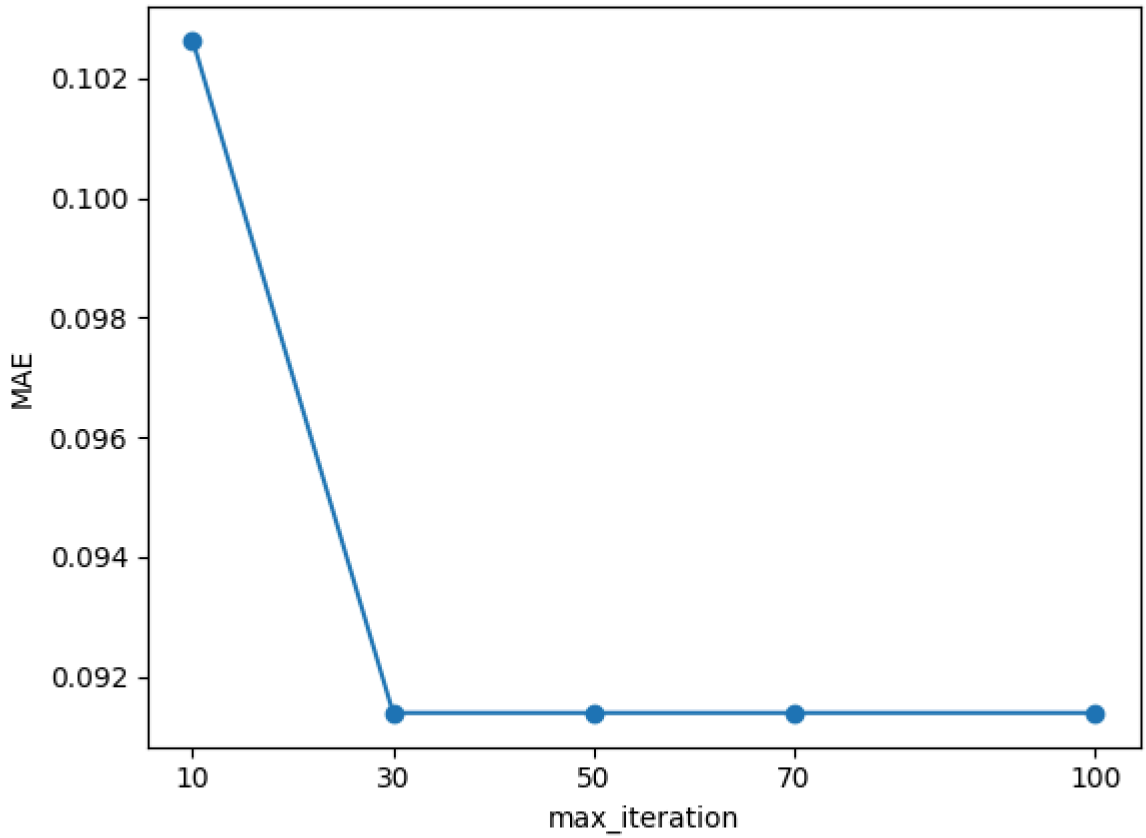
Out[20]:

	pop_size	max_iteration	mutation	MAE
4	200	10	0.0	0.082448
2	50	10	0.0	0.102636
3	100	10	0.0	0.109003
1	30	10	0.0	0.343511
0	10	10	0.0	0.755009

In [21]:

```
# varing the maximum iteration
params = {
    'pop_size': [50],
    'max_iteration': [10, 30, 50, 70, 100,],
    'mutation': [0.0],
}

result = do_grid_search(
    estimator=GA_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='max_iteration',

    )
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



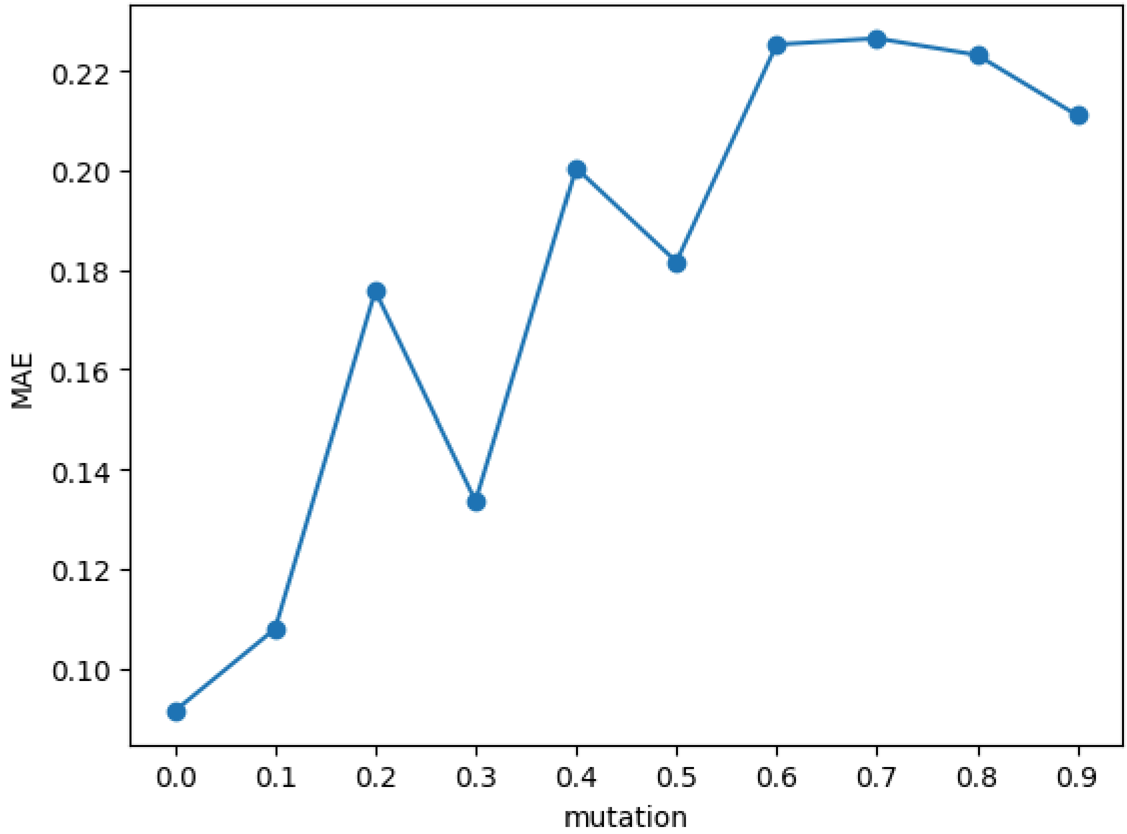
Out[21]:

	pop_size	max_iteration	mutation	MAE
1	50	30	0.0	0.091389
2	50	50	0.0	0.091389
3	50	70	0.0	0.091389
4	50	100	0.0	0.091389
0	50	10	0.0	0.102636

In [22]:

```
# varying the mutation probability
params = {
    'pop_size': [50],
    'max_iteration': [30],
    'mutation': [x*0.1 for x in range(0,10)],
}

result = do_grid_search(
    estimator=GA_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='mutation',
    )
result
```

```
Fitting 7 folds for each of 10 candidates, totalling 70 fits
```



Out[22]:

	pop_size	max_iteration	mutation	MAE
0	50	30	0.0	0.091389
1	50	30	0.1	0.107893
3	50	30	0.3	0.133579
2	50	30	0.2	0.175807
5	50	30	0.5	0.181660
4	50	30	0.4	0.200507
9	50	30	0.9	0.211136
8	50	30	0.8	0.223277
6	50	30	0.6	0.225369
7	50	30	0.7	0.226610

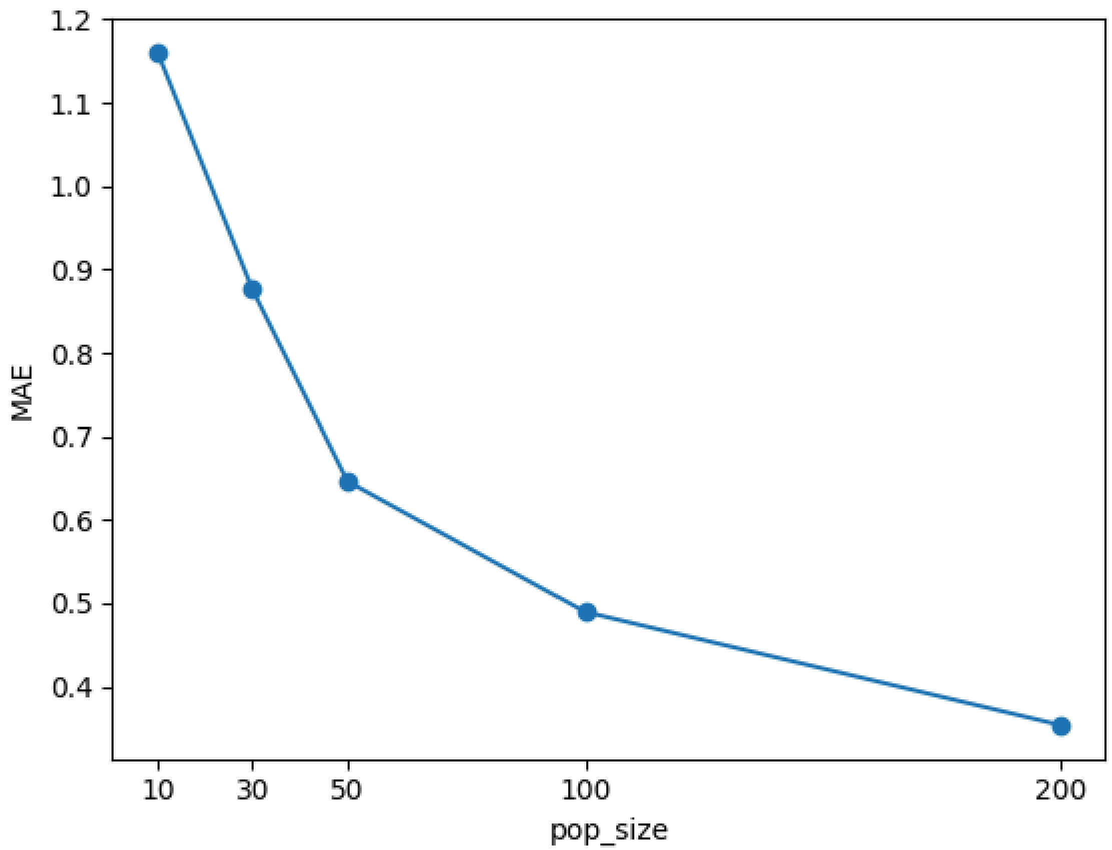
In [23]:
```
best_ga= GA_Optimizer(
    max_iteration=50,
    pop_size=200,
    mutation=0.1,
)
```

DE Hyperparameters Selection

In [24]:
```
# varing the population size
params = {
    'pop_size': [10, 30, 50, 100, 200],
    'max_iteration': [10],
    'mutation': [0.0],
}
```

```
result=do_grid_search(
    estimator=DE_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='pop_size',
    )
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



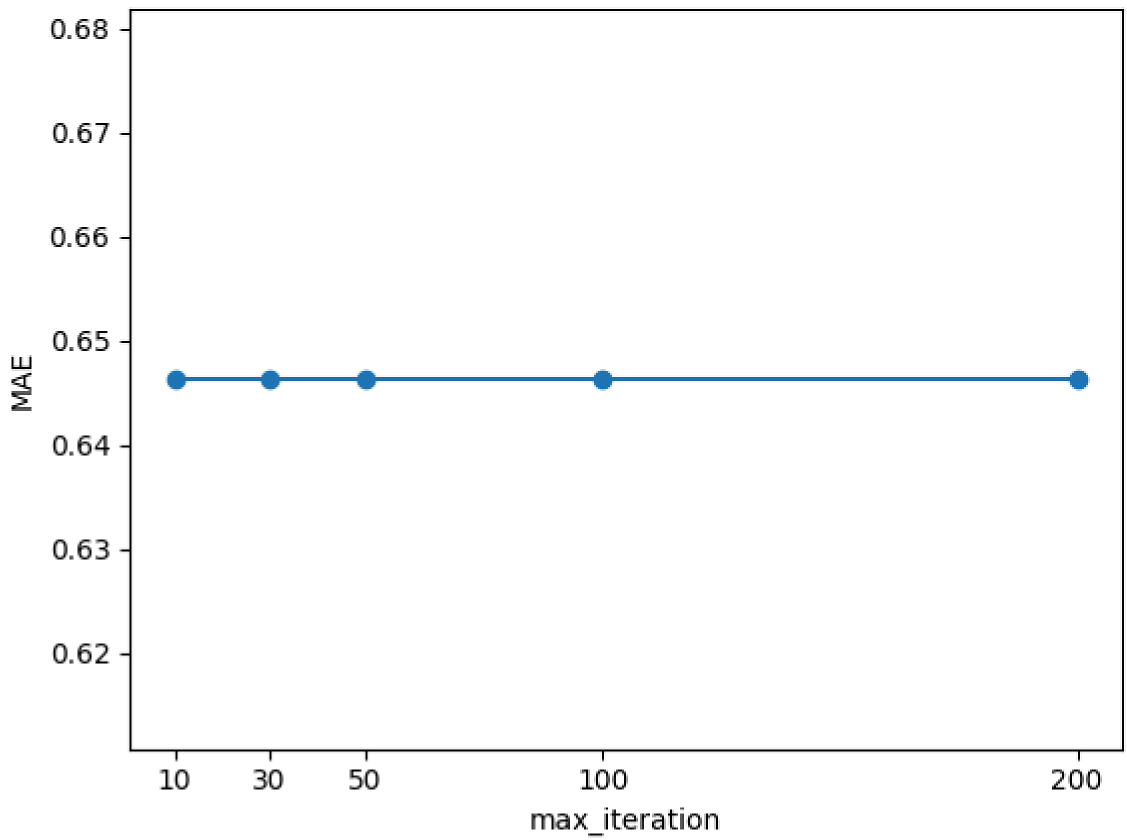
Out[24]:

	pop_size	max_iteration	mutation	MAE
4	200	10	0.0	0.353903
3	100	10	0.0	0.489629
2	50	10	0.0	0.646348
1	30	10	0.0	0.875871
0	10	10	0.0	1.160889

In [25]:

```
# varing the max_iteration
params = {
    'pop_size': [50],
    'max_iteration': [10, 30, 50,100,200],
    'mutation': [0.0],
}

result=do_grid_search(
    estimator=DE_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='max_iteration',
    )
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



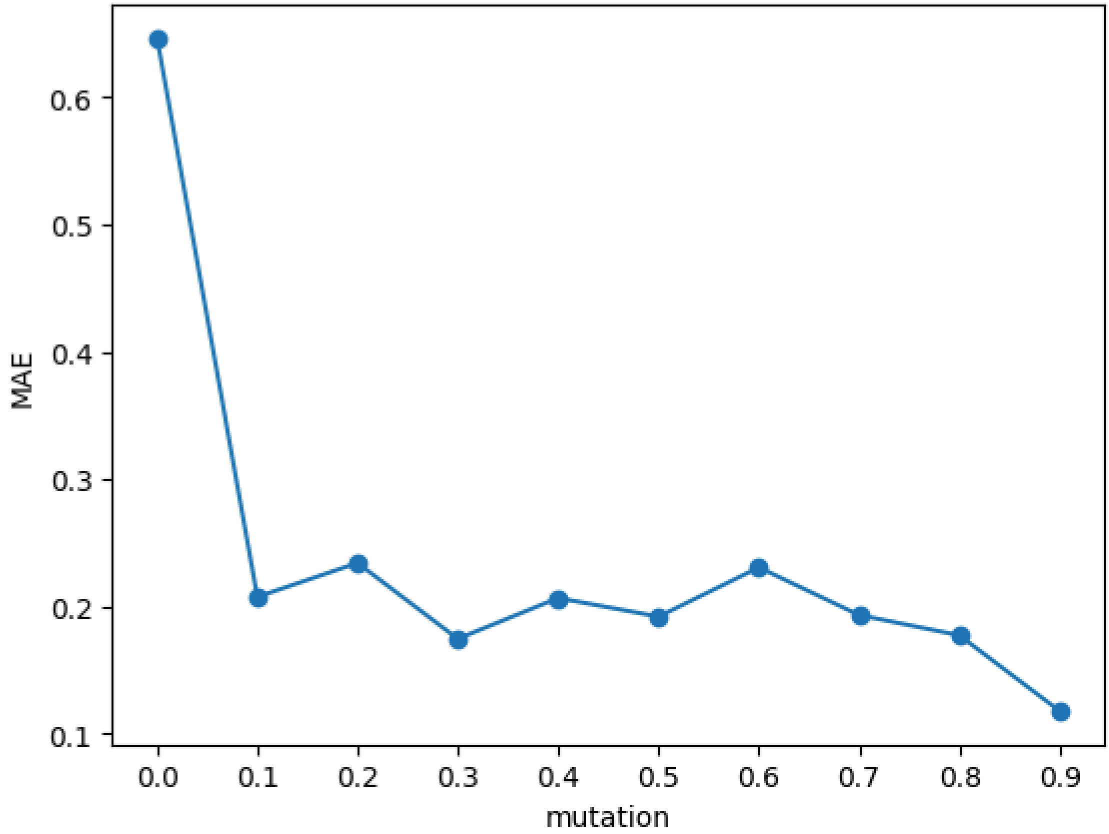
Out[25]:

	pop_size	max_iteration	mutation	MAE
0	50	10	0.0	0.646348
1	50	30	0.0	0.646348
2	50	50	0.0	0.646348
3	50	100	0.0	0.646348
4	50	200	0.0	0.646348

In [26]:

```
# varing the probability mutation
params = {
    'pop_size': [50],
    'max_iteration': [10,],
    'mutation': [x*0.1 for x in range(0,10)],
}

result=do_grid_search(
    estimator=DE_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='mutation',
    )
result
```

```
Fitting 7 folds for each of 10 candidates, totalling 70 fits
```



Out[26]:

	pop_size	max_iteration	mutation	MAE
9	50	10	0.9	0.117777
3	50	10	0.3	0.174451
8	50	10	0.8	0.177221
5	50	10	0.5	0.191906
7	50	10	0.7	0.193149
4	50	10	0.4	0.206472
1	50	10	0.1	0.207397
6	50	10	0.6	0.230605
2	50	10	0.2	0.234121
0	50	10	0.0	0.646348

In [27]:

```
best_de=DE_Optimizer(
    pop_size=200,
    max_iteration=50,
    mutation=0.9
)
```

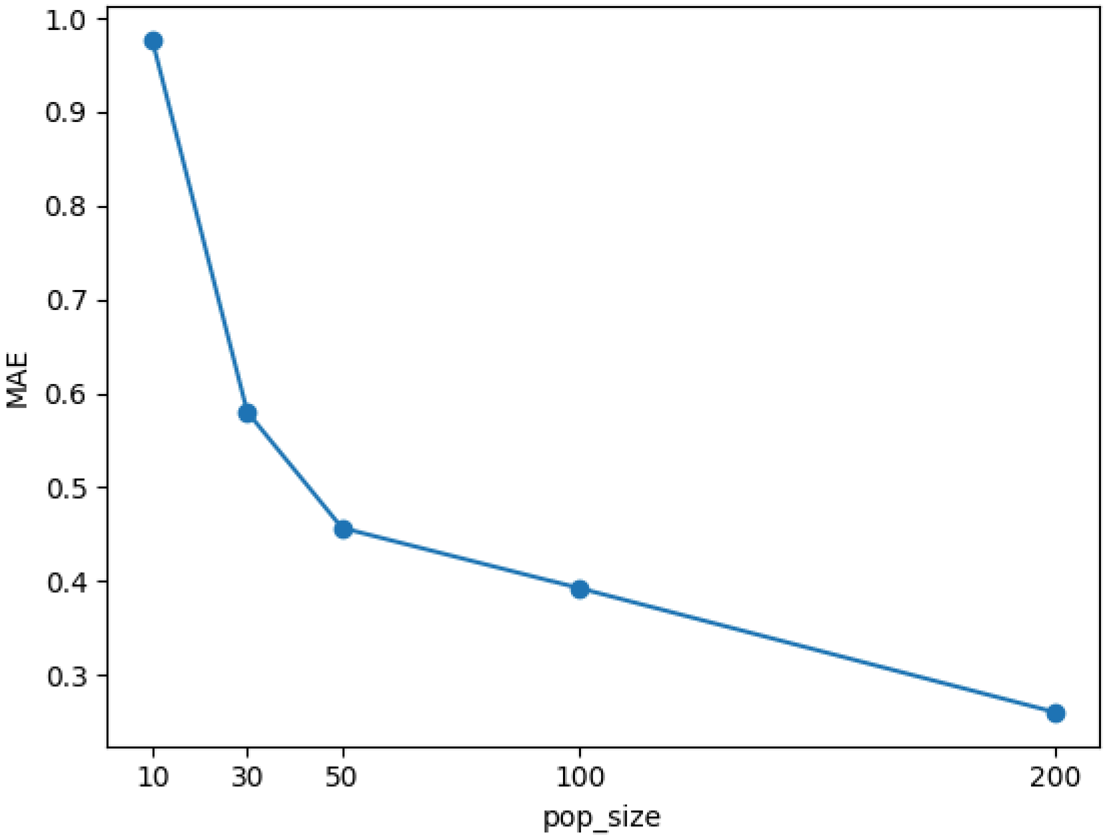
PSO Hyperparameters Selection

In [28]:

```
# varing the population size
params = {
    'pop_size': [10, 30, 50, 100, 200],
    'max_iteration': [10],
    "inertia": [0.1],
    "cognitive_param": [0.1],
    "social_param": [0.1]
```

```
}

result = do_grid_search(
    estimator=PSO_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='pop_size',
)
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



Out[28]:

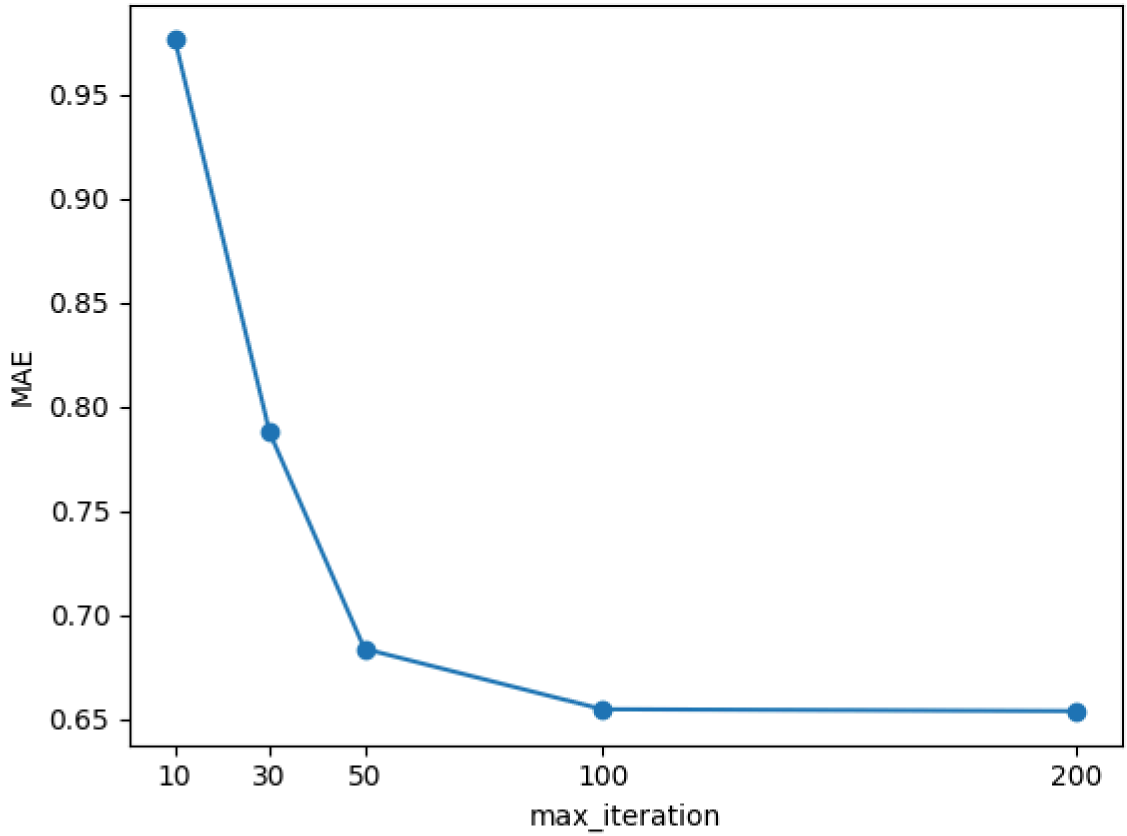
	pop_size	max_iteration	inertia	cognitive_param	social_param	MAE
4	200	10	0.1	0.1	0.1	0.260409
3	100	10	0.1	0.1	0.1	0.392450
2	50	10	0.1	0.1	0.1	0.456814
1	30	10	0.1	0.1	0.1	0.580813
0	10	10	0.1	0.1	0.1	0.977069

In [29]:

```
# varing the max_iteration
params = {
    'pop_size': [10],
    'max_iteration': [10, 30, 50, 100, 200],
    "inertia" : [0.1],
    "cognitive_param" : [0.1],
    "social_param" : [0.1]
}


result = do_grid_search(
    estimator=PSO_Optimizer(),
    params=params,
    X=pos_choices,
```

```
    y=angle_choices,
    x_plot='max_iteration',
)
result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



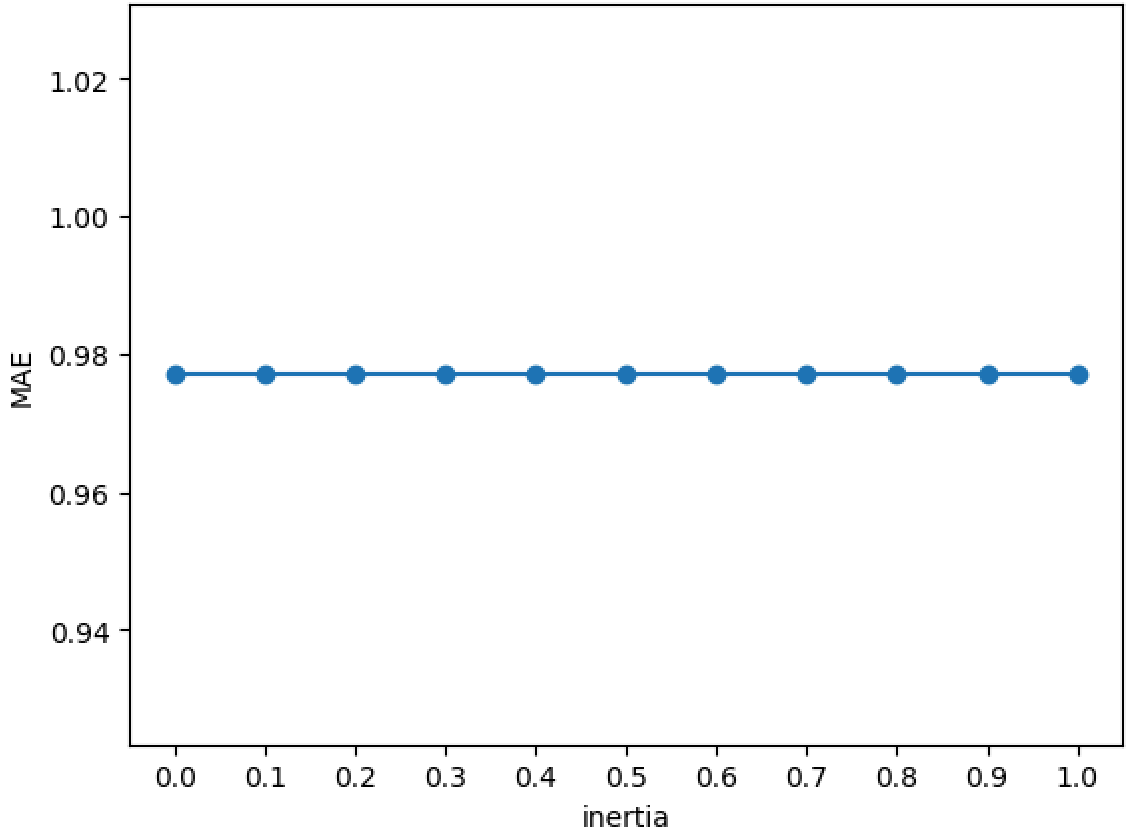
Out[29]:

	pop_size	max_iteration	inertia	cognitive_param	social_param	MAE
4	10	200	0.1	0.1	0.1	0.653666
3	10	100	0.1	0.1	0.1	0.654531
2	10	50	0.1	0.1	0.1	0.683623
1	10	30	0.1	0.1	0.1	0.787767
0	10	10	0.1	0.1	0.1	0.977069

In [30]:

```
# varing the inertia
params = {
    'pop_size': [10],
    'max_iteration': [10],
    "inertia" : [x*0.1 for x in range(11)],
    "cognitive_param" : [0.1],
    "social_param" : [0.1]
}

result = do_grid_search(
    estimator=PSO_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='inertia',
)
result
```

```
Fitting 7 folds for each of 11 candidates, totalling 77 fits
```



Out[30]:

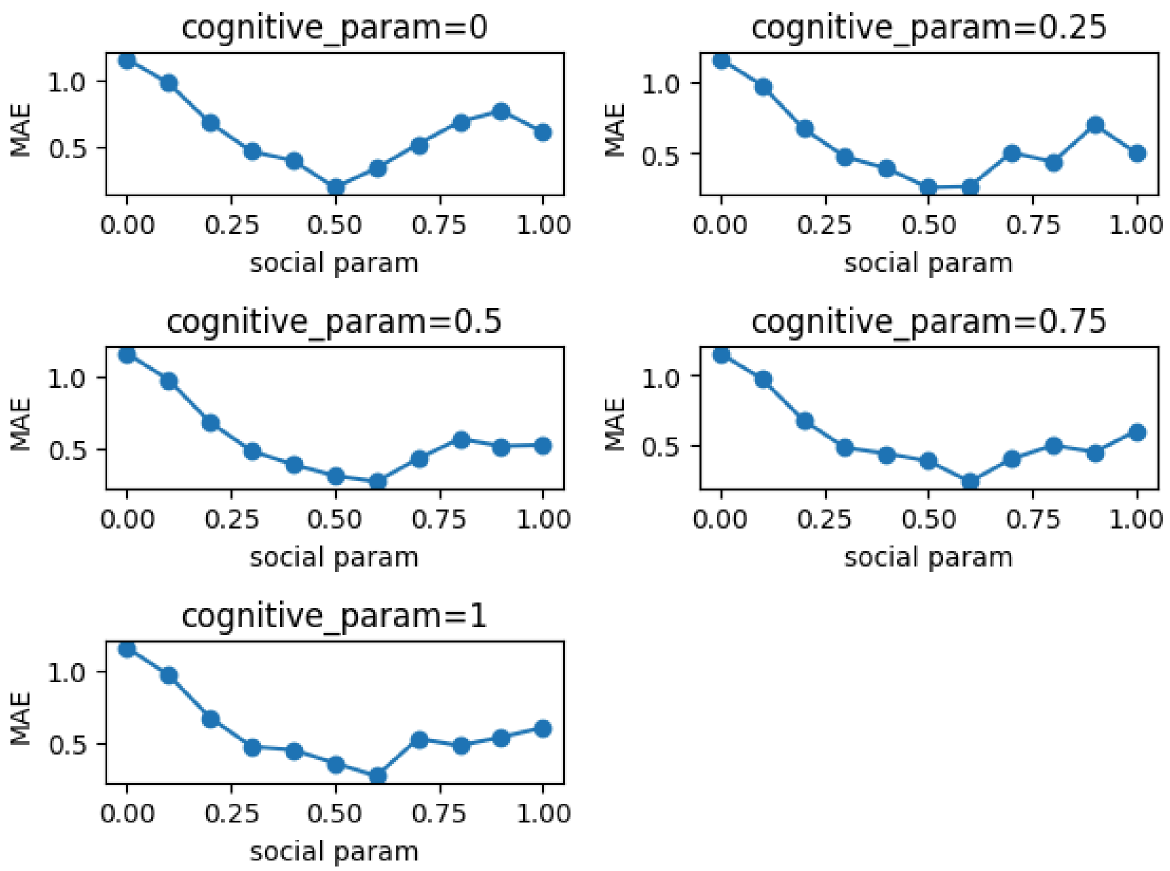
	pop_size	max_iteration	inertia	cognitive_param	social_param	MAE
0	10	10	0.0	0.1	0.1	0.977069
1	10	10	0.1	0.1	0.1	0.977069
2	10	10	0.2	0.1	0.1	0.977069
3	10	10	0.3	0.1	0.1	0.977069
4	10	10	0.4	0.1	0.1	0.977069
5	10	10	0.5	0.1	0.1	0.977069
6	10	10	0.6	0.1	0.1	0.977069
7	10	10	0.7	0.1	0.1	0.977069
8	10	10	0.8	0.1	0.1	0.977069
9	10	10	0.9	0.1	0.1	0.977069
10	10	10	1.0	0.1	0.1	0.977069

In [31]:

```
# varing the cognitive_param and social_param simultaneously

fig = plt.figure()


interval = [0,  0.25, 0.5,  0.75,  1]
for count, i in enumerate(interval, 1):
    ax = fig.add_subplot(3, 2, count)
    params = {
        'pop_size': [10],
        'max_iteration': [10],
        "inertia": [0.1],
        "cognitive_param": [i],
        "social_param": [x*0.1 for x in range(11)],
    }
```

```
    result = do_grid_search(
        estimator=PSO_Optimizer(),
        params=params,
        X=pos_choices,
        y=angle_choices,
    )
    result = result.sort_values('social_param')
    ax.plot(result['social_param'].values, result['MAE'].values, marker='o')
    ax.set_title(f'cognitive_param={i}')
    ax.set_ylabel('MAE')
    ax.set_xlabel('social param')
    # ax.set_xticks(list(result['social_param'].values))

fig.tight_layout()

plt.show()
```

```
Fitting 7 folds for each of 11 candidates, totalling 77 fits
Fitting 7 folds for each of 11 candidates, totalling 77 fits
Fitting 7 folds for each of 11 candidates, totalling 77 fits
Fitting 7 folds for each of 11 candidates, totalling 77 fits
Fitting 7 folds for each of 11 candidates, totalling 77 fits
```

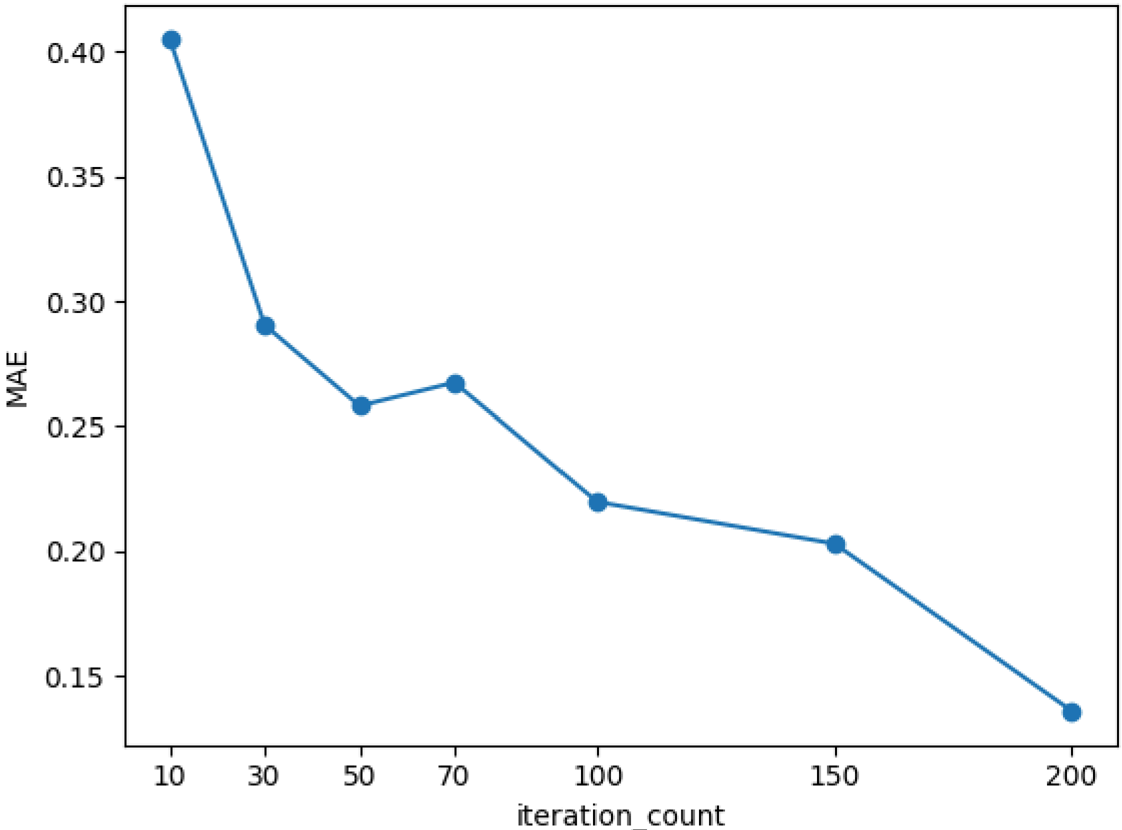


In [32]:
```
best_pso=PSO_Optimizer(
    pop_size=200,
    max_iteration=100,
    cognitive_param=0.25,
    social_param=0.5,
    inertia=0.1,
)
```

SA Hyperparameters Selection

In [33]:
```
# varing the iteration_count
params = {
    'iteration_count':[10, 30, 50,70, 100,150, 200],
    'T_max': [10],
    'T_min': [0.1]
}

result = do_grid_search(
    estimator=SA_Optimizer(),
    params=params,
    X=pos_choices,
    y=angle_choices,
    x_plot='iteration_count'
)
result
```

Fitting 7 folds for each of 7 candidates, totalling 49 fits



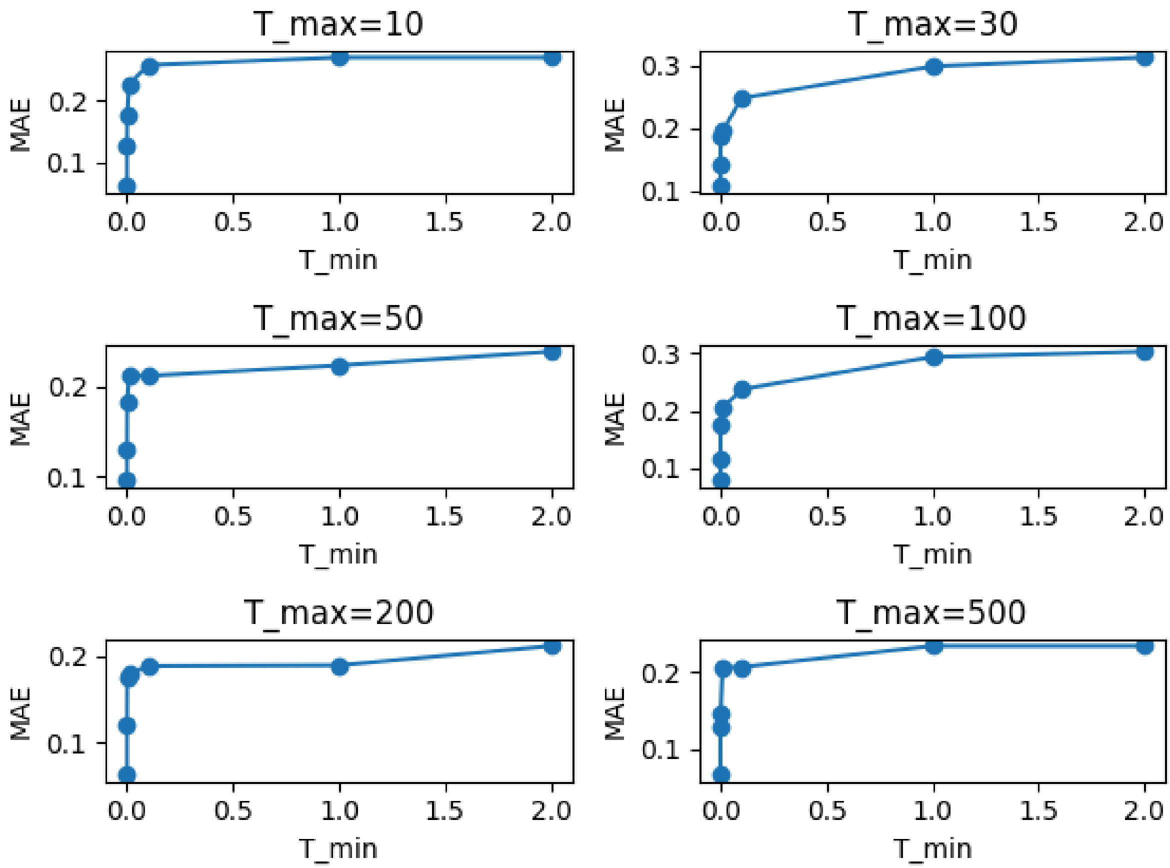
Out[33]:

	iteration_count	T_max	T_min	MAE
6	200	10	0.1	0.136070
5	150	10	0.1	0.203034
4	100	10	0.1	0.219811
2	50	10	0.1	0.258056
3	70	10	0.1	0.267426
1	30	10	0.1	0.290436
0	10	10	0.1	0.405041

In [34]:
```
# varing the T_max and T_min simultaneously
fig = plt.figure()


interval = [10, 30, 50, 100, 200,500]
```

```
for count, i in enumerate(interval, 1):
    ax = fig.add_subplot(3, 2, count)
    params = {
        'iteration_count': [50],
        'T_max': [i],
        'T_min': [1e-5,1e-4,1e-3,1e-2,1e-1,1,2]
    }
    result = do_grid_search(
        estimator=SA_Optimizer(),
        params=params,
        X=pos_choices,
        y=angle_choices,
    )
    result = result.sort_values('T_min')
    ax.plot(result['T_min'].values, result['MAE'].values, marker='o')
    ax.set_title(f'T_max={i}')
    ax.set_ylabel('MAE')
    ax.set_xlabel('T_min')
    # ax.set_xticks(list(result['social_param'].values))

fig.tight_layout()

plt.show()
```

```
Fitting 7 folds for each of 7 candidates, totalling 49 fits
Fitting 7 folds for each of 7 candidates, totalling 49 fits
Fitting 7 folds for each of 7 candidates, totalling 49 fits
Fitting 7 folds for each of 7 candidates, totalling 49 fits
Fitting 7 folds for each of 7 candidates, totalling 49 fits
Fitting 7 folds for each of 7 candidates, totalling 49 fits
```

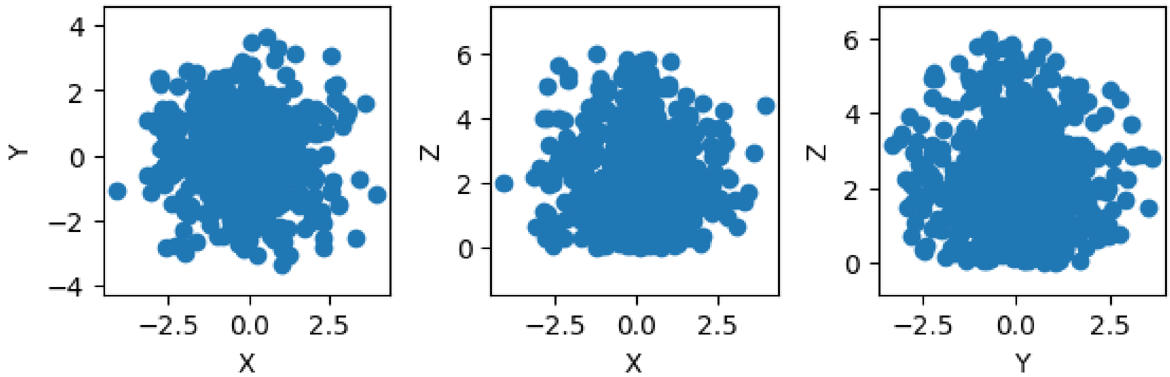


In [35]:
```
best_sa=SA_Optimizer(
    iteration_count=200,
    T_max=100,
    T_min=1e-5,
)
```

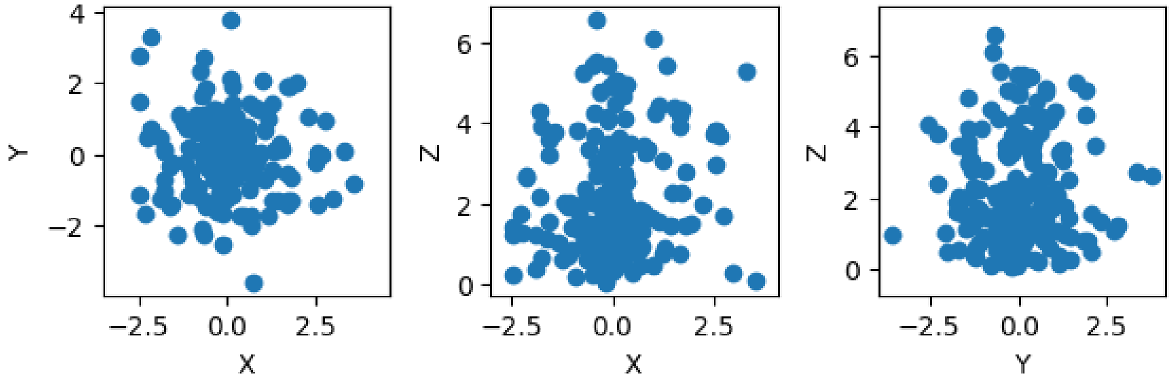
Data Splitting For Model Training

In [36]:
```
from sklearn.model_selection import train_test_split

# Split the data into training and test sets
# 80% of the data will be used for training, and 20% for testing
# Random state is set for reproducibility
df_train: pd.DataFrame  # Define variable for training set
df_test: pd.DataFrame  # Define variable for test set
df_train, df_test = train_test_split(
    df, test_size=0.2, random_state=10,)

# Print information about the data
print('DF')  # Print heading for the data
print('Training Size: ', len(df_test))  # Print size of training set
plot_positions(df_train[['x', 'y', 'z']].values)  # Plot positions for trai
print('Test Size: ', len(df_test))  # Print size of test set
plot_positions(df_test[['x', 'y', 'z']].values)  # Plot positions for test s
```

```
DF
Training Size:  200
```



```
Test Size:  200
```



In [37]:
```
# Define the list of features
features = [
    'x',
    'y',
    'z',
    'r',
    'rho',
    'theta',
    'phi'
]

# Define the maximum values for each feature
features_max_values = {
```

```
    'x': 6,
    'y': 6,
    'z': 6,
    'r': 6,
    'rho': 6,
    'theta': 2 * np.pi,
    'phi': np.pi,
    **{joint_name: joint_angle for joint_name, joint_angle in list(zip(join
}

# Define the minimum values for each feature
features_min_values = {
    'x': 0,
    'y': 0,
    'z': 0,
    'r': 0,
    'rho': 0,
    'theta': 0,
    'phi': 0,
    **{joint_name: joint_angle for joint_name, joint_angle in list(zip(join
}

# Create DataFrames for maximum and minimum values of features
features_max_df = pd.DataFrame(features_max_values, index=[0])
features_min_df = pd.DataFrame(features_min_values, index=[0])

# Create a combined DataFrame containing both maximum and minimum values
features_combined_df = pd.DataFrame(
    [features_min_values, features_max_values], index=[0, 1])


def do_max_scaling(features: list[str], dataframe: pd.DataFrame):
    '''
    Function to perform max scaling on specified features of a DataFrame

    Args:
        features (list[str]): List of feature names to be scaled
        dataframe (pd.DataFrame): DataFrame containing the features

    Returns:
        pd.DataFrame: DataFrame with the scaled features
    '''
    modified_df = dataframe[features].values / features_max_df[features].va
    return pd.DataFrame(modified_df, columns=features)


def undo_max_scaling(features: list[str], array: np.array):
    '''
    Function to undo max scaling on specified features of a NumPy array

    Args:
        features (list[str]): List of feature names to be unscaled
        array (np.array): NumPy array containing the scaled features

    Returns:
        pd.DataFrame: DataFrame with the unscaled features
    '''
    modified_array = array * features_max_df[features].values
    return pd.DataFrame(modified_array, columns=features)
```

In [38]:
```
# List of feature combinations
features_combinations = [
    ['x', 'y', 'z'],
    ['z', 'rho', 'theta'],
```

```
    ['r', 'theta', 'phi'],
    ['x', 'y', 'z', 'r', 'rho', 'theta', 'phi'],
    ['z', 'r', 'rho', 'theta', 'phi'],
    ['x', 'y', 'z', 'theta', 'phi'],
    ['r', 'rho', 'theta', 'phi'],
    ['x', 'y', 'z', 'r', 'rho', 'theta'],
    ['rho', 'theta', 'phi'],
]
```

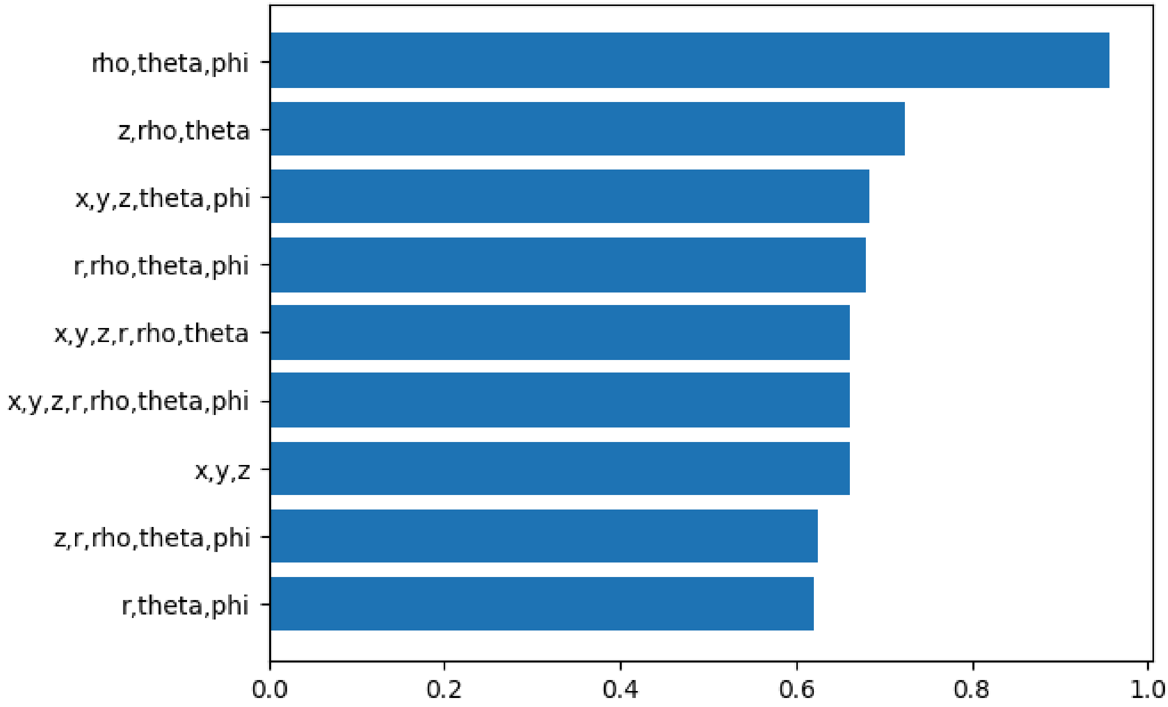
Decision Tree Regressor Hyperparameters Selection

In [39]:

```python
from sklearn.tree import DecisionTreeRegressor

# Initialize a list to store the results
data = []

# Loop through each feature combination
for features in features_combinations:

    # Extract training and test data based on current feature combination
    X_train = df_train[features].values
    Y_train = df_train[joint_names].values
    X_test = df_test[features].values

    # Initialize DecisionTreeRegressor with hyperparameters
    tree = DecisionTreeRegressor(
        max_depth=30,
        max_features=7,
        min_samples_split=2,
        min_samples_leaf=1,
        random_state=10,
    )

    # Fit the model on training data
    tree = tree.fit(X_train, Y_train)

    # Make predictions on test data
    y_pred = tree.predict(X_test)

    # Calculate Mean Absolute Error (MAE) without scaling
    mae_without_scaling = evaluate_prediction(
        df_test[['x', 'y', 'z']].values, y_pred)

    # Append results to the data list
    data.append([','.join(features), mae_without_scaling])

# Convert the results to a DataFrame
data = pd.DataFrame(data, columns=['features', 'MAE'])

# Sort the DataFrame based on MAE
data = data.sort_values('MAE')

# Plot a horizontal bar chart showing MAE for each feature combination
plt.barh(data['features'], data['MAE'])
```

Out[39]:

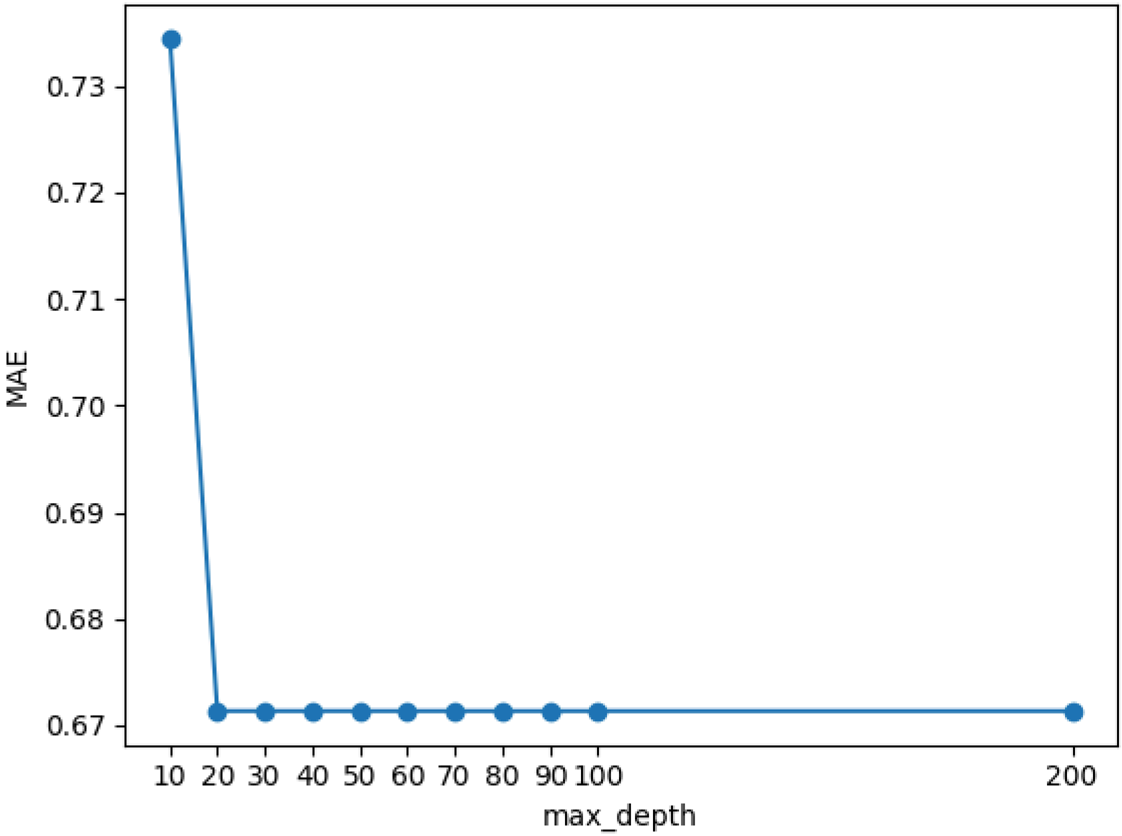
```
<BarContainer object of 9 artists>
```



In [40]:
```
# Define the list of features selected as the best by the decision tree mode
best_tree_features = ['r', 'theta', 'phi']
```

In [41]:
```
# varying the max_depth
from sklearn.tree import DecisionTreeRegressor


X_train = df_train[best_tree_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_tree_features].values

param_grid = {
    "max_depth": [10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200],
    "max_features": [7,],
    "min_samples_split": [2,],
    "min_samples_leaf": [1],
    "random_state": [10],
}


result = do_grid_search(
    DecisionTreeRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='max_depth'
)

result
```

```
Fitting 7 folds for each of 11 candidates, totalling 77 fits
```



Out[41]:

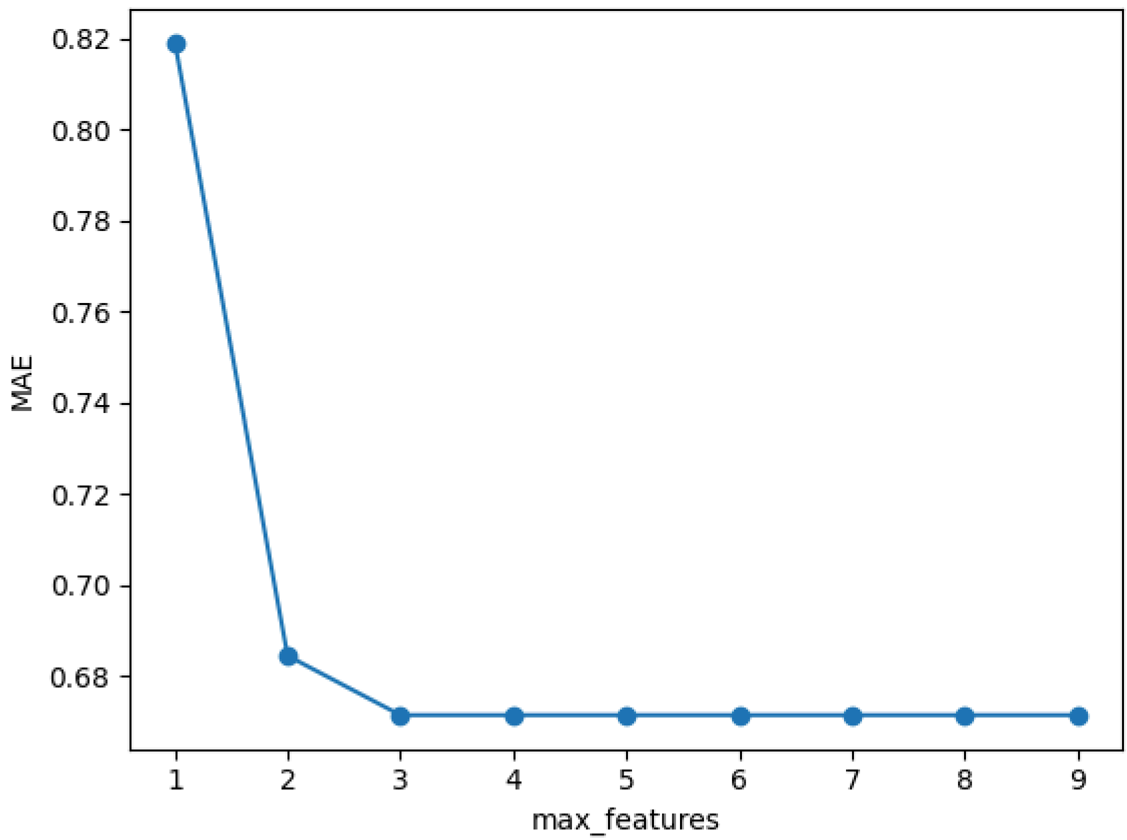
	max_depth	max_features	min_samples_split	min_samples_leaf	random_state	MA
1	20	7	2	1	10	0.67134
2	30	7	2	1	10	0.67134
3	40	7	2	1	10	0.67134
4	50	7	2	1	10	0.67134
5	60	7	2	1	10	0.67134
6	70	7	2	1	10	0.67134
7	80	7	2	1	10	0.67134
8	90	7	2	1	10	0.67134
9	100	7	2	1	10	0.67134
10	200	7	2	1	10	0.67134
0	10	7	2	1	10	0.73450

In [42]:

```
# varying the max_features
from sklearn.tree import DecisionTreeRegressor


X_train = df_train[best_tree_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_tree_features].values

param_grid = {
        "max_depth": [30],
        "max_features": [1,2,3,4,5,6,7,8,9],
        "min_samples_split": [2,],
        "min_samples_leaf": [1],
        "random_state": [10],
    }
```

```
result = do_grid_search(
    DecisionTreeRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='max_features'
)

result
```

```
Fitting 7 folds for each of 9 candidates, totalling 63 fits
```



Out[42]:

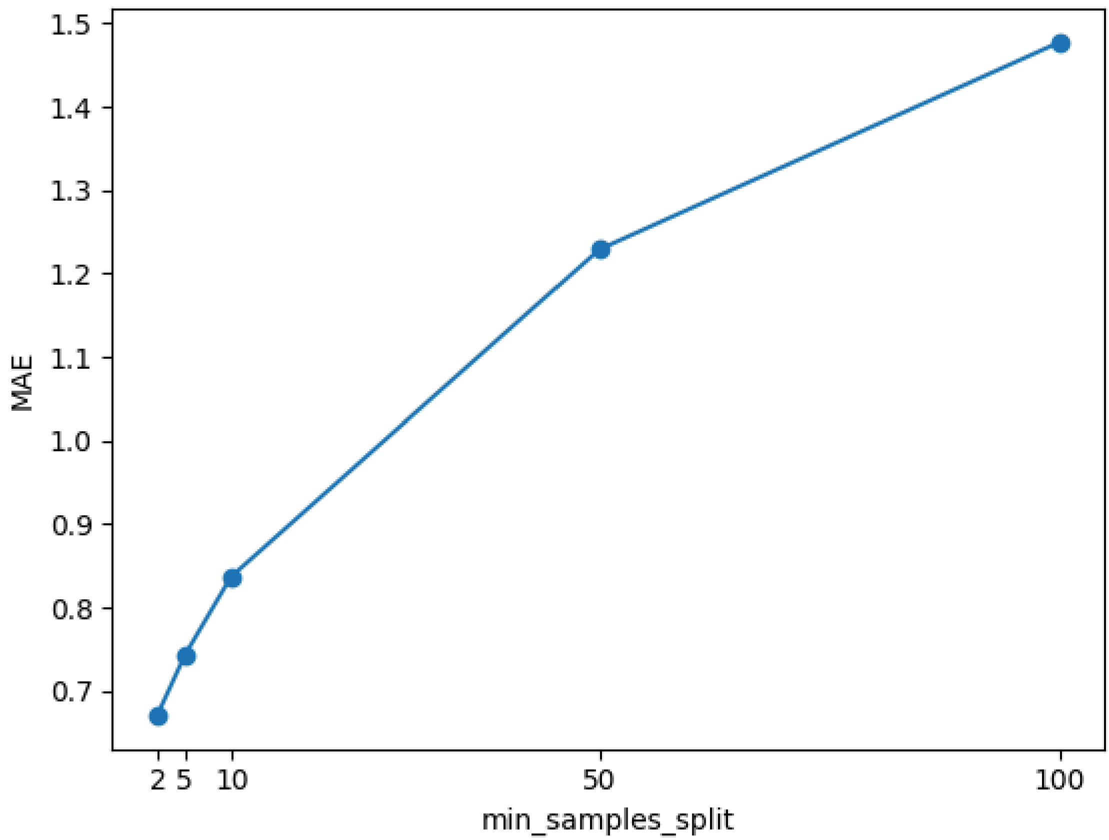
	max_depth	max_features	min_samples_split	min_samples_leaf	random_state	MAI
2	30	3	2	1	10	0.67134
3	30	4	2	1	10	0.67134
4	30	5	2	1	10	0.67134
5	30	6	2	1	10	0.67134
6	30	7	2	1	10	0.67134
7	30	8	2	1	10	0.67134
8	30	9	2	1	10	0.67134
1	30	2	2	1	10	0.68438
0	30	1	2	1	10	0.81915

In [43]:

```
# varying the min_samples_split

from sklearn.tree import DecisionTreeRegressor


X_train = df_train[best_tree_features].values
```

```
Y_train = df_train[joint_names].values
X_test = df_test[best_tree_features].values

param_grid = {
        "max_depth": [30],
        "max_features": [7],
        "min_samples_split": [2,5,10,50,100],
        "min_samples_leaf": [1],
        "random_state": [10],
    }


result = do_grid_search(
    DecisionTreeRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='min_samples_split'
)

result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



Out[43]:

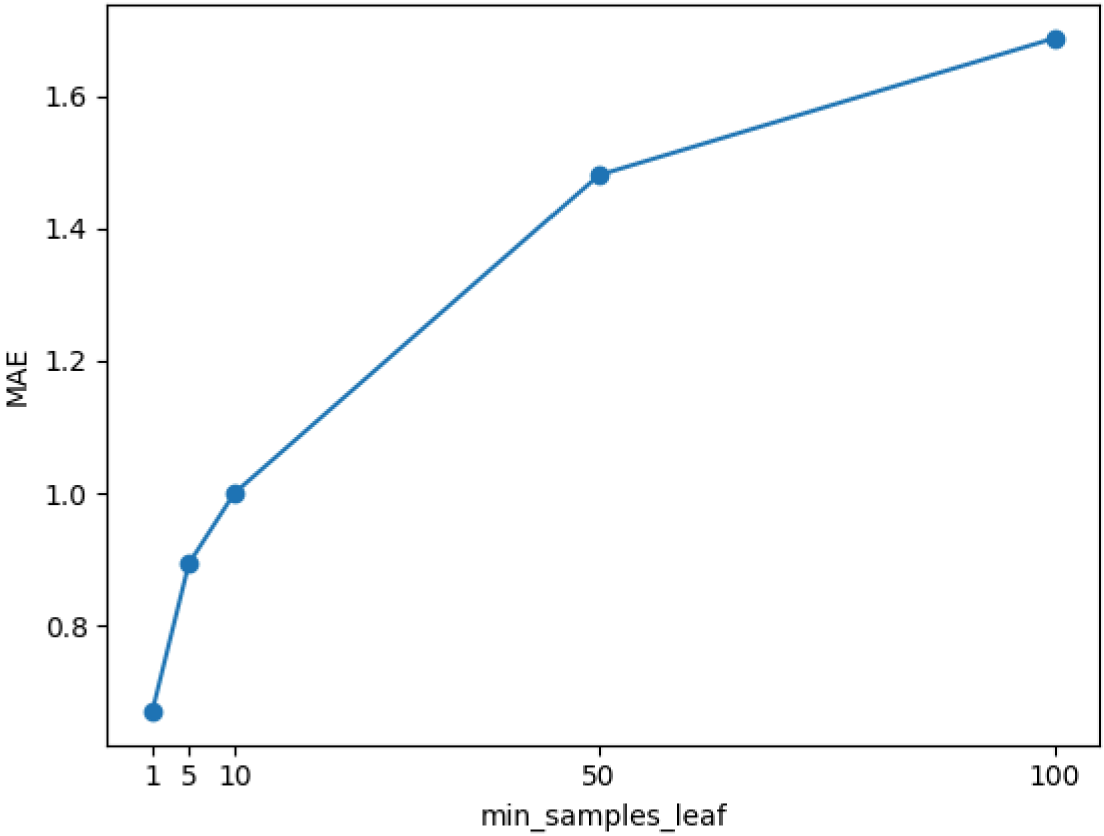
	max_depth	max_features	min_samples_split	min_samples_leaf	random_state	MAE
0	30	7	2	1	10	0.671342
1	30	7	5	1	10	0.743469
2	30	7	10	1	10	0.837039
3	30	7	50	1	10	1.228862
4	30	7	100	1	10	1.477298

In [44]:

```
# varying the min_samples_leaf

from sklearn.tree import DecisionTreeRegressor
```

```
X_train = df_train[best_tree_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_tree_features].values

param_grid = {
        "max_depth": [30],
        "max_features": [7],
        "min_samples_split": [2,],
        "min_samples_leaf": [1,5,10,50,100],
        "random_state": [10],
    }


result = do_grid_search(
    DecisionTreeRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='min_samples_leaf'
)

result
```

```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



Out[44]:

	max_depth	max_features	min_samples_split	min_samples_leaf	random_state	MAE
0	30	7	2	1	10	0.671342
1	30	7	2	5	10	0.893656
2	30	7	2	10	10	1.000134
3	30	7	2	50	10	1.480432
4	30	7	2	100	10	1.687194

In [45]:
```
from sklearn.tree import DecisionTreeRegressor

tree = DecisionTreeRegressor(
    max_depth=30,
    max_features=7,
    min_samples_leaf=1,
    min_samples_split=2,
    random_state=10,
)
X_train = df_train[best_tree_features]
Y_train = df_train[joint_names]
X_test = df_test[best_tree_features]
best_tree = tree.fit(X_train, Y_train)
```

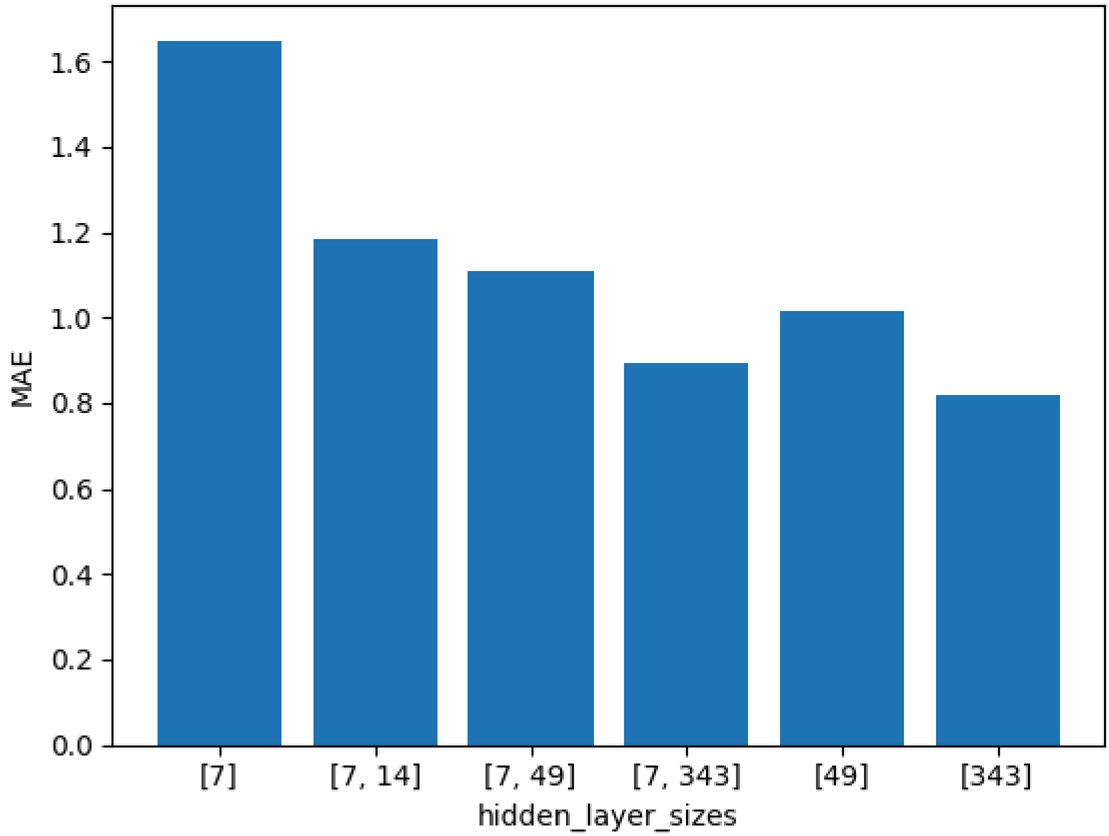
MLP Hyperparameters Selection

In [46]:
```
best_mlp_features=['x', 'y', 'z', 'r', 'rho', 'theta', 'phi']
```

In [47]:
```
# varying the hidden_layer_sizes
from sklearn.neural_network import MLPRegressor


X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7],
        [7, 14],
        [7, 7**2],
        [7**2],
        [7**3],
        [7,7**3],
    ],
    "activation": ['relu'],
    "solver": ['adam'],
    "max_iter": [10],
    "learning_rate": ['constant'],
    "learning_rate_init": [0.001],
    "random_state": [10],
    "batch_size": [5],
}


result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
```

```
    x_plot='hidden_layer_sizes',
    stringify_xplot=True,
    bar_plot=True
)
```

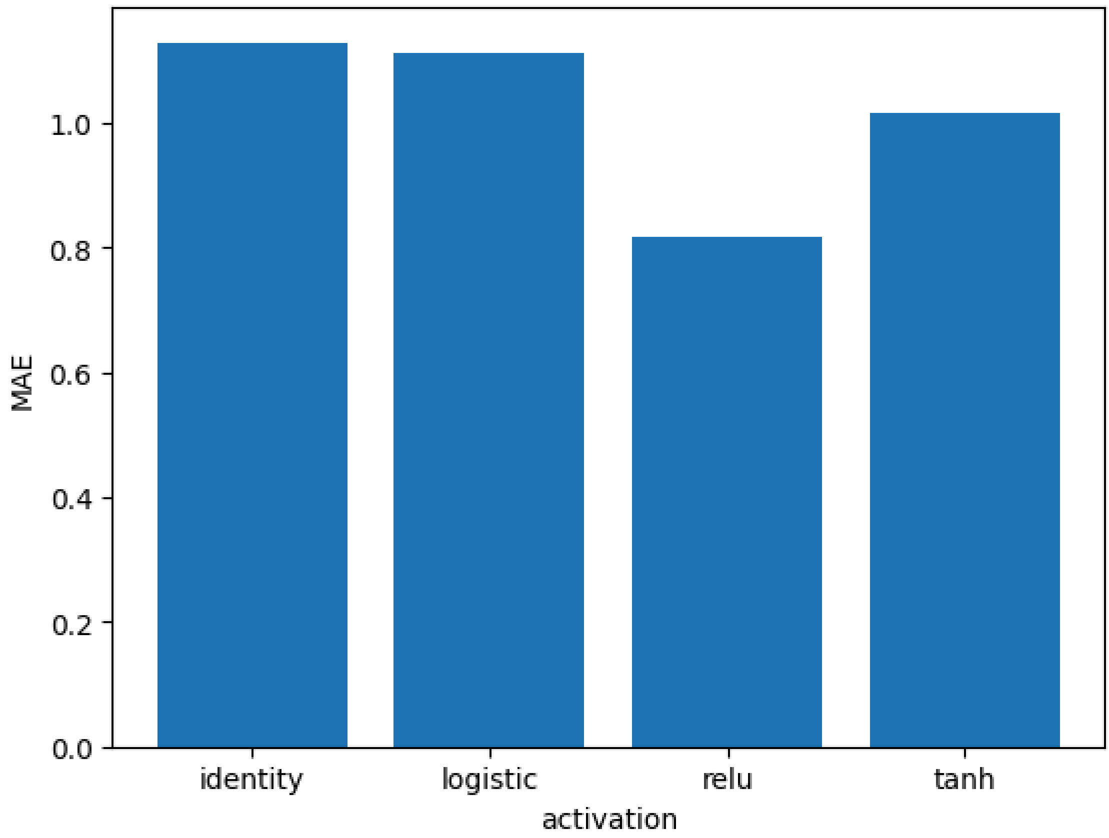
```
Fitting 7 folds for each of 6 candidates, totalling 42 fits
```



In [48]:

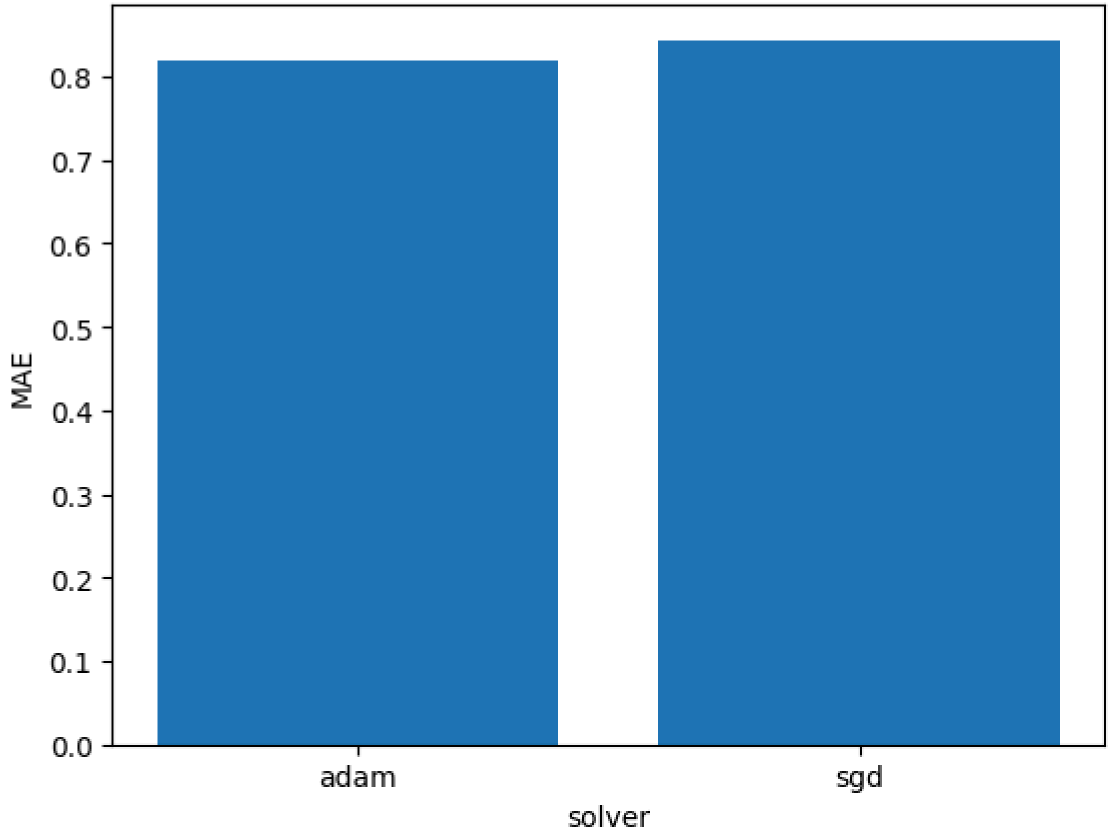
```
# varying the activation function
from sklearn.neural_network import MLPRegressor


X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7**3],
    ],
    "activation": ['identity', 'logistic', 'tanh', 'relu',],
    "solver": ['adam'],
    "max_iter": [10],
    "learning_rate": ['constant'],
    "learning_rate_init": [0.001],
    "random_state": [10],
    "batch_size": [5],
}


result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='activation',
    bar_plot=True
)
```

```
Fitting 7 folds for each of 4 candidates, totalling 28 fits
```



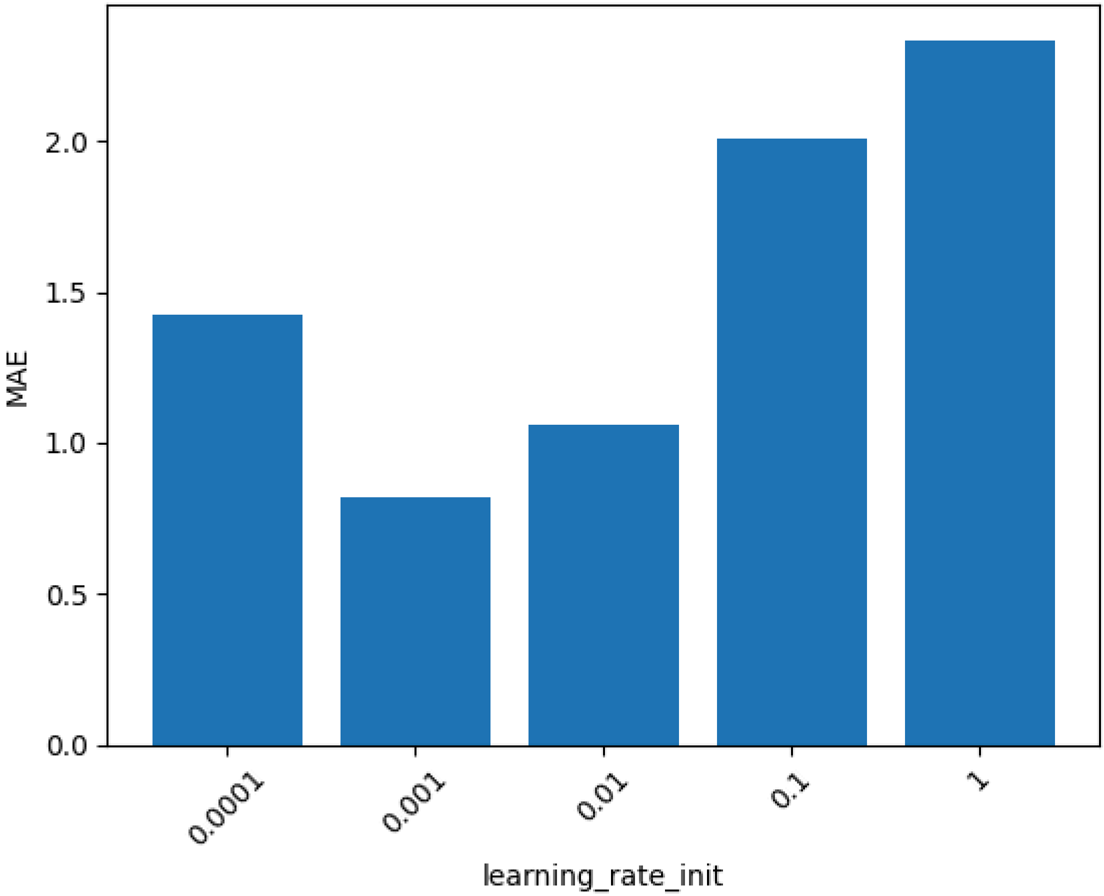
In [49]:
```python
# varying the solver
from sklearn.neural_network import MLPRegressor


X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7**3],
    ],
    "activation": ['relu'],
    "solver": ['adam','sgd'],
    "max_iter": [10],
    "learning_rate": ['constant'],
    "learning_rate_init": [0.001],
    "random_state": [10],
    "batch_size": [5],
}


result = do_grid_search(MLPRegressor(), param_grid, X_train, Y_train)

result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='solver',
    bar_plot=True
)
```

```
Fitting 7 folds for each of 2 candidates, totalling 14 fits
Fitting 7 folds for each of 2 candidates, totalling 14 fits
```



In [50]:
```
# varying the learning_rate_init
from sklearn.neural_network import MLPRegressor

X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7**3],
    ],
    "activation": ['relu'],
    "solver": [ 'adam'],
    "max_iter": [10],
    "learning_rate": ['constant'],
    "learning_rate_init": [1e-4,1e-3,1e-2,1e-1,1],
    "random_state": [10],
    "batch_size": [5],
}


result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='learning_rate_init',
    xticks_rotation=45,
    stringify_xplot=True,
    bar_plot=True
)
```

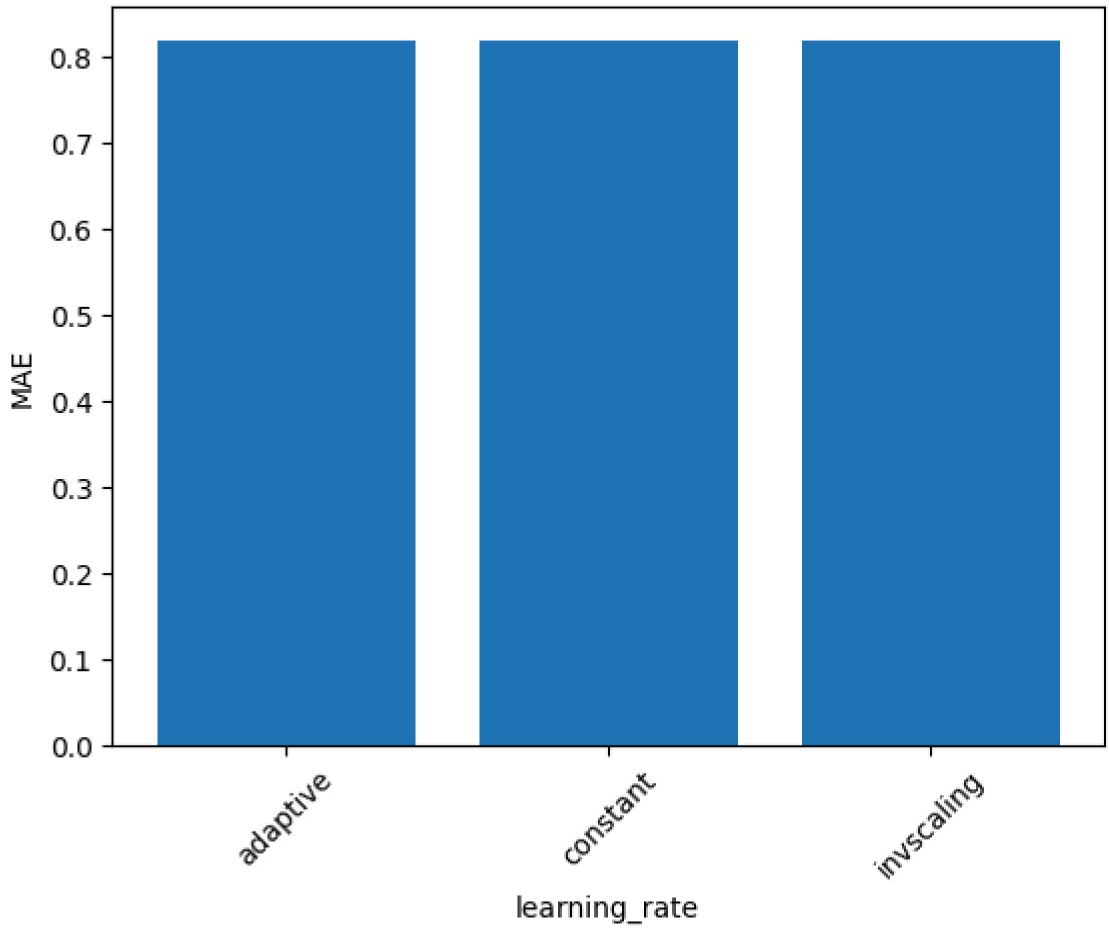
```
Fitting 7 folds for each of 5 candidates, totalling 35 fits
```



In [51]:

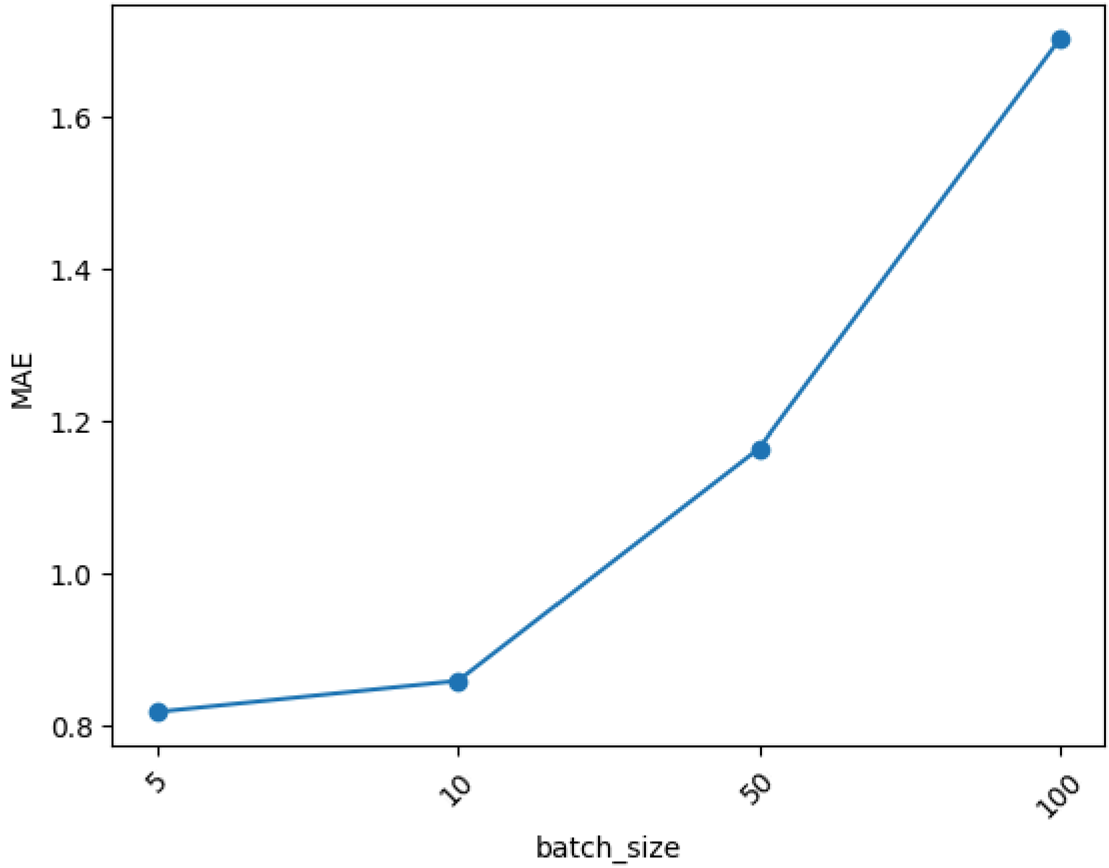
```
# varying the learning_rate strategy
from sklearn.neural_network import MLPRegressor

X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7**3],

    ],
    "activation": ['relu'],
    "solver": [ 'adam'],
    "max_iter": [10],
    "learning_rate": ['constant', 'invscaling', 'adaptive'],
    "learning_rate_init": [0.001],
    "random_state": [10],
    "batch_size": [5],
}


result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='learning_rate',
    xticks_rotation=45,
    stringify_xplot=True,
    bar_plot=True
)
```

```
Fitting 7 folds for each of 3 candidates, totalling 21 fits
```



In [52]:
```
# varying the batch_size
from sklearn.neural_network import MLPRegressor


X_train = df_train[best_mlp_features].values
Y_train = df_train[joint_names].values
X_test = df_test[best_mlp_features].values

param_grid = {
    "hidden_layer_sizes": [
        [7**3],
    ],
    "activation": ['relu'],
    "solver": [ 'adam'],
    "max_iter": [10],
    "learning_rate": ['constant'],
    "learning_rate_init": [0.001],
    "random_state": [10],
    "batch_size": [5,10,50,100],
}


result = do_grid_search(
    MLPRegressor(),
    param_grid,
    X_train,
    Y_train,
    x_plot='batch_size',
    xticks_rotation=45,
    stringify_xplot=True,
    # bar_plot=True
)
```

```
Fitting 7 folds for each of 4 candidates, totalling 28 fits
```



In [53]:

```
from sklearn.neural_network import MLPRegressor

mlp1=MLPRegressor(
    hidden_layer_sizes= [7**3],
    activation='relu',
    solver='adam',
    max_iter=200,
    learning_rate='constant',
    learning_rate_init=0.001,
    random_state=10,
    batch_size=5,

)
X_train = df_train[best_mlp_features]
Y_train = df_train[joint_names]
X_test = df_test[best_mlp_features]
best_mlp = mlp1.fit(X_train, Y_train)
```

Cross-comparison of the best estimators from each category

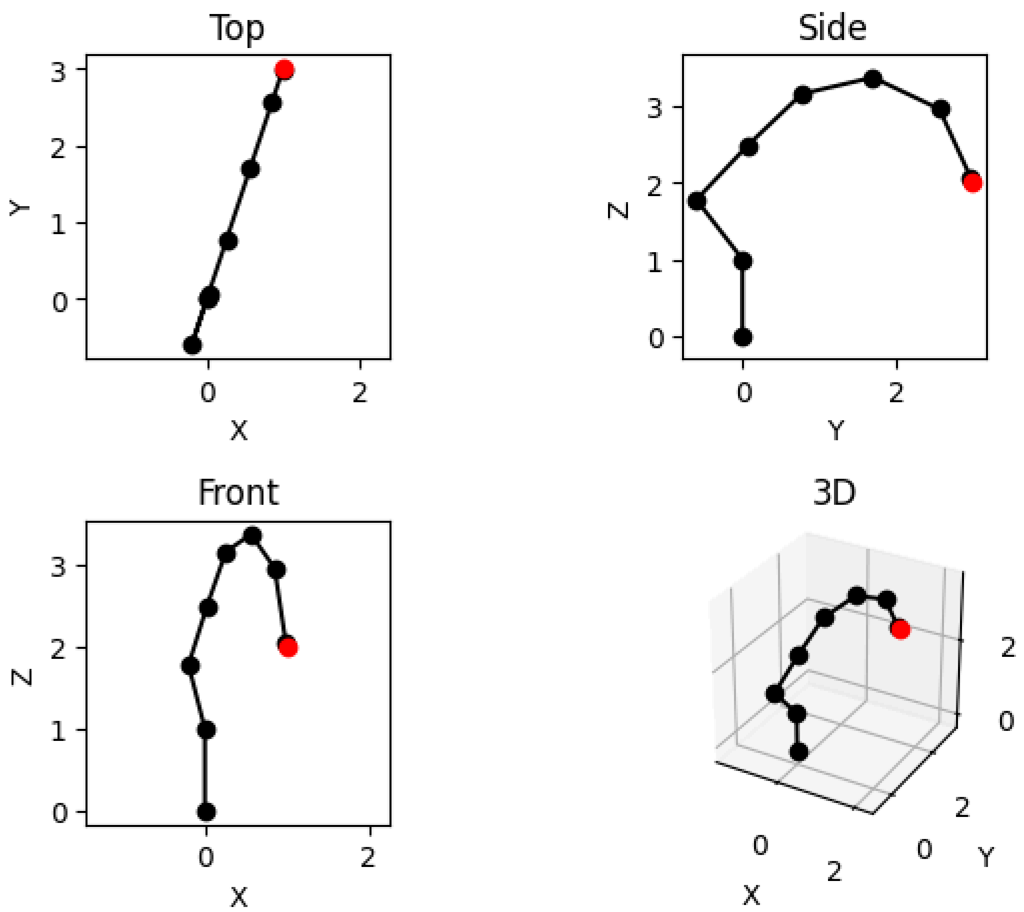
In [61]:

```
np.random.seed(5)
positions = np.asarray([[1,3,2]])
```

In [62]:

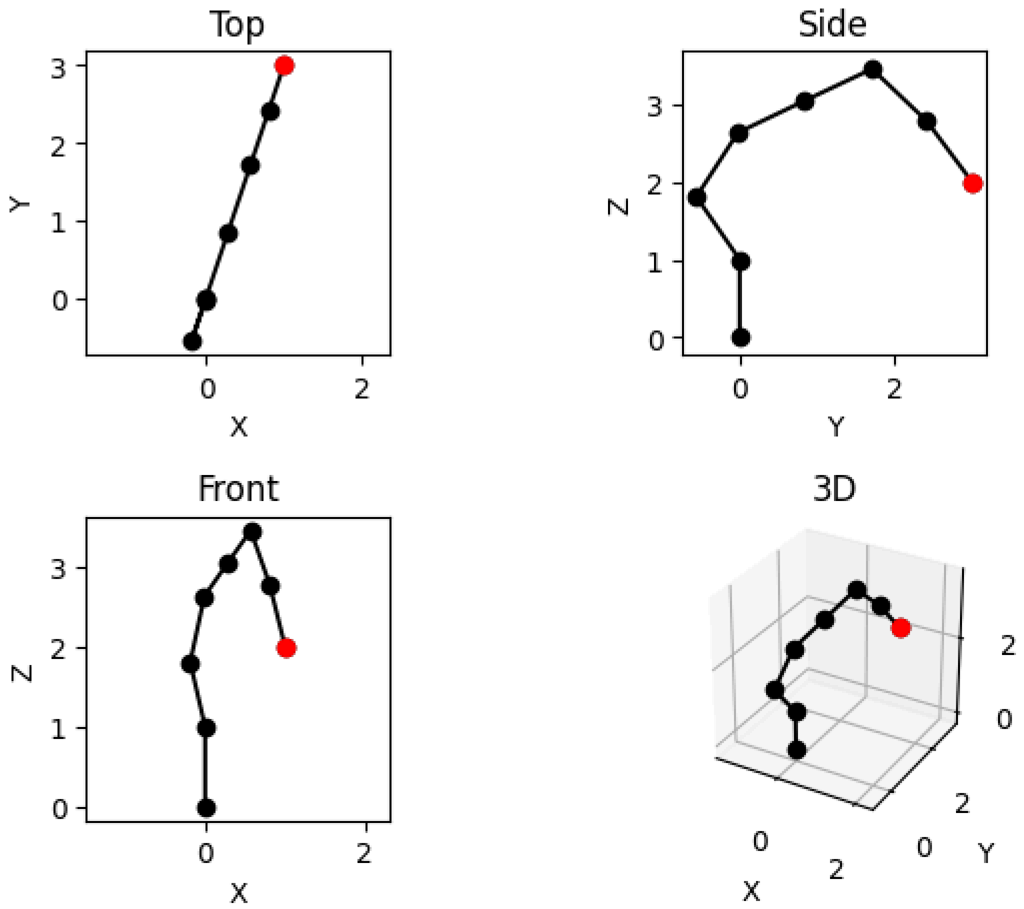
```
predictions=best_ga.predict(positions)

print('Best GA')
print('MAE: ',evaluate_prediction(positions,predictions))

for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

```
Best GA
MAE:  0.062
```



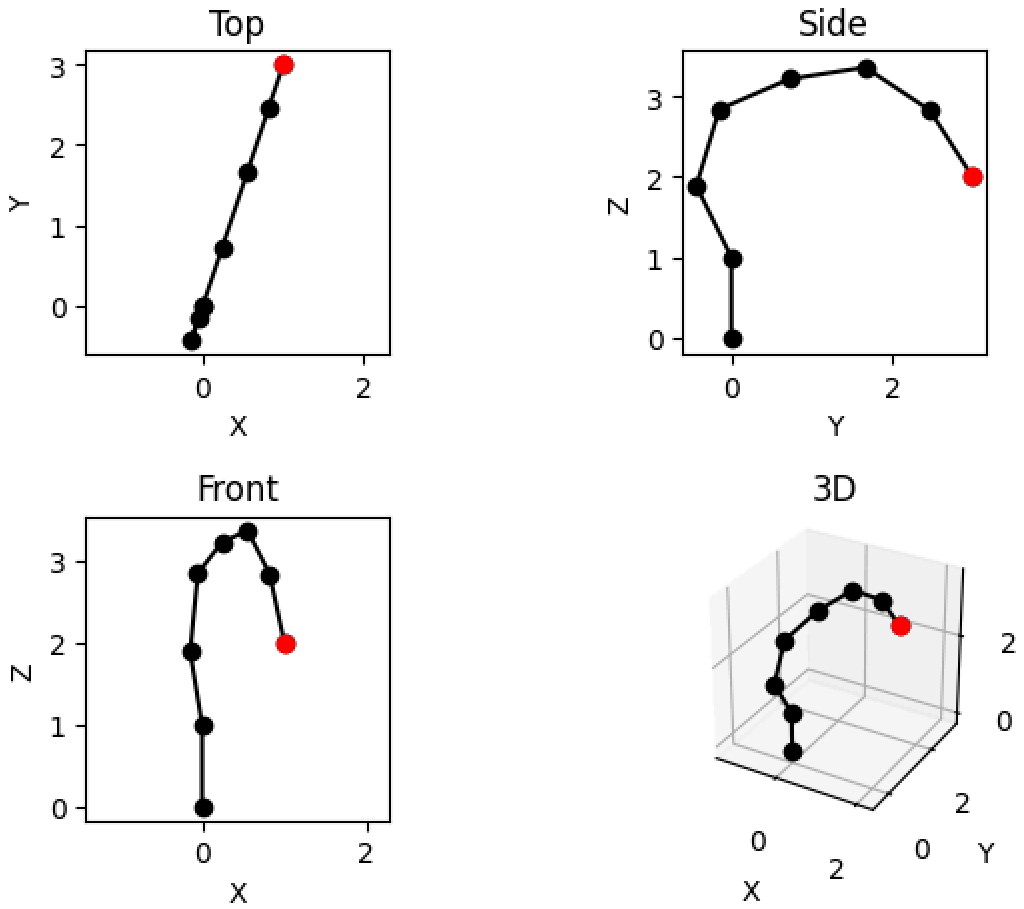
In [63]:
```python
predictions=best_de.predict(positions)
print('Best DE')
print('MAE: ',evaluate_prediction(positions,predictions))
for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

```
Best DE
MAE:  0.006
```



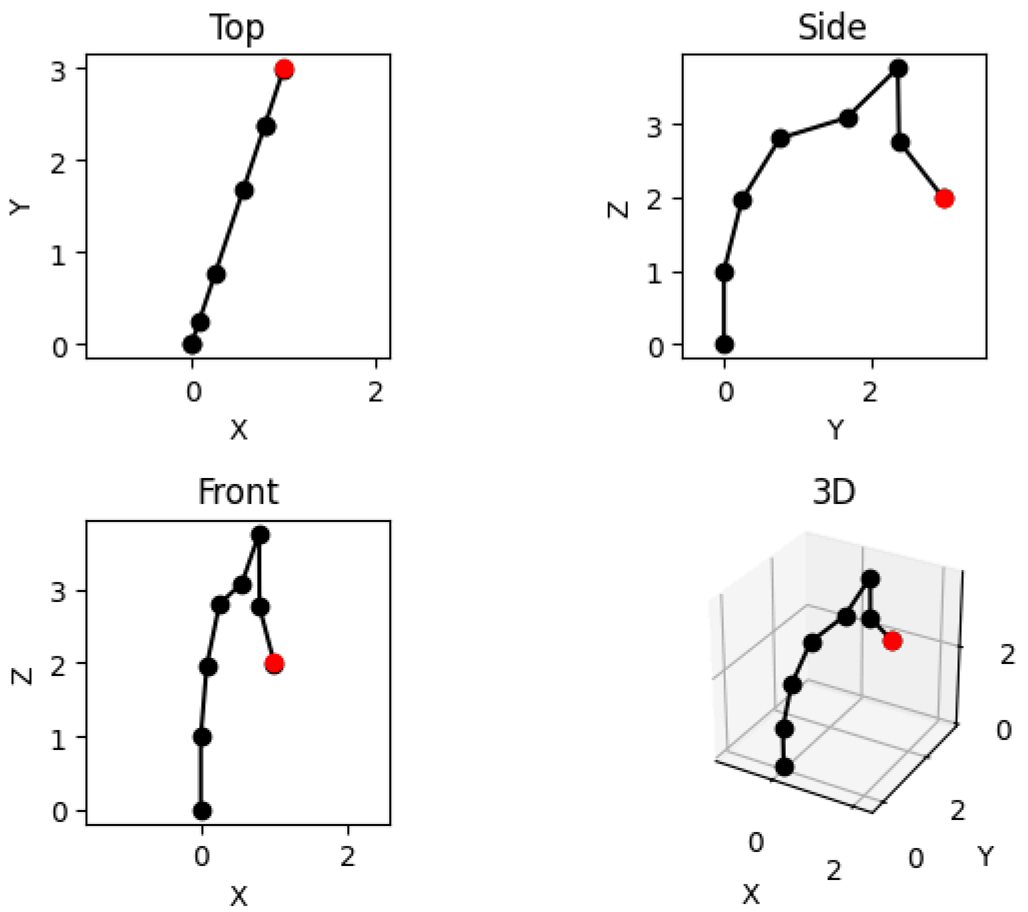
In [64]:
```
predictions=best_pso.predict(positions)
print('Best PSO')
print('MAE: ',evaluate_prediction(positions,predictions))
for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

```
Best PSO
MAE:  0.0
```



In [65]:
```
predictions=best_sa.predict(positions)
print('Best SA')
print('MAE: ',evaluate_prediction(positions,predictions))
for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

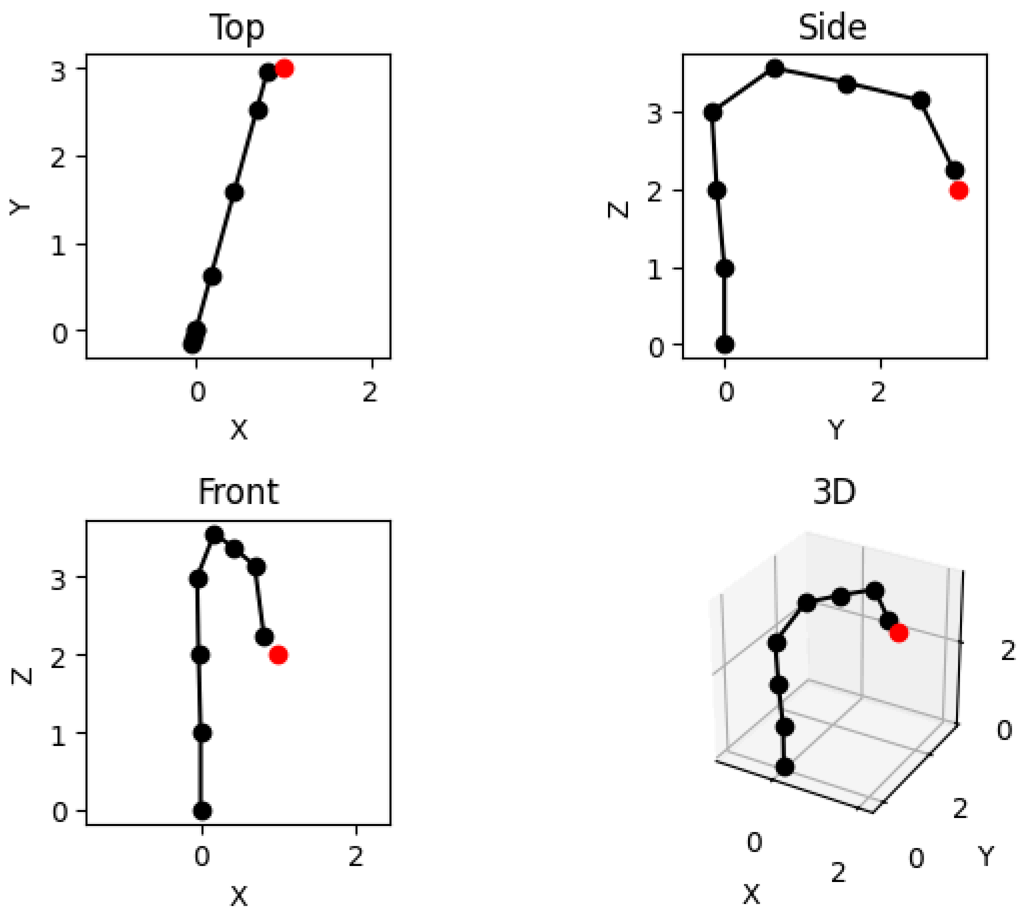
```
Best SA
MAE:  0.014
```



In [66]:

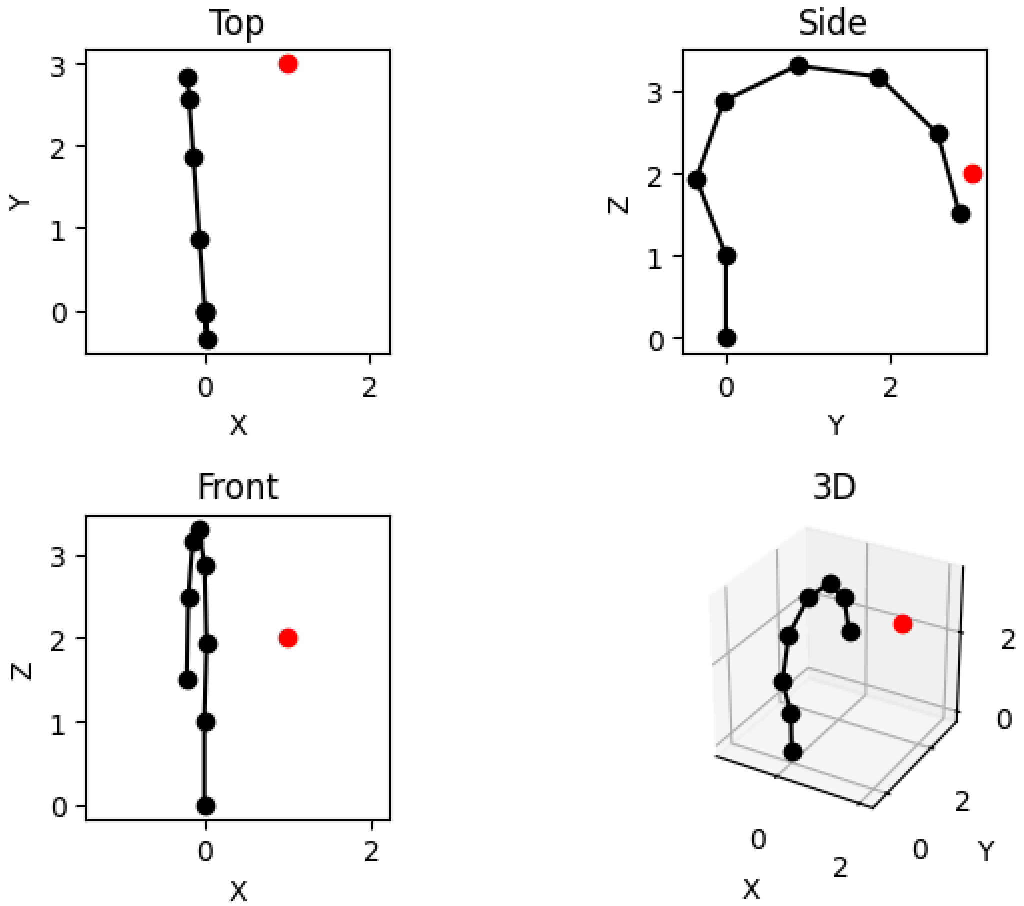
```
expanded_features=pd.DataFrame(expand_features(*positions[0,:]),index=[0])

predictions=best_tree.predict(expanded_features[best_tree_features])

print('Best DTR')
print('MAE: ',evaluate_prediction(positions,predictions))

for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

```
Best DTR
MAE:  0.315
```



In [67]:
```
expanded_features=pd.DataFrame(expand_features(*positions[0,:]),index=[0])[l

predictions=best_mlp.predict(expanded_features)

print('Best MLP')
print('MAE: ',evaluate_prediction(positions,predictions))

for prediction,position in zip(predictions,positions):
    plot_robot(prediction,position)
```

```
Best MLP
MAE:  1.316
```


Top
Y
X
Side
Z
Y
Front
Z
X
3D
X
Y