In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm
import pandas as pd
from scipy.integrate import odeint
from scipy.integrate import solve_ivp
```

Opening predator-prey dataset

In [2]:

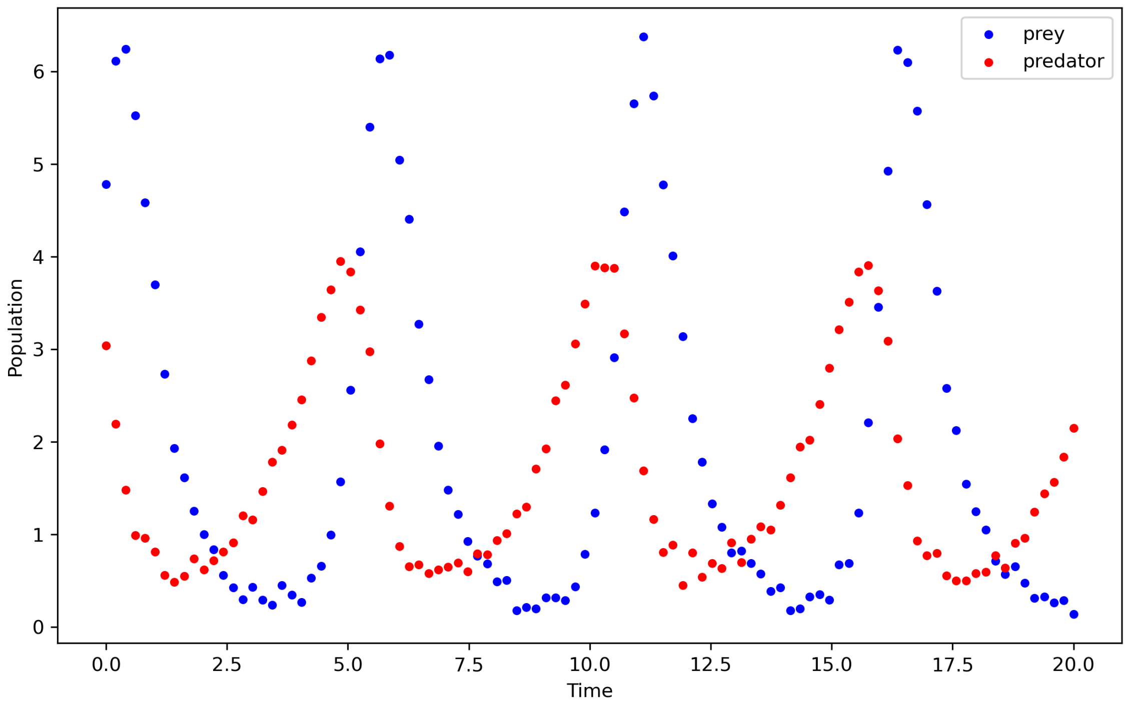
```
df = pd.read_csv('predator-prey-data.csv', index_col=False)
df.head()
```

Out[2]:

	Unnamed: 0	t	x	y
0	0	0.000000	4.781635	3.035257
1	1	0.202020	6.114005	2.189746
2	2	0.404040	6.238361	1.478907
3	3	0.606061	5.520524	0.989836
4	4	0.808081	4.582546	0.957827

In [3]:
```
# Loading data into read-only numpy arrays
data = df[['t','x','y']].values
# data[1], data[2] = data[2].copy(), data[1].copy()
data.flags.writeable = False


# Plotting
plt.figure(dpi =300, figsize=(10, 6))
point_width = 13
plt.scatter(data[:,0], data[:,1], label = 'prey', color = 'blue', s =pc
plt.scatter(data[:,0], data[:,2], label = 'predator', color = 'red', s=
plt.ylabel('Population')
plt.xlabel('Time')
plt.legend()

```

Out[3]: <matplotlib.legend.Legend at 0x13fc52f10>



Objective functions

Defining volterra equations function

In [4]:
```
def predator_prey_odes(initial_conditions,time ,alpha, beta, delta, gam
    x = initial_conditions[0]  # initial predator population
    y = initial_conditions[1]  # initial prey population
    dxdt = (alpha * x) - (beta * x * y)  # Prey ODE
    dydt = (delta * x * y) - (gamma * y)  # Predator ODE
    return [dxdt, dydt]

```

In [5]:
```
#Function that will return the data for predator and prey for a given s
def predator_prey_integration(time,initial_conditions,parameters):
    alpha,beta,delta,gamma = parameters
    results = odeint(predator_prey_odes,initial_conditions, time, args=
    predator_values,prey_values = results[:,0], results[:,1]
    return np.array([predator_values,prey_values]).T


```

Defining objective functions

In [101]:
```
def weighted_sse(actual, predicted):
    '''Weighted sum of squared erros'''

    sd = 0.01

    sd_list = sd*actual #List of estimated standard deviations

    inv_sd = 1/sd_list #List of inverted standard deviations from sd_li

    weighted_sse =  np.sum(sd_list*((actual - predicted)**2))

    #weighted_sse =

    return weighted_sse


def MAE(actual, predicted):
    '''Mean absolute error'''
    return np.mean(np.abs(actual - predicted))



def MSE(actual, predicted):
    '''Mean squared error'''
    return np.mean((actual - predicted)**2)
```

In [7]:
```
test = np.array([1,2,3])

mult = 3*test
print(mult)

sum = np.sum(mult*test)

print(sum)
```

```
[3 6 9]
42
```

Algorithms & Optimisation

Simulated Annealing

In [8]:
```
def random_walk_annealing(parameters): #A random walk designed for anne
    lst = [parameter + np.random.normal(0, 0.5) for parameter in parame
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                lst[indx] = max(0, parameters[indx] + np.random.normal(

    return lst



def simulated_annealing(initial_temp,cooling_constant, data, time, init

    temp = initial_temp #Scaling factor for random movement. We square
    start = parameters #Initial starting parameters
    x_n = start
    scores = [] #A score is just the value of the objective function ev

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est) #The current value of
    scores.append(current_score) #Keeping track of the values of the ob

    #cur = function(x) #The function value of the current x solution
    history = [x_n] #Stores previously searched x values

    for i in range (max_iterations):

        proposal = random_walk_annealing(x_n) #A new proposal for the p
        new_est = predator_prey_integration(time, initial_conditions, p
        new_score = objective(data, new_est) #Calculate new value of ob

        delta = new_score - current_score #Difference in objective func

        #if proposal < 0 or proposal > 1:
           #proposal = x_n # Reject proposal by setting it equal to pre

        acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate

        #if delta < 0:
           #x_n = proposal ##Accept proposal
            #current_score = new_score

        if np.random.rand() < acceptance_probability: #else if it is no
            x_n = proposal #Accept proposal
            current_score = new_score

        scores.append(current_score)
        temp = cooling_constant**i * initial_temp #Cool temperature
        #print(temp)
        history.append(x_n) #Add to history

    return x_n, scores
```

In [90]:

```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
initial_temp = 20
cooling_constant = 0.10

# Using MSE
x_best, scores = simulated_annealing(initial_temp,cooling_constant, inp
```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

In [184]:

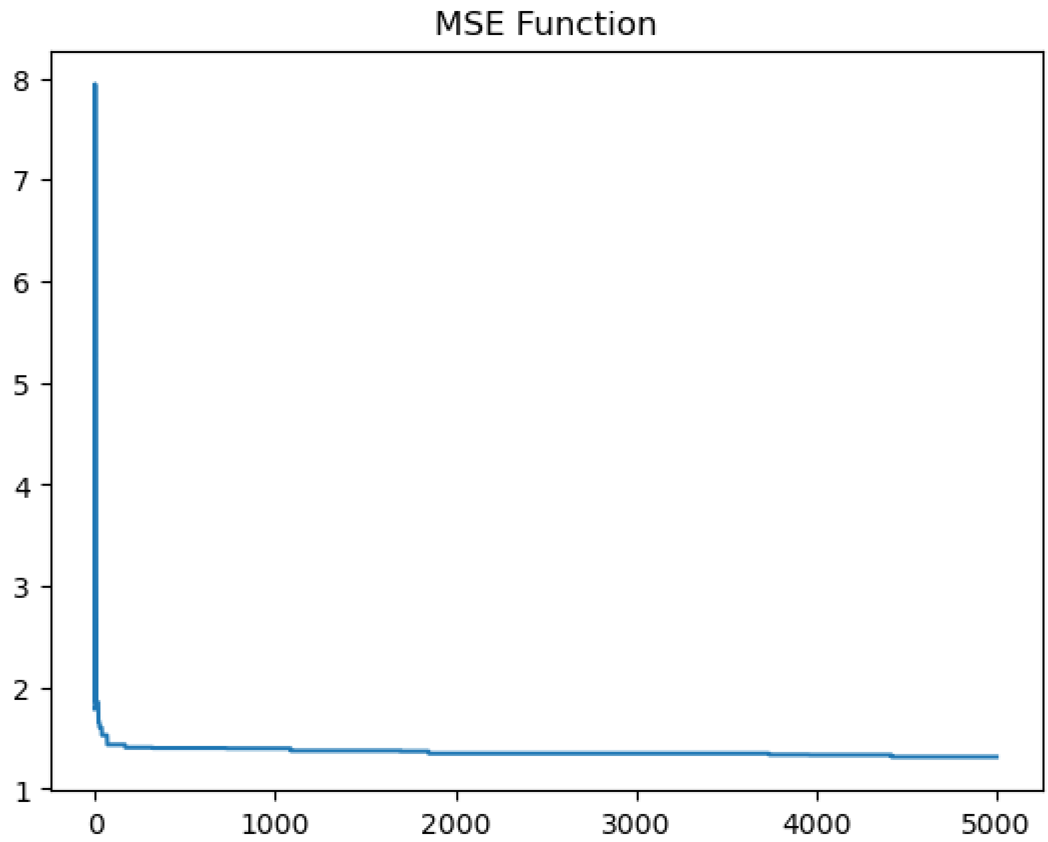
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
initial_temp = 20
cooling_constant = 0.10

# Using MSE
x_best, scores = simulated_annealing(initial_temp,cooling_constant, inp
```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

Solution discovery over iterations

In [185]:
```python
xvalues = [x for x in range(0,len(scores))]



plt.plot(xvalues,scores)
plt.title("MSE Function")

print("LOWEST MSE: " + str(scores[-1]))
```

```
LOWEST MSE: 1.3145243092280952
```

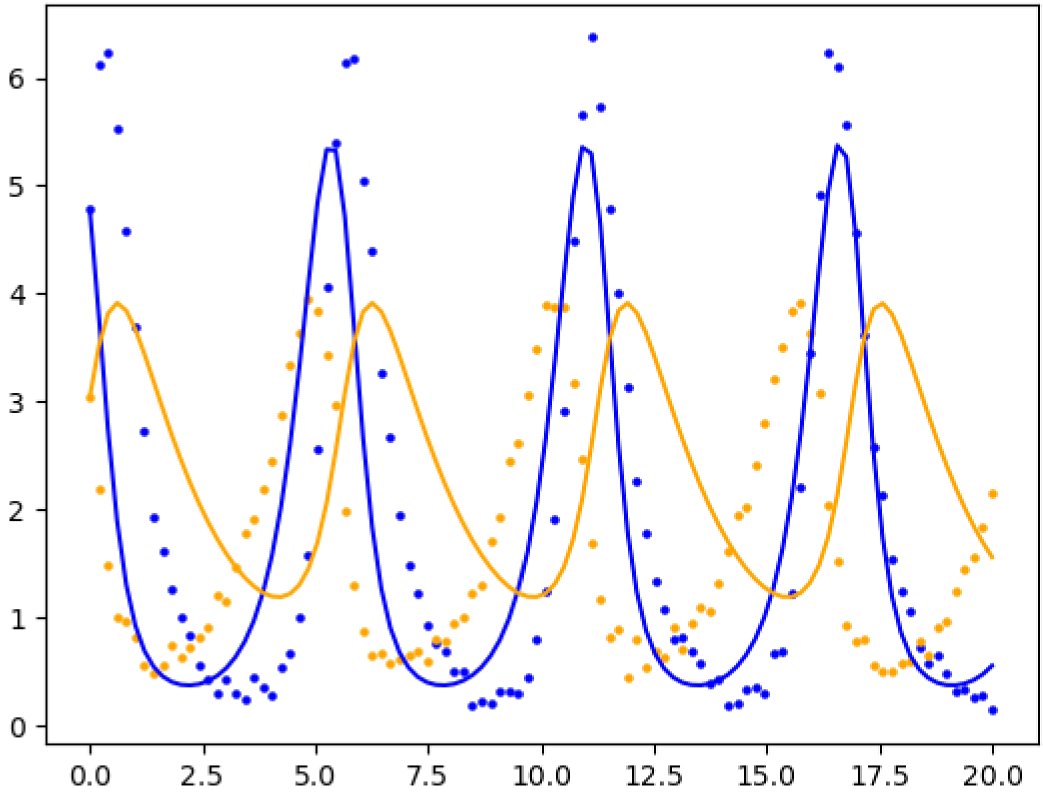


Curve fit

In [186]:

```
# t, x ,y = data
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
scaling = 2

parameters = x_best

# Using MSE
x = predator_prey_integration(t,initial_conditions,parameters)

#plt.figure(dpi =300, figsize=(6, 5))
point_width = 13
plt.plot(t, x[:,0],color = "b")
plt.plot(t, x[:,1],color = "orange")

plt.scatter(t, data[:,1], color= 'blue', s = 5)
plt.scatter(t, data[:,2], color= 'orange', s = 5)

#mse_prey = MSE(data[:,1],x[:,0]) #MSE for fitted curve
#mse_predator = MSE(data[:,2],x[:,1])
#mse_total = mse_prey + mse_predator
print("MAE: " +str(scores[-1]))
```

```
MAE: 1.3145243092280952
```



Calculation of mean and variance

In [96]:
```
### Distribution of parameters for multiple runs

def multiple_runs_annealing(initial_temp,cooling_constant,input_data,t,

    mse_total_list = []


    for i in range(n_runs):

        x_best, scores = simulated_annealing(initial_temp,cooling_const

        mse = scores[-1]

        mse_total_list.append(mse) #Add total MSE for this simulation t

    return mse_total_list

```

In [106]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20
cooling_constant = 0.10

mse_total_list = multiple_runs_annealing(initial_temp,cooling_constant,

#print(mse_total_list)
```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_58892/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_58892/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_58892/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/Users/alex_1/anaconda3/lib/python3.11/site-packages/scipy/integrate/_odep
ack_py.py:248: ODEintWarning: Excess work done on this call (perhaps wrong
Dfun type). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
```

In [107]:
```
print(mse_total_list)
```

```
[2.6473227546360665, 2.7464957827676564, 2.8201901313461293, 2.68480725254
8282, 2.6589224841462658, 2.5022908556330266, 2.4583578426621084, 2.439019
9669793287, 2.460643513633285, 2.543829159819853]
```

In [108]:
```python

mean_mse_annealing = np.mean(mse_total_list)
std_mse_annealing = np.std(mse_total_list)

print("Average MSE = " + str(mean_mse_annealing))
print("Standard deviation of MSE = " + str(std_mse_annealing))
```

```
Average MSE = 2.5961879744172007
Standard deviation of MSE = 0.12680792857239243
```

FOR WEIGHTED SSE

In [189]:
```python


input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20
cooling_constant = 0.10

mse_total_list = multiple_runs_annealing(initial_temp,cooling_constant,

```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

In [190]:
```python
print(mse_total_list)
print(np.std(mse_total_list))
```

```
[1.4283946885408745, 1.3067741402910857, 1.4442398586927112, 1.28940092054
71197, 1.4204590248705167, 1.4440930616053458, 1.3031423818937582, 1.35896
96758657763, 1.3465599587990993, 1.3043258816810026]
0.06051240976134452
```

Comparison of cooling schedules

In [221]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20

cooling_constants = np.arange(0.10,1,0.10)

mean_mse_per_simulation = [] #The mean MSE per simulation
sd_mse_per_simulation = [] #The standard deviation per simulation

for constant in cooling_constants:

    mse_total_list = multiple_runs_annealing(initial_temp,constant,inpu
    mean_mse_annealing = np.mean(mse_total_list)
    std_mse_annealing = np.std(mse_total_list)
    mean_mse_per_simulation.append(mean_mse_annealing)
    sd_mse_per_simulation.append(std_mse_annealing)
```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/Users/alex_1/anaconda3/lib/python3.11/site-packages/scipy/integrate/_odep
ack_py.py:248: ODEintWarning: Excess work done on this call (perhaps wrong
Dfun type). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

In [222]:

```
mean_mae_per_simulation = []
sd_mae_per_simulation = []

for constant in cooling_constants:

    mae_total_list = multiple_runs_annealing(initial_temp,constant,inpu
    mean_mae_annealing = np.mean(mae_total_list)
    std_mae_annealing = np.std(mae_total_list)
    mean_mae_per_simulation.append(mean_mae_annealing)
    sd_mae_per_simulation.append(std_mae_annealing)

```

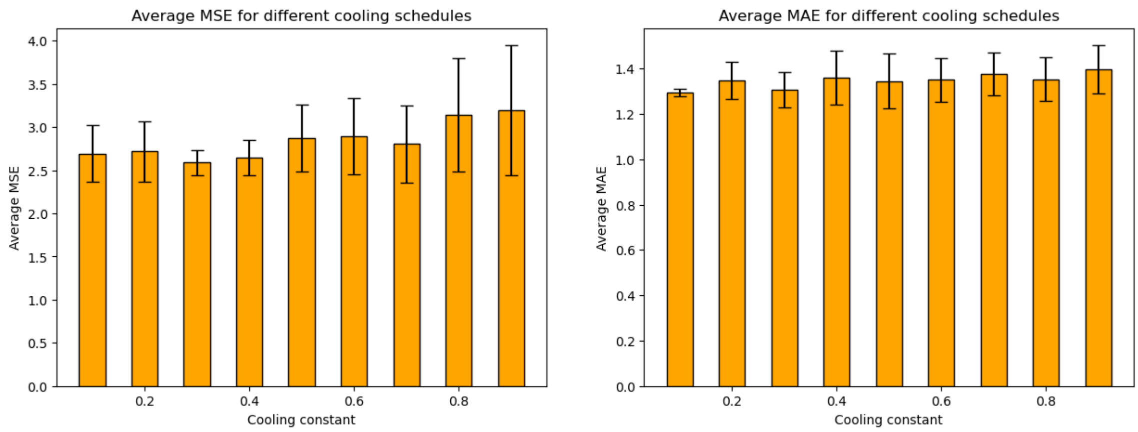
```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

In [223]:

```python

fig, axes = plt.subplots(1, 2, figsize=(15, 5))

bar_width = 0.05

axes[0].bar(cooling_constants, mean_mse_per_simulation, yerr = sd_mse_p
axes[1].bar(cooling_constants, mean_mae_per_simulation, yerr = sd_mae_p

axes[0].set_xlabel("Cooling constant")
axes[1].set_xlabel("Cooling constant")

axes[0].set_ylabel("Average MSE")
axes[1].set_ylabel("Average MAE")

axes[0].set_title("Average MSE for different cooling schedules")
axes[1].set_title("Average MAE for different cooling schedules")



#plt.bar(cooling_constants, mean_per_simulation, yerr = sd_per_simulati
#plt.ylabel("Average MSE")
#plt.xlabel("Cooling constant")
#plt.title("Average MSE for different cooling schedules (30 simulations

#plt.show()

```

Out[223]:

```
Text(0.5, 1.0, 'Average MAE for different cooling schedules')
```



Hill climbing

In [238]:
```python


def random_walk(parameters):
    lst = [parameter + np.random.normal(0, 0.5) for parameter in parame
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                lst[indx] = max(0, parameters[indx] + np.random.normal(

    return lst

def hill_climbing(data, time, initial_conditions, parameters, objective
    '''Tries to find the best solution using random walker'''
    # Initialize starting parameter state
    scores = []
    x_n = parameters

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est)
    scores.append(current_score)

    for _ in range(max_iterations):
        # Generate a random walk for parameters
        x_n_1 = random_walk(x_n)

        # Calculate the current and next estimations
        current_est = predator_prey_integration(time, initial_conditior
        new_estimation = predator_prey_integration(time, initial_condit
        new_score = objective(data, new_estimation)

        # If the next estimation is better, update the parameters
        if new_score < current_score:
            current_score = new_score
            x_n = x_n_1
            scores.append(current_score)

    return x_n, scores

```

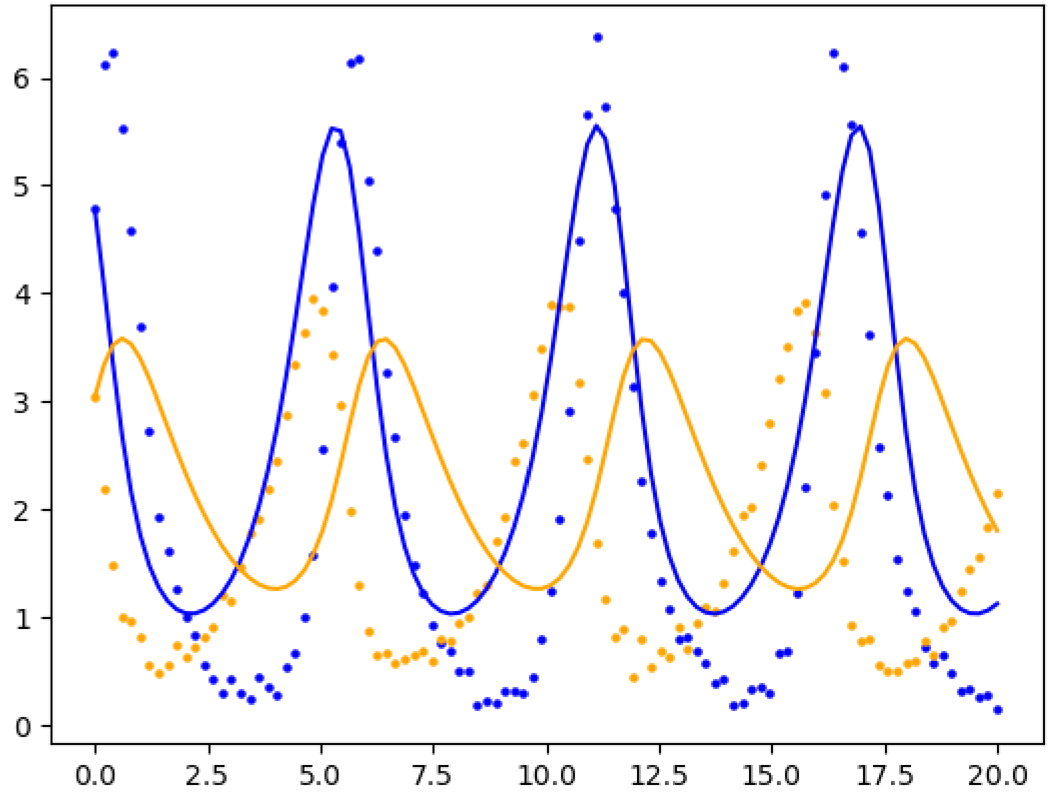
In [239]:
```python
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]

# Using MSE
x_best,scores = hill_climbing(input_data, t, input_data[0], parameters,
```

Curve fit

In [241]:

```
# t, x ,y = data
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

parameters = x_best

# Using MSE
x = predator_prey_integration(t,initial_conditions,parameters)



point_width = 13
plt.plot(t, x[:,0],color = "b")
plt.plot(t, x[:,1],color = "orange")

plt.scatter(t, data[:,1], color= 'blue', s = 5)
plt.scatter(t, data[:,2], color= 'orange', s = 5)

mse_prey = MSE(data[:,1],x[:,0]) #MSE for fitted curve
mse_predator = MSE(data[:,2],x[:,1])
mse_total = mse_prey + mse_predator
print("Mean Square Error: " +str(mse_total))

```

```
Mean Square Error: 5.385424572357688
```



In [195]:
```
def multiple_runs_hill_climbing(input_data, t, initial_conditions, para

    mse_total_list = []

    for i in range(n_runs):

        x_best = hill_climbing(input_data, t, input_data[0], parameters

        x = predator_prey_integration(t,initial_conditions,x_best)

        mse_prey = MSE(data[:,1],x[:,0])
        mse_predator = MSE(data[:,2],x[:,1])
        mse_total = mse_prey + mse_predator

        mse_total_list.append(mse_total) #Add total MSE for this simula

    return mse_total_list

```

In [32]:
```
mean_mse_hill_climbing = np.mean(mse_total_list)
std_mse_hill_climbing = np.std(mse_total_list)

print("Average MSE = " + str(mean_mse_hill_climbing))
print("Standard deviation of MSE = " + str(std_mse_hill_climbing))
```

```
Average MSE = 7.020538795747848
Standard deviation of MSE = 0.525718488225756
```

Comparison of Optimisation Algorithms

MSE objecive function

In [228]:

```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20
cooling_constant = 0.10

mse_total_list_annealing = multiple_runs_annealing(initial_temp,cooling
mean_mse_annealing = np.mean(mse_total_list_annealing)
std_mse_annealing = np.std(mse_total_list_annealing)

```

```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/Users/alex_1/anaconda3/lib/python3.11/site-packages/scipy/integrate/_odep
ack_py.py:248: ODEintWarning: Excess work done on this call (perhaps wrong
Dfun type). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
```

In [229]:

```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]


mse_total_list_hill = multiple_runs_hill_climbing(input_data, t, initia
mean_mse_hill_climbing = np.mean(mse_total_list_hill)
std_mse_hill_climbing = np.std(mse_total_list_hill)
```

MAE objective function

In [230]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20
cooling_constant = 0.10

mae_total_list_annealing = multiple_runs_annealing(initial_temp,cooling
mean_mae_annealing = np.mean(mae_total_list_annealing)
std_mae_annealing = np.std(mae_total_list_annealing)
```

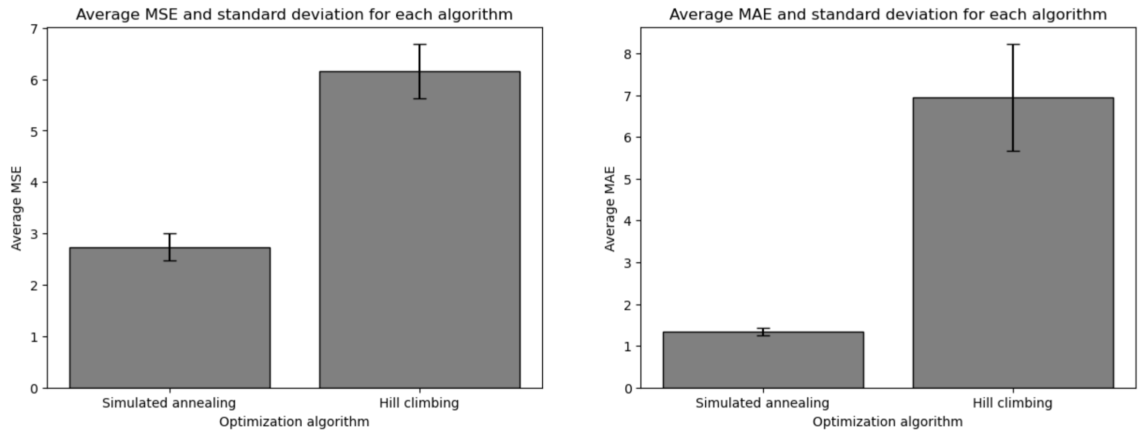
```
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
/var/folders/rc/tn2ys5g55157vhhlmn0_vfwr0000gq/T/ipykernel_70535/385309489
9.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

In [231]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]


mae_total_list_hill = multiple_runs_hill_climbing(input_data, t, initia
mean_mae_hill_climbing = np.mean(mae_total_list_hill)
std_mae_hill_climbing = np.std(mae_total_list_hill)
```

In [237]:

```
##PLOTTING

fig, axes = plt.subplots(1, 2, figsize=(15, 5))


x = ["Simulated annealing", "Hill climbing"]
mse_list = [mean_mse_annealing,mean_mse_hill_climbing] #Stores the mean
std_mse_list = [std_mse_annealing,std_mse_hill_climbing]

mae_list = [mean_mae_annealing,mean_mae_hill_climbing] #Stores the mean
std_mae_list = [std_mae_annealing,std_mae_hill_climbing]

axes[0].bar(x, mse_list, yerr = std_mse_list,color = "grey",ec = "black
axes[1].bar(x, mae_list, yerr = std_mae_list,color = "grey",ec = "black



axes[0].set_xlabel("Optimization algorithm")
axes[1].set_xlabel("Optimization algorithm")

axes[0].set_ylabel("Average MSE")
axes[1].set_ylabel("Average MAE")

axes[0].set_title("Average MSE and standard deviation for each algorith
axes[1].set_title("Average MAE and standard deviation for each algorith



#plt.bar(x, mse_list, yerr = std_list,color = "grey",ec = "black", ecol
#plt.title("Bar plot comparing the means and errors of the MSE")
#plt.ylabel("MSE")
#plt.xlabel("Optimization algorithm")
```

Out[237]: Text(0.5, 1.0, 'Average MAE and standard deviation for each algorithm')



In [ ]:

```

```

In [ ]:

```

```

In [3]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm
import pandas as pd
from scipy.integrate import odeint
from scipy.integrate import solve_ivp
import statistics
import random
import scipy.stats
```

Opening predator-prey dataset

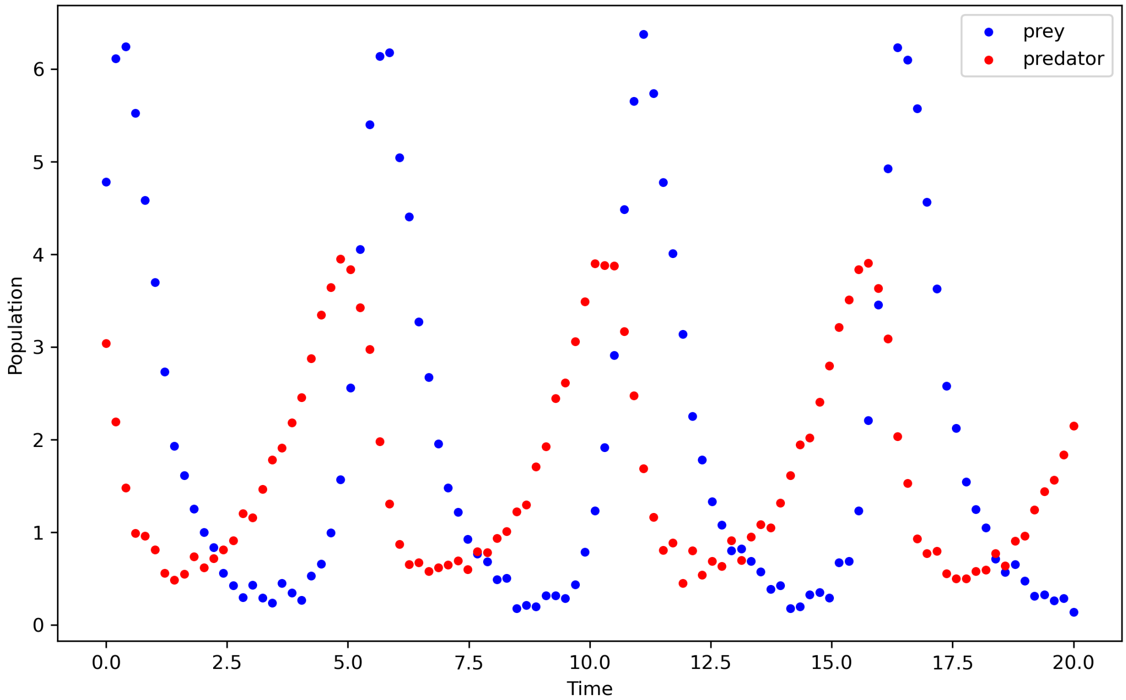
In [4]:
```
df = pd.read_csv('predator-prey-data.csv', index_col=False)
df.head()

```

Out[4]:

	Unnamed: 0	t	x	y
0	0	0.000000	4.781635	3.035257
1	1	0.202020	6.114005	2.189746
2	2	0.404040	6.238361	1.478907
3	3	0.606061	5.520524	0.989836
4	4	0.808081	4.582546	0.957827

In [5]:
```
# Loading data into read-only numpy arrays
data = df[['t','x','y']].values
# data[1], data[2] = data[2].copy(), data[1].copy()
data.flags.writeable = False


# Plotting
plt.figure(dpi =300, figsize=(10, 6))
point_width = 13
plt.scatter(data[:,0], data[:,1], label = 'prey', color = 'blue', s =pc
plt.scatter(data[:,0], data[:,2], label = 'predator', color = 'red', s=
plt.ylabel('Population')
plt.xlabel('Time')
plt.legend()

```

Out[5]:
```
<matplotlib.legend.Legend at 0x1108369be50>
```



Objective functions

Defining volterra equations function

In [6]:
```
def predator_prey_odes(initial_conditions,time ,alpha, beta, delta, gan
    x = initial_conditions[0]  # initial predator population
    y = initial_conditions[1]  # initial prey population
    dxdt = (alpha * x) - (beta * x * y)  # Prey ODE
    dydt = (delta * x * y) - (gamma * y)  # Predator ODE
    return [dxdt, dydt]

```

In [7]:
```
#Function that will return the data for predator and prey for a given s
def predator_prey_integration(time,initial_conditions,parameters):
    alpha,beta,delta,gamma = parameters
    results = odeint(predator_prey_odes,initial_conditions, time, args=
    predator_values,prey_values = results[:,0], results[:,1]
    return np.array([predator_values,prey_values]).T


```

Defining objective functions

In [8]:
```
def negative_log_likelihood(actual, predicted, variance=1.0):
    '''Log likelyhood function'''
    # Assuming a normal distribution for simplicity
    log_likelihoods1 =norm.logpdf(actual[0], loc=predicted[0], scale=np
    log_likelihoods2 = norm.logpdf(actual[1], loc=predicted[1], scale=n

    return -np.sum((log_likelihoods1,log_likelihoods2))

def MSE(actual, predicted):
    '''Mean squared error'''
    return np.mean((actual - predicted)**2)
```

Algorithms & Optimisation

Simulated Annealing

In [9]:

```
def random_walk_annealing(parameters): #A random walk designed for anne
    lst = [parameter + np.random.normal(0, 0.5) for parameter in parame
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                lst[indx] = max(0, parameters[indx] + np.random.normal(

    return lst



def simulated_annealing(initial_temp,cooling_constant, data, time, init

    temp = initial_temp #Scaling factor for random movement. We square
    start = parameters #Initial starting parameters
    x_n = start
    scores = [] #A score is just the value of the objective function ev

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est) #The current value of
    scores.append(current_score) #Keeping track of the values of the ob

    #cur = function(x) #The function value of the current x solution
    history = [x_n] #Stores previously searched x values

    for i in range (max_iterations):

        proposal = random_walk_annealing(x_n) #A new proposal for the p
        new_est = predator_prey_integration(time, initial_conditions, p
        new_score = objective(data, new_est) #Calculate new value of ob

        delta = new_score - current_score #Difference in objective func

        #if proposal < 0 or proposal > 1:
           #proposal = x_n # Reject proposal by setting it equal to pre

        acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate

        #if delta < 0:
           #x_n = proposal ##Accept proposal
            #current_score = new_score

        if np.random.rand() < acceptance_probability: #else if it is no
            x_n = proposal #Accept proposal
            current_score = new_score

        scores.append(current_score)
        temp = cooling_constant**i * initial_temp #Cool temperature
        #print(temp)
        history.append(x_n) #Add to history

    return x_n, scores
```

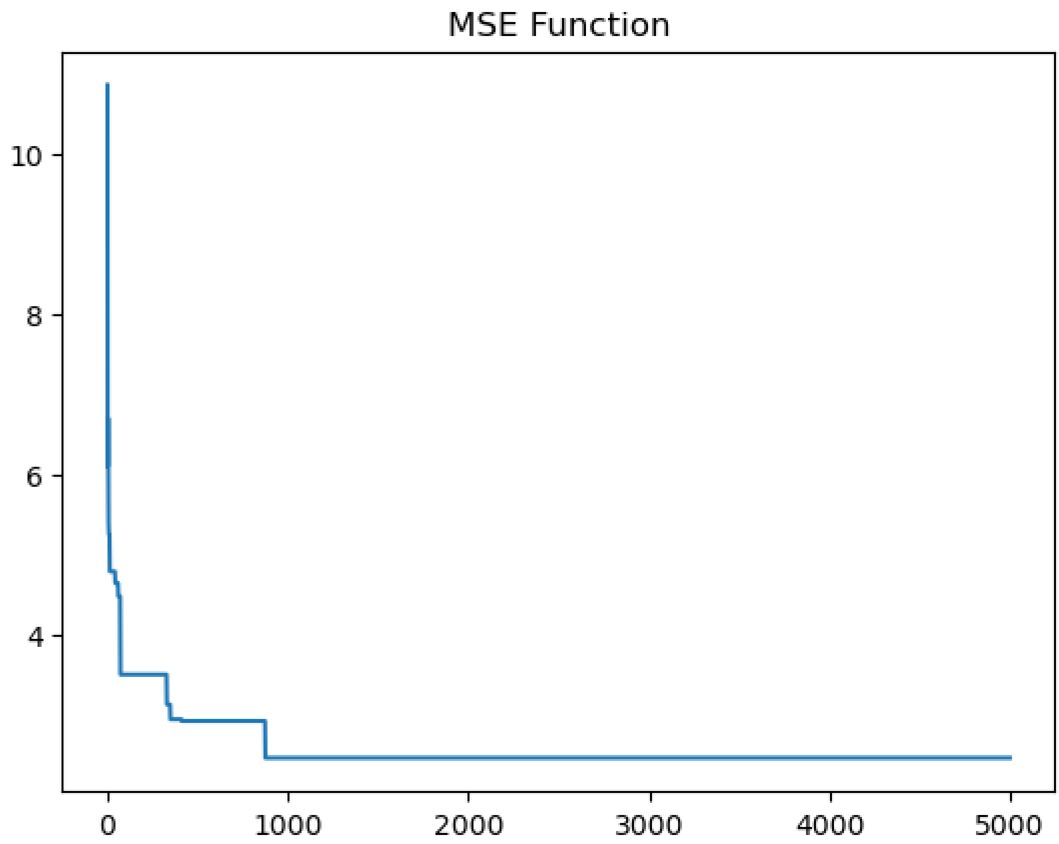
In [8]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
initial_temp = 20
cooling_constant = 0.10

# Using MSE
x_best, scores = simulated_annealing(initial_temp,cooling_constant, inp
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

Solution discovery over iterations

In [9]:
```
xvalues = [x for x in range(0,len(scores))]



plt.plot(xvalues,scores)
plt.title("MSE Function")

print("LOWEST MSE: " + str(scores[-1]))
```

```
LOWEST MSE: 2.4498445634217485
```

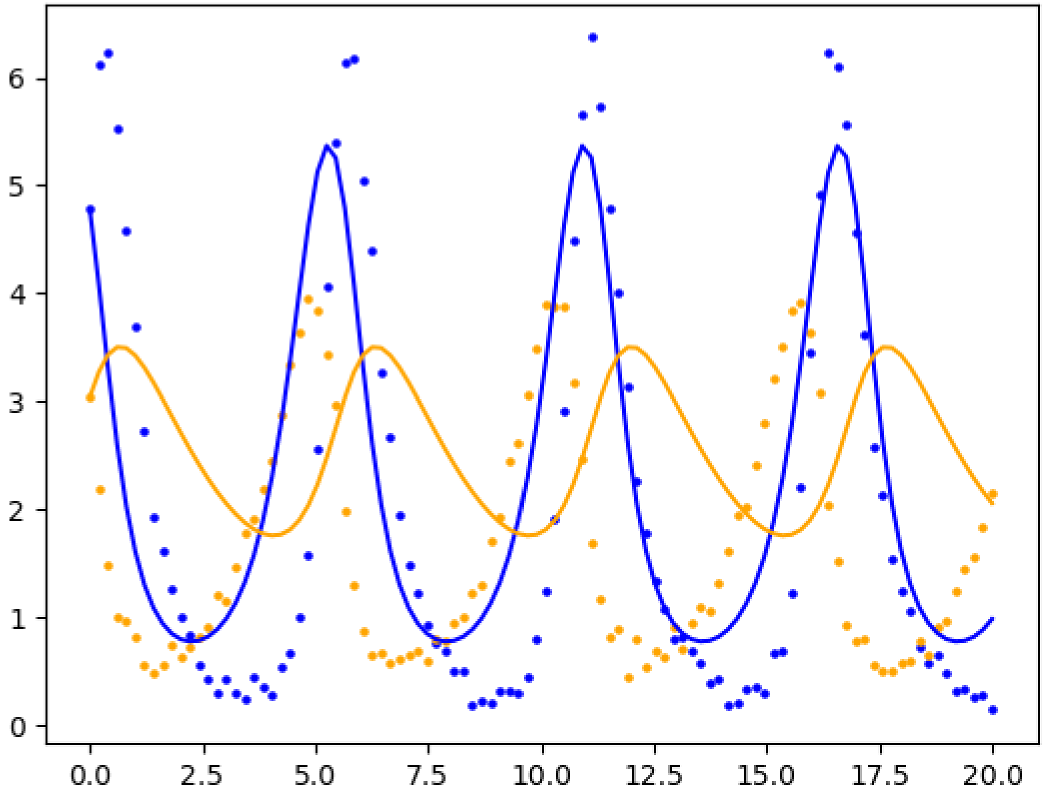


Curve fit

In [10]:

```
# t, x ,y = data
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
scaling = 2

parameters = x_best

# Using MSE
x = predator_prey_integration(t,initial_conditions,parameters)

#plt.figure(dpi =300, figsize=(6, 5))
point_width = 13
plt.plot(t, x[:,0],color = "b")
plt.plot(t, x[:,1],color = "orange")

plt.scatter(t, data[:,1], color= 'blue', s = 5)
plt.scatter(t, data[:,2], color= 'orange', s = 5)

mse_prey = MSE(data[:,1],x[:,0]) #MSE for fitted curve
mse_predator = MSE(data[:,2],x[:,1])
mse_total = mse_prey + mse_predator
print("Mean Square Error: " +str(mse_total))
```

```
Mean Square Error: 4.899689126843497
```



Calculation of mean and variance

In [10]:

```
### Distribution of parameters for multiple runs

def multiple_runs_annealing(initial_temp,cooling_constant,input_data,t,

    mse_total_list = []


    for i in range(n_runs):

        x_best, scores = simulated_annealing(initial_temp,cooling_const

        x = predator_prey_integration(t,initial_conditions,x_best)
        mse_prey = MSE(data[:,1],x[:,0])
        mse_predator = MSE(data[:,2],x[:,1])
        mse_total = mse_prey + mse_predator

        mse_total_list.append(mse_total) #Add total MSE for this simula

    return mse_total_list

```

In [12]:

```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20
cooling_constant = 0.10

mse_total_list = multiple_runs_annealing(initial_temp,cooling_constant,

#print(mse_total_list)
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\anaconda3\Lib\site-packages\scipy\integrate\_odepack_py.py:
248: ODEintWarning: Excess work done on this call (perhaps wrong Dfun typ
e). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
```

In [13]:

```

mean_mse_annealing = np.mean(mse_total_list)
std_mse_annealing = np.std(mse_total_list)

print("Average MSE = " + str(mean_mse_annealing))
print("Standard deviation of MSE = " + str(std_mse_annealing))
```

```
Average MSE = 5.337976129896431
Standard deviation of MSE = 0.7116981017582293
```

Comparison of cooling schedules

In [11]:

```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

initial_temp = 20

cooling_constants = np.arange(0.10,1,0.10)

mean_and_sd_per_simulation = []

for constant in cooling_constants:
    print(constant)
    mse_total_list = multiple_runs_annealing(initial_temp,constant,inpu
    mean_mse_annealing = np.mean(mse_total_list)
    std_mse_annealing = np.std(mse_total_list)
    mean_and_sd_per_simulation.append([(mean_mse_annealing,std_mse_anne


```

```
0.1

C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Excess work done on this call (perhaps w
rong Dfun type). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
```

```
---------------------------------------------------------------------------
-
KeyboardInterrupt                         Traceback (most recent call las
t)
Cell In[11], line 20
     18 for constant in cooling_constants:
     19     print(constant)
---> 20     mse_total_list = multiple_runs_annealing(initial_temp,constan
t,input_data,t,parameters,MSE,10)
     21     mean_mse_annealing = np.mean(mse_total_list)
     22     std_mse_annealing = np.std(mse_total_list)

Cell In[10], line 10, in multiple_runs_annealing(initial_temp, cooling_con
stant, input_data, t, parameters, objective_function, n_runs)
      5 mse_total_list = []
      8 for i in range(n_runs):
---> 10     x_best, scores = simulated_annealing(initial_temp,cooling_cons
tant, input_data, t, input_data[0], parameters, objective_function, max_it
erations=5000)
     12     x = predator_prey_integration(t,initial_conditions,x_best)
     13     mse_prey = MSE(data[:,1],x[:,0])

Cell In[9], line 30, in simulated_annealing(initial_temp, cooling_constan
t, data, time, initial_conditions, parameters, objective, max_iterations)
     27 for i in range (max_iterations):
     29     proposal = random_walk_annealing(x_n) #A new proposal for the
parameters is generated by taking a random walk scaled by the scale
---> 30     new_est = predator_prey_integration(time, initial_conditions,
proposal) #Calculate new function values based on proposal parameters
     31     new_score = objective(data, new_est) #Calculate new value of o
bjective function based on new function values
     33     delta = new_score - current_score #Difference in objective fun
ction values

Cell In[7], line 4, in predator_prey_integration(time, initial_conditions,
parameters)
      2 def predator_prey_integration(time,initial_conditions,parameters):
      3     alpha,beta,delta,gamma = parameters
----> 4     results = odeint(predator_prey_odes,initial_conditions, time,
args=(alpha,beta,delta,gamma))
      5     predator_values,prey_values = results[:,0], results[:,1]
      6     return np.array([predator_values,prey_values]).T

File ~\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_odepack_
py.py:241, in odeint(func, y0, t, args, Dfun, col_deriv, full_output, ml,
mu, rtol, atol, tcrit, h0, hmax, hmin, ixpr, mxstep, mxhnil, mxordn, mxord
s, printmessg, tfirst)
    236     raise ValueError("The values in t must be monotonically increa
sing "
    237                      "or monotonically decreasing; repeated values
are "
    238                      "allowed.")
    240 t = copy(t)
--> 241 y0 = copy(y0)
    242 output = _odepack.odeint(func, y0, t, args, Dfun, col_deriv, ml, m
u,
    243                          full_output, rtol, atol, tcrit, h0, hmax,
hmin,
    244                          ixpr, mxstep, mxhnil, mxordn, mxords,
    245                          int(bool(tfirst)))
    246 if output[-1] < 0:
```

```
File ~\AppData\Local\anaconda3\Lib\copy.py:84, in copy(x)
     82 copier = getattr(cls, "__copy__", None)
     83 if copier is not None:
---> 84     return copier(x)
     86 reductor = dispatch_table.get(cls)
     87 if reductor is not None:

KeyboardInterrupt:
```

In [12]:

```
print(mean_and_sd_per_simulation)

plt.bar()
```

```
[]

---------------------------------------------------------------------------
-
TypeError                                 Traceback (most recent call las
t)
Cell In[12], line 3
      1 print(mean_and_sd_per_simulation)
----> 3 plt.bar()

TypeError: bar() missing 2 required positional arguments: 'x' and 'height'
```

Hill climbing

In [13]:

```


def random_walk(parameters):
    lst = [parameter + np.random.normal(0, 1) for parameter in paramete
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                lst[indx] = max(0, parameters[indx] + np.random.normal(

    return lst

def hill_climbing(initial_temp,cooling_constant, data, time, initial_cc
    '''Tries to find the best solution using random walker'''
    # Initialize starting parameter state
    scores = []
    x_n = parameters

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est)
    scores.append(current_score)

    for _ in range(max_iterations):
        # Generate a random walk for parameters
        x_n_1 = random_walk(x_n)

        # Calculate the current and next estimations
        current_est = predator_prey_integration(time, initial_conditior
        new_estimation = predator_prey_integration(time, initial_condit
        new_score = objective(data, new_estimation)

        # If the next estimation is better, update the parameters
        if new_score < current_score:
            current_score = new_score
            x_n = x_n_1
            scores.append(current_score)

    return [x_n, scores]

```

In [35]:

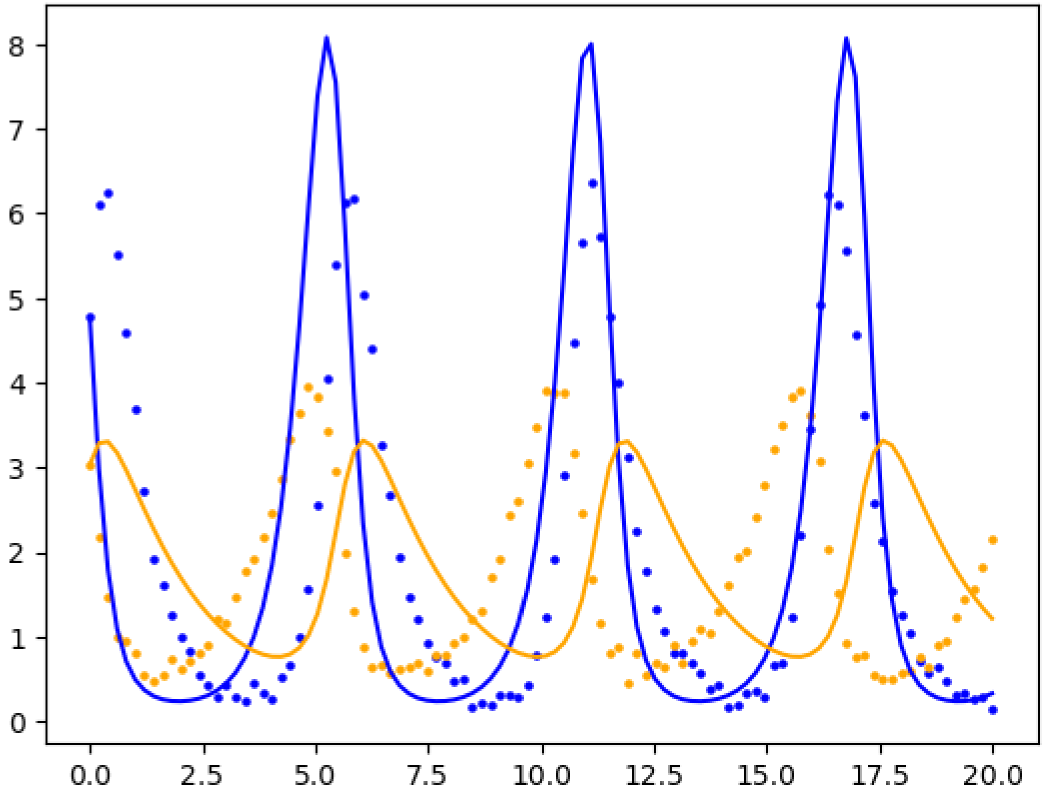
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]

# Using MSE
x_best = hill_climbing(initial_temp,cooling_constant, input_data, t, ir

```

Curve fit

In [17]:

```
# t, x ,y = data
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

parameters = x_best

# Using MSE
x = predator_prey_integration(t,initial_conditions,parameters)

point_width = 13
plt.plot(t, x[:,0],color = "b")
plt.plot(t, x[:,1],color = "orange")

plt.scatter(t, data[:,1], color= 'blue', s = 5)
plt.scatter(t, data[:,2], color= 'orange', s = 5)

mse_prey = MSE(data[:,1],x[:,0]) #MSE for fitted curve
mse_predator = MSE(data[:,2],x[:,1])
mse_total = mse_prey + mse_predator
print("Mean Square Error: " +str(mse_total))

```

```
Mean Square Error: 6.016318958977161
```



In [36]:
```
def multiple_runs_hill_climbing(initial_temp,cooling_constant, input_da

    mse_total_list = []

    for i in range(n_runs):

        x_best = hill_climbing(initial_temp,cooling_constant, input_dat

        x = predator_prey_integration(t,initial_conditions,x_best)

        mse_prey = MSE(data[:,1],x[:,0])
        mse_predator = MSE(data[:,2],x[:,1])
        mse_total = mse_prey + mse_predator

        mse_total_list.append(mse_total) #Add total MSE for this simula

    return mse_total_list

```

In [37]:
```
input_data = data[:,1:3]
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]


mse_total_list = multiple_runs_hill_climbing(initial_temp,cooling_const
```

In [20]:
```
mean_mse_hill_climbing = np.mean(mse_total_list)
std_mse_hill_climbing = np.std(mse_total_list)

print("Average MSE = " + str(mean_mse_hill_climbing))
print("Standard deviation of MSE = " + str(std_mse_hill_climbing))
```

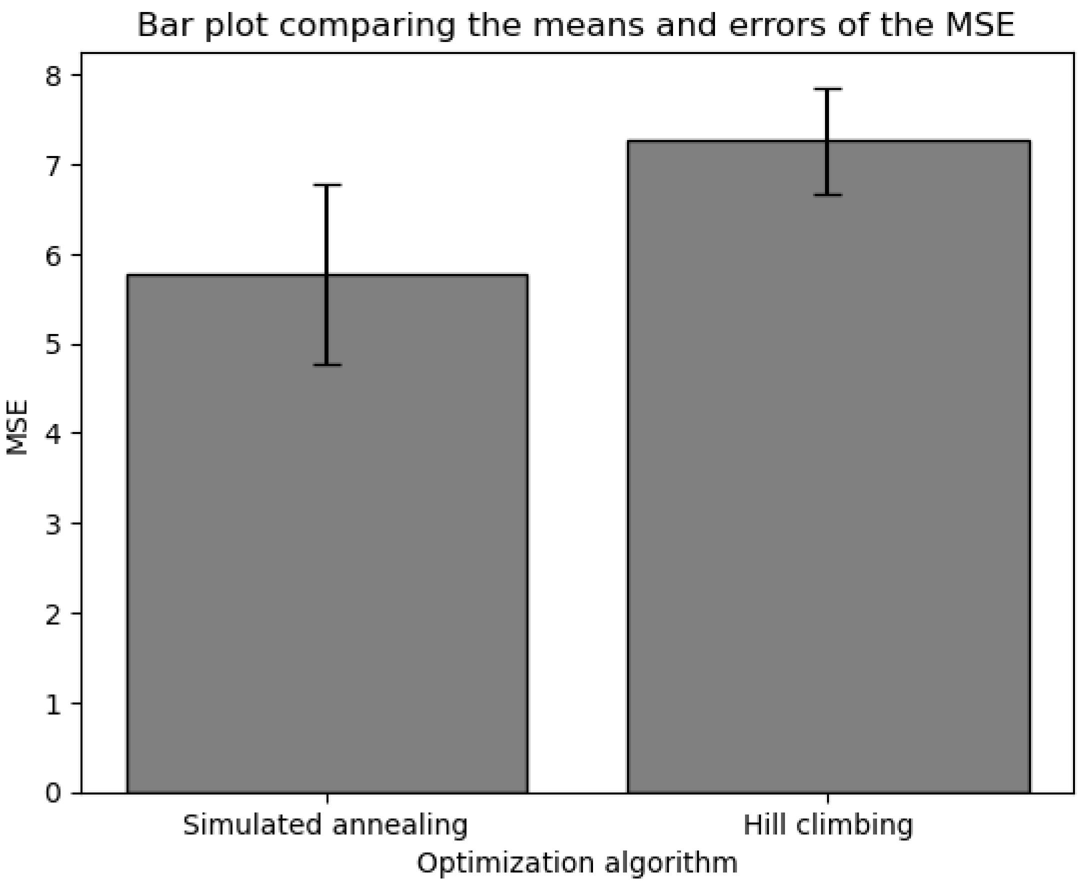
```
Average MSE = 7.258042040055488
Standard deviation of MSE = 0.5962174191554426
```

Comparison of Optimisation Algorithms

MSE objecive function

In [21]:
```
x = ["Simulated annealing", "Hill climbing"]
mse_list = [mean_mse_annealing,mean_mse_hill_climbing] #Stores the mear
std_list = [std_mse_annealing,std_mse_hill_climbing]

plt.bar(x, mse_list, yerr = std_list,color = "grey",ec = "black", ecolc
plt.title("Bar plot comparing the means and errors of the MSE")
plt.ylabel("MSE")
plt.xlabel("Optimization algorithm")
```

Out[21]:
```
Text(0.5, 0, 'Optimization algorithm')
```



In [48]:
```

good= data[:,1:3]
bad = np.zeros_like(good)

print(negative_log_likelihood(x,good))
print()
print(negative_log_likelihood(x,bad))
```

Reverse engineering with removal of points targeted

In [18]:
```
def MSE2(actual, predicted):
    '''Mean squared error'''
    x1 = actual[:, 0]
    y1 = actual[:, 1]

    #Getting useful indexes
    indx_x = np.where(~np.isnan(x1))
    indx_y = np.where(~np.isnan(y1))

    x2, y2 = predicted[:, 0], predicted[:, 1]
    err1 = (x1[indx_x] - x2[indx_x])**2
    err2 = (y1[indx_y] - y2[indx_y])**2
    err = np.concatenate([err1, err2])

    return np.nanmean([err])

def MAE(actual, predicted):
    '''Mean absolute error'''
    return np.mean(np.abs(actual - predicted))

def MAE2(actual, predicted):
    x1 = actual[0]
    y1 = actual[1]

    #Getting useful indexes
    indx_x = np.where(~np.isnan(x1))
    indx_y = np.where(~np.isnan(y1))

    x2, y2 = predicted[:, 0], predicted[:, 1]
    err1 = abs(x1[indx_x] - x2[indx_x])
    err2 = abs(y1[indx_y] - y2[indx_y])
    err = np.concatenate([err1, err2])
    err = np.concatenate([err1, err2])

    return np.nanmean([err])


def point_removal(time, input_data, points_removed, Focus = 0):
    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # initialize set up for removing points randomly given the bounds
    removal_options = np.arange(0,len(time))

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(removal_options, k = points

    # remove points based on choices for points to be removed
    if Focus == 0:
        for i in removed_points_indices:
            prey[i] = None
            predator[i] = None

    elif Focus == 1:
        for i in removed_points_indices:
            prey[i] = None

    elif Focus == 2:
```

```
        for i in removed_points_indices:
            predator[i] = None

    return np.array(time), np.array(prey), np.array(predator)

```

In [19]:
```
def extrema_removal(time, input_data, points_removed, Focus = 0):
    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # Calculate mean and variance to set regions for data
    mean_prey_population, mean_predator_population = np.mean(prey), np.
    variance_prey, variance_predator = statistics.variance(prey), stati

    # set upper bound and lower bound for point removals
    ub_prey, lb_prey = mean_prey_population + 0.45 * variance_prey, mea
    ub_predator, lb_predator = mean_predator_population + 0.9 *variance

    # initialize set up for removing points randomly given the bounds
    prey_options = []
    predator_options = []
    # enumerate through list of stored points
    for index, prey_count in enumerate(prey):
        # check if they are in specified region
        if prey_count >= ub_prey or prey_count <= lb_prey:
            prey_options.append([index, prey_count, predator[index]])
    for index, predator_count in enumerate(predator):
        if predator_count >= ub_predator or predator_count <= lb_predat
            predator_options.append([index, prey[index], predator_count

    # remove points from list depending on which focus is set
    removal_options = []
    if Focus == 0:
        removal_options = removal_options + prey_options + predator_opt
    elif Focus == 1:
        removal_options = removal_options + prey_options
    elif Focus == 2:
        removal_options = removal_options + predator_options
    else:
        print('Error: Removal option not known. Try either both, prey,

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(np.array(removal_options).T

    # turn the list into integers so we can remove them based on the in
    integer_array = []
    for counter in range(len(removed_points_indices)):
        integer_array.append(int(removed_points_indices[counter]))

    # update the lists based on points we wanted to remove
    if Focus == 0:
        for i in integer_array:
            prey[i] = None
            predator[i] = None

    elif Focus == 1:
        for i in integer_array:
            prey[i] = None

    elif Focus == 2:
        for i in integer_array:
            predator[i] = None

    return np.array(time), np.array(prey), np.array(predator)
```

In [314]:
```
def midpoint_removal(time, input_data, points_removed, Focus = 0):
    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # Calculate mean and variance to set regions for data
    mean_prey_population, mean_predator_population = np.mean(prey), np.
    variance_prey, variance_predator = statistics.variance(prey), stati

    # set upper bound and lower bound for point removals
    ub_prey, lb_prey = mean_prey_population + 0.45 * variance_prey, mea
    ub_predator, lb_predator = mean_predator_population + 0.9 *variance

    # initialize set up for removing points randomly given the bounds
    prey_options = []
    predator_options = []
    # enumerate through list of stored points
    for index, prey_count in enumerate(prey):
        # check if they are in specified region
        if prey_count <= ub_prey and prey_count >= lb_prey:
            prey_options.append([index, prey_count, predator[index]])
    for index, predator_count in enumerate(predator):
        if predator_count <= ub_predator and predator_count >= lb_preda
            predator_options.append([index, prey[index], predator_count

    # remove points from list depending on which focus is set
    removal_options = []
    if Focus == 0:
        removal_options = removal_options + prey_options + predator_opt
    elif Focus == 1:
        removal_options = removal_options + prey_options
    elif Focus == 2:
        removal_options = removal_options + predator_options
    else:
        print('Error: Removal option not known. Try either both, prey,

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(np.array(removal_options).T

    # turn the list into integers so we can remove them based on the in
    integer_array = []
    for counter in range(len(removed_points_indices)):
        integer_array.append(int(removed_points_indices[counter]))

    # update the lists based on points we wanted to remove
    if Focus == 0:
        for i in integer_array:
            prey[i] = None
            predator[i] = None

    elif Focus == 1:
        for i in integer_array:
            prey[i] = None

    elif Focus == 2:
        for i in integer_array:
            predator[i] = None

    return np.array(time), np.array(prey), np.array(predator)
```

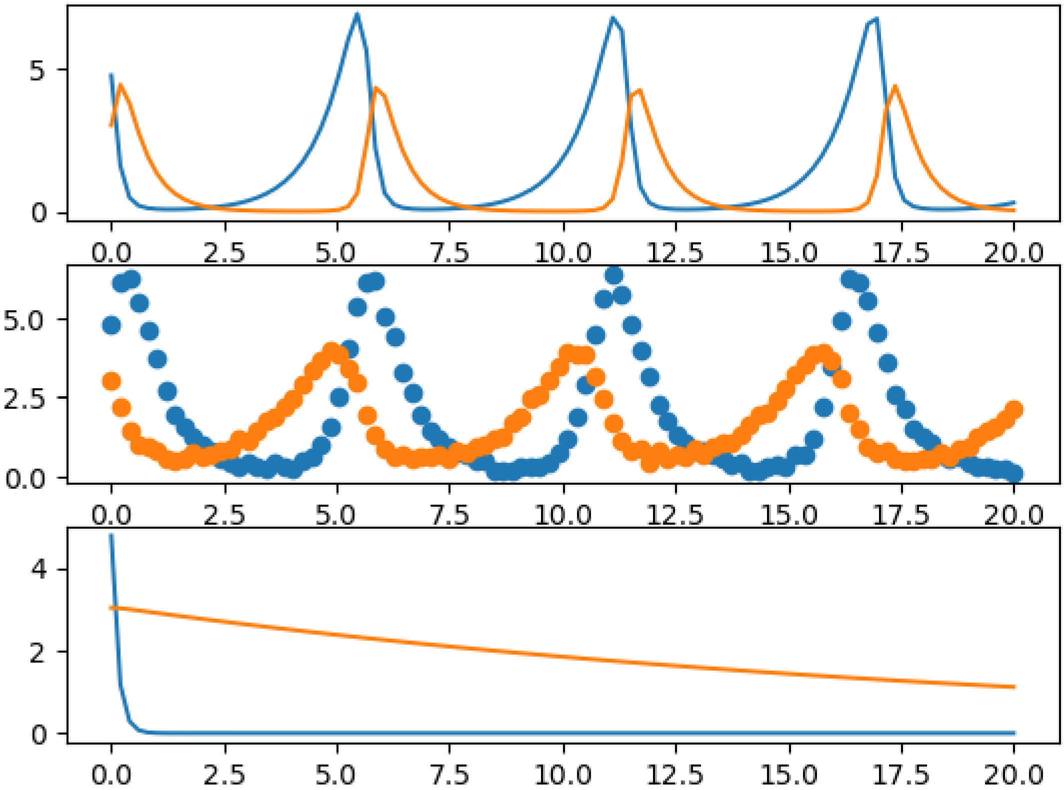
```
midpoint_removal(time, input_data, points_removed, 0)
```

Out[314]:
```
(array([ 0.        ,  0.2020202 ,  0.4040404 ,  0.60606061,  0.80808081,
         1.01010101,  1.21212121,  1.41414141,  1.61616162,  1.81818182,
         2.02020202,  2.22222222,  2.42424242,  2.62626263,  2.82828283,
         3.03030303,  3.23232323,  3.43434343,  3.63636364,  3.83838384,
         4.04040404,  4.24242424,  4.44444444,  4.64646465,  4.84848485,
         5.05050505,  5.25252525,  5.45454545,  5.65656566,  5.85858586,
         6.06060606,  6.26262626,  6.46464646,  6.66666667,  6.86868687,
         7.07070707,  7.27272727,  7.47474747,  7.67676768,  7.87878788,
         8.08080808,  8.28282828,  8.48484848,  8.68686869,  8.88888889,
         9.09090909,  9.29292929,  9.49494949,  9.6969697 ,  9.8989899 ,
        10.1010101 , 10.3030303 , 10.50505051, 10.70707071, 10.90909091,
        11.11111111, 11.31313131, 11.51515152, 11.71717172, 11.91919192,
        12.12121212, 12.32323232, 12.52525253, 12.72727273, 12.92929293,
        13.13131313, 13.33333333, 13.53535354, 13.73737374, 13.93939394,
        14.14141414, 14.34343434, 14.54545455, 14.74747475, 14.94949495,
        15.15151515, 15.35353535, 15.55555556, 15.75757576, 15.95959596,
        16.16161616, 16.36363636, 16.56565657, 16.76767677, 16.96969697,
        17.17171717, 17.37373737, 17.57575758, 17.77777778, 17.97979798,
        18.18181818, 18.38383838, 18.58585859, 18.78787879, 18.98989899,
        19.19191919, 19.39393939, 19.5959596 , 19.7979798 , 20.        ]),
 array([4.78163509, 6.11400461, 6.23836095, 5.52052405, 4.58254575,
        3.69549338, 2.73241063, 1.93007859,        nan, 1.25280509,
        0.99647646, 0.83616635, 0.55796464, 0.42574735, 0.29284544,
        0.42998578, 0.29047429, 0.23623108,        nan, 0.34584789,
        0.26683052, 0.52841771, 0.65807025,        nan,        nan,
        2.55628162, 4.05272265, 5.39827216, 6.13430431, 6.17559672,
        5.04337145, 4.40335325, 3.26795378, 2.66918471, 1.95164064,
        1.47972638, 1.21762543, 0.92610618, 0.76317457, 0.68336557,
        0.48930524, 0.50292464, 0.17631951, 0.21193155, 0.19391247,
        0.31392994,        nan, 0.2876866 , 0.43413798, 0.78532619,
        1.23239764, 1.91250492,        nan, 4.48294454, 5.65027253,
        6.37322741, 5.73552279, 4.77653998, 4.00597789, 3.13453968,
        2.25261307, 1.78222451, 1.33145956, 1.07897012, 0.79924317,
        0.82105872, 0.68730727, 0.57397704,        nan, 0.42231647,
        0.17771466, 0.19526324, 0.32527476, 0.34995521, 0.28914043,
        0.67309272, 0.68659273, 1.23055182, 2.20768819, 3.45148561,
        4.92302552, 6.22992039, 6.0991116 , 5.57323872, 4.56083925,
        3.62460823, 2.57661795, 2.1230354 , 1.5435279 , 1.24764464,
               nan, 0.71257577,        nan, 0.65039322,        nan,
        0.31034585, 0.32459509, 0.25808311, 0.28367985, 0.13595587]),
 array([3.03525736, 2.18974589, 1.47890677, 0.98983604, 0.95782741,
        0.8089764 , 0.5550991 , 0.48259774,        nan, 0.7378781 ,
        0.61912135, 0.71381421, 0.80913925, 0.90709674, 1.20019798,
        1.15551425, 1.4620071 , 1.7790317 ,        nan, 2.18036662,
        2.45451334, 2.87645734, 3.34293736,        nan,        nan,
        3.83569514, 3.42440295, 2.97234104, 1.97992361, 1.30265342,
        0.8702643 , 0.65378973, 0.67275523, 0.57794837, 0.61721216,
        0.64514385, 0.69083686, 0.59946108, 0.79222153, 0.78077762,
        0.93441085, 1.00700856, 1.21962625, 1.29428758, 1.70666312,
        1.92431547,        nan, 2.61408082, 3.05851749, 3.4901669 ,
        3.90039401, 3.88133056,        nan, 3.16769416, 2.47120556,
        1.68769771, 1.16042605, 0.80690056, 0.88570405, 0.44751714,
        0.7982129 , 0.53985993, 0.68495287, 0.63356906, 0.90963702,
        0.69373712, 0.94734264, 1.08333741,        nan, 1.31674353,
        1.61225858, 1.9424163 , 2.01694512, 2.40634827, 2.79703811,
        3.21140628, 3.50568978, 3.83378881, 3.90396118, 3.63260061,
        3.08637832, 2.03180558, 1.52594296, 0.93100161, 0.77101994,
        0.79666992, 0.55440616, 0.49615381, 0.49720865, 0.57677885,
               nan, 0.77056314,        nan, 0.9048621 ,        nan,
        1.24188957, 1.43725675, 1.56281031, 1.83417075, 2.14706546]))
```

In [16]:
```
def inferance_removal(initial_temp,cooling_constant, objective, algorit
    # define input data based on number of points we want to remove
    new_data_set = removal_type(time, input_data, points_removed, Focus
    time_new = new_data_set[0]
    prey_new = new_data_set[1]
    predator_new = new_data_set[2]

    # prepare data to match input requirements of algorithm (so far onl
    input_data_new = []
    for i in range(len(time_new)):
        input_data_tulple = [prey_new[i], predator_new[i]]
        input_data_new.append(input_data_tulple)

    # apply algorithm to find best fitted parameters given new data set
    x_best, scores = algorithm(initial_temp,cooling_constant, np.array(

    return x_best, scores

# parameters = [0.5, 0.6, 0.7, 0.8]
# x = inferance_removal(initial_temp,cooling_constant, MSE2, simulated_
# print(x[0])
```

In [268]:
```
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]
time = t
input_data = data[:,1:3]

best = inferance_removal(initial_temp,cooling_constant, MSE2, simulated
removed = inferance_removal(initial_temp,cooling_constant, MSE2, simula

best_params_tests = best[0]
reduced_params_test = removed[0]

res1 = predator_prey_integration(time,initial_conditions,best_params_te
res2 = predator_prey_integration(time,initial_conditions,reduced_params

MSE_ = MSE2(res1, input_data)
MSE = MSE2(res2, input_data)

print(MSE_, MSE)

plt.figure()
plt.subplot(311)
plt.plot(data[:,0], res1[:,0])
plt.plot(data[:,0], res1[:,1])

plt.subplot(312)
plt.scatter(time, data[:,1])
plt.scatter(time, data[:, 2])

plt.subplot(313)
plt.plot(data[:,0], res2[:,0])
plt.plot(data[:,0], res2[:,1])
plt.show()
plt.close
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

WARNING: Maximum number of points that can be removed has been exceeded. A
ll points possible within the given bound have now been removed.
3.7074011653569787 4.557827773152935
```



Out[268]: <function matplotlib.pyplot.close(fig=None)>

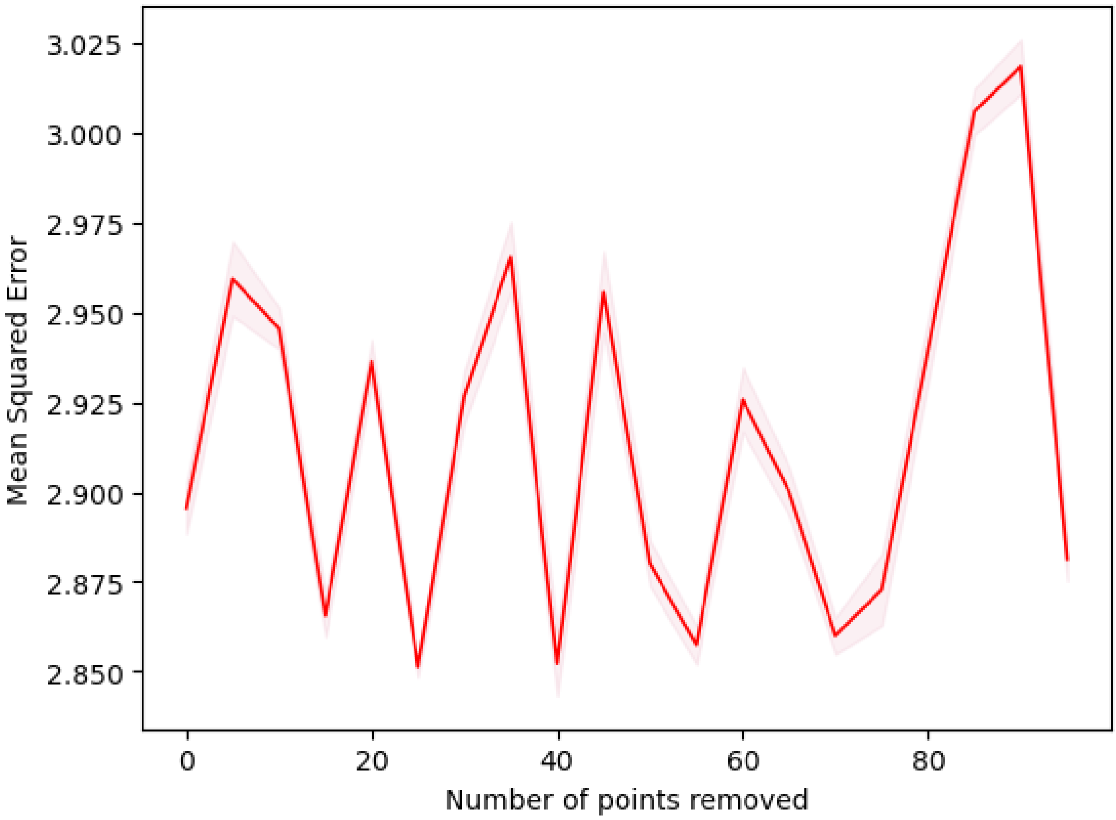
In [378]:

```
def multirun_SA_point_removal(iterations, simulations, initial_temperat
    # initialize objective score sufficiently high
    Lowest_MSE = [100000]
    best_param_overall = []
    # start simulated annealing from varying initial parameters
    for simulation_count in range(simulations):
        init_conditions = original_data[0]
        initial_parameter_guess = [np.random.uniform(0,1), np.random.ur
        # iterate several times for each initial condition
        for iteration_count in range(iterations):
            # find parameters best fitted
            best_found_parameters = inferance_removal(initial_temperatu
            # integrate
            Reversed_curve = predator_prey_integration(timestep,init_cc
            # compute objective function
            MSE = objective(original_data, Reversed_curve)
            # check if current objective lower than initial ones and if
            if MSE < Lowest_MSE[-1]:
                best_param_overall.append(best_found_parameters[0])
                Lowest_MSE.append(MSE)
    return best_param_overall[-1], Lowest_MSE[-1]

```

In [425]:

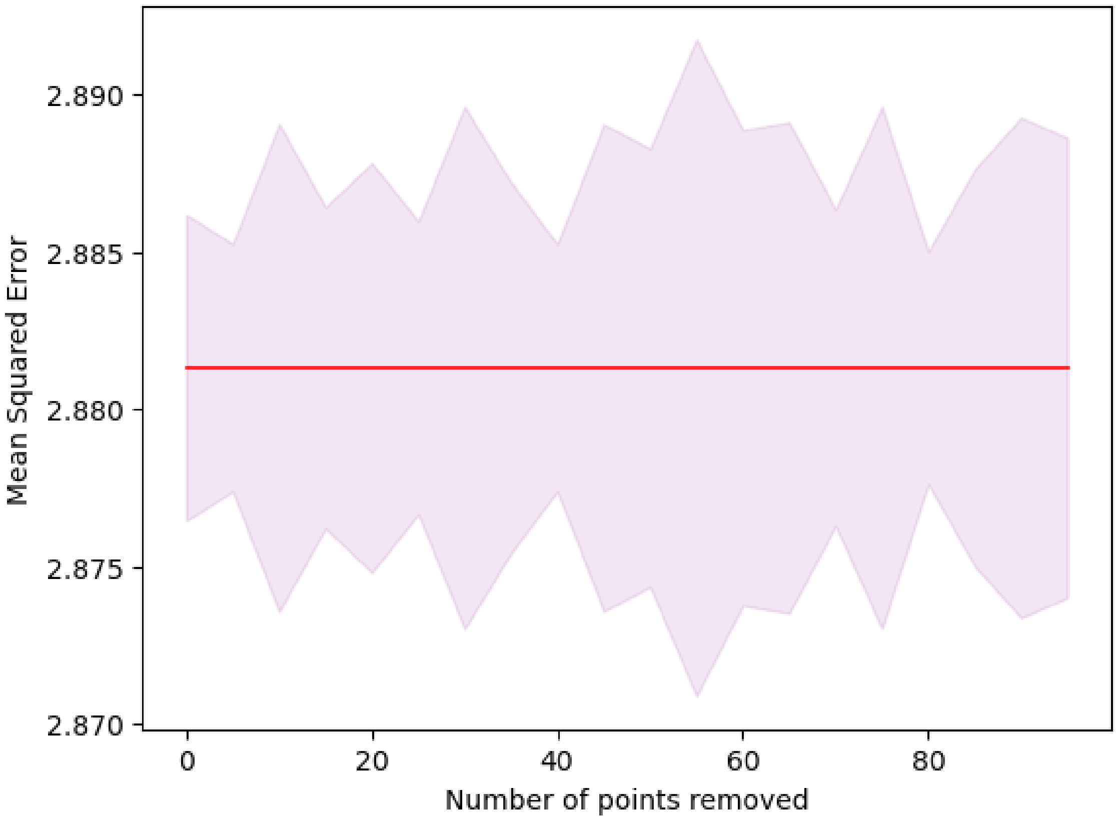
```
# Points removed with aggressive cooling for prey population, simulatec
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey = []
plt.figure(dpi = 300)
for counter in range(25):
    # storage
    paramets_prey = []
    objective_results_prey = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal = multirun_SA_point_removal(
        paramets_prey.append(best_parameters_found_prey_removal[0])
        objective_results_prey.append(best_parameters_found_prey_remova
    all_scores_prey.append(objective_results_prey)
means_scores_prey = []
variance_scores_prey = []
for index in range(len(npoints)):
    current_score_count = np.array(all_scores_prey)[:,index]
    means_scores_prey.append(np.mean(current_score_count))
    variance_scores_prey.append(statistics.variance(current_score_count
ci = 1.96 * np.array(variance_scores_prey)/25
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey, linewidth = '1.2', color = 'red')
ax.fill_between(npoints, (np.array(means_scores_prey)-ci), (np.array(me
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

<Figure size 1920x1440 with 0 Axes>
```


3.025
3.000
2.975
2.950
2.925
2.900
2.875
2.850
Mean Squared Error
0
20
40
60
80
Number of points removed

In [429]:
```
# Points removed with aggressive cooling for prey population, simulatec
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_predprey = []
plt.figure(dpi = 300)
for counter in range(25):
    # storage
    paramets_predprey = []
    objective_results_predprey = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_predprey_removal = multirun_SA_point_remc
        paramets_predprey.append(best_parameters_found_predprey_removal
        objective_results_predprey.append(best_parameters_found_predpre
    all_scores_predprey.append(objective_results_predprey)
means_scores_predprey = []
variance_scores_predprey = []
for index in range(len(npoints)):
    current_score_count_predprey = np.array(all_scores_predprey)[:,inde
    means_scores_predprey.append(np.mean(current_score_count))
    variance_scores_predprey.append(statistics.variance(current_score_c
ci_predprey = 1.96 * np.array(variance_scores_predprey)/25
plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_predprey, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_predprey)-ci_predprey),
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

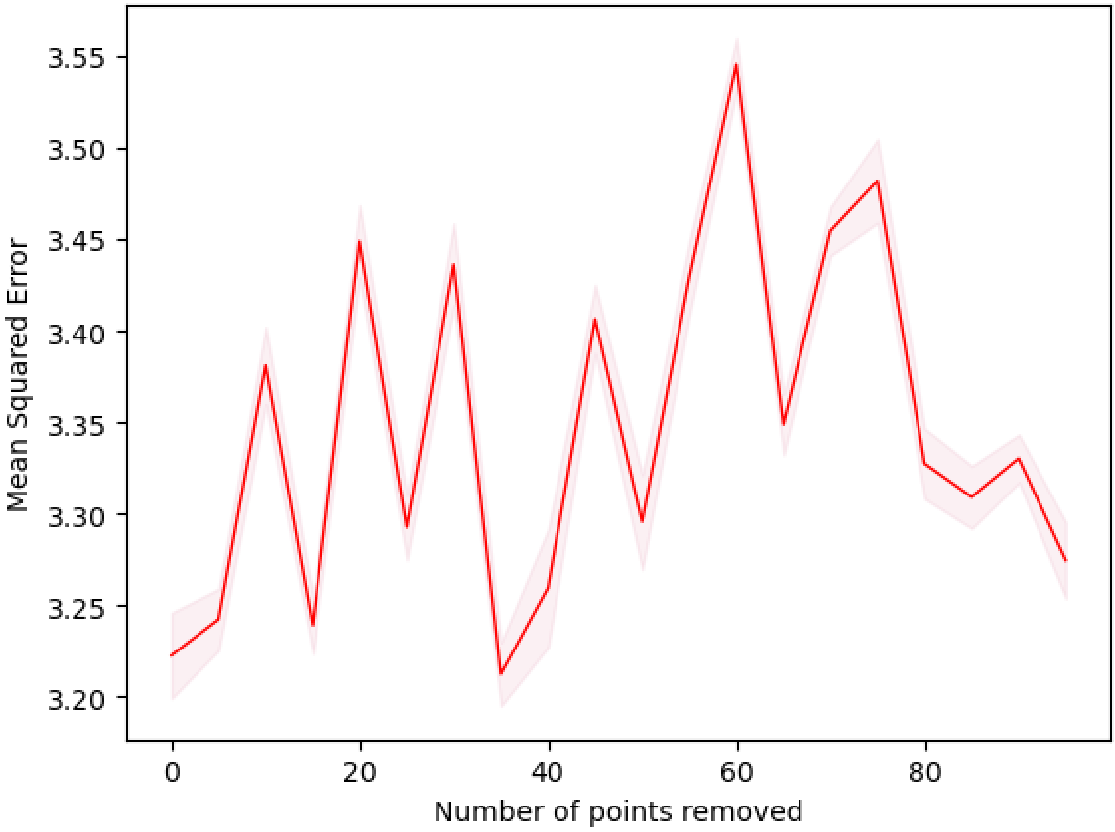
```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

<Figure size 1920x1440 with 0 Axes>

<Figure size 1920x1440 with 0 Axes>
```


2.890
2.885
2.880
2.875
2.870
Mean Squared Error
0
20
40
60
80
Number of points removed

In [424]:

```
# Points removed with slower cooling simulated annealing and slower coo
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.9
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_predator = []
plt.figure(dpi = 300)
for counter in range(25):
    # storage
    paramets_predator = []
    objective_results_predator = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_predator_removal = multirun_SA_point_remo
        paramets_predator.append(best_parameters_found_predator_removal
        objective_results_predator.append(best_parameters_found_predato
    all_scores_predator.append(objective_results_predator)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_scores_predator = []
variance_scores_predator = []
for index in range(len(npoints)):
    current_score_count_predator = np.array(all_scores_predator)[:,inde
    means_scores_predator.append(np.mean(current_score_count_predator))
    variance_scores_predator.append(statistics.variance(current_score_c
ci_predator = 1.96 * np.array(variance_scores_predator)/25
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_predator, linewidth = '1', color = 'red')
ax.fill_between(npoints, (np.array(means_scores_predator)-ci_predator),
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

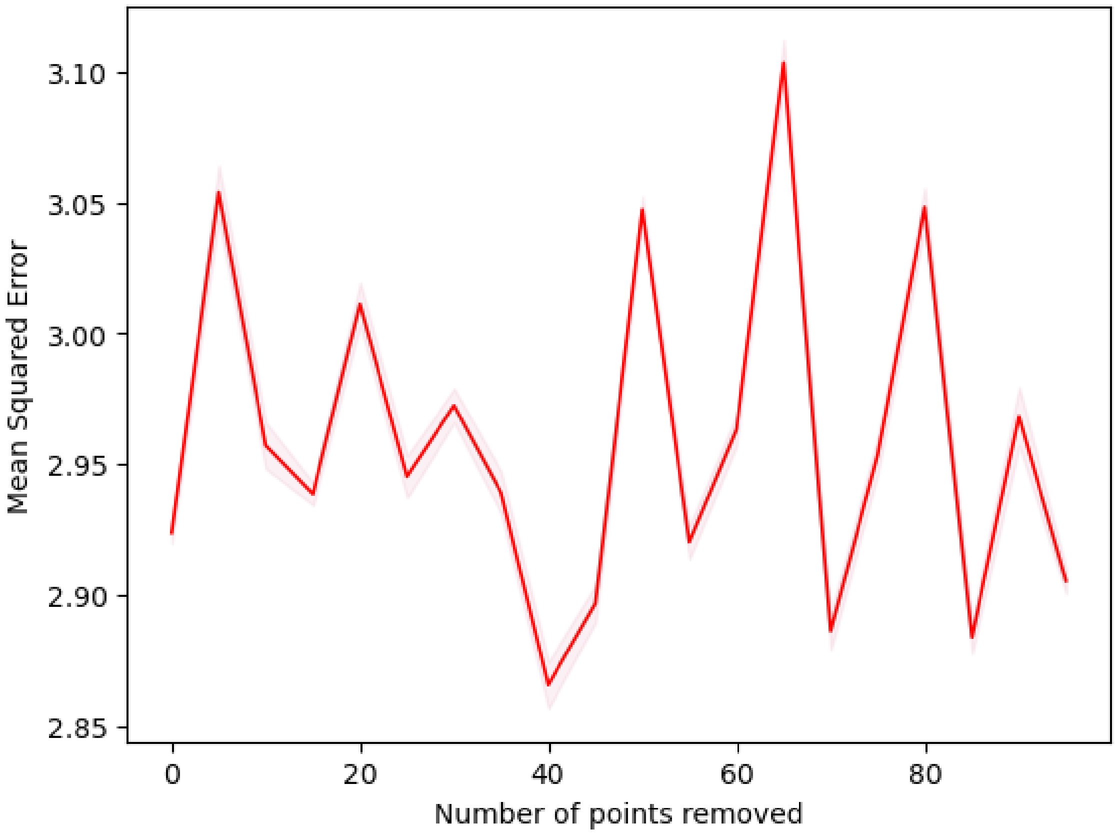
```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:11: Runtime
Warning: overflow encountered in square
  err1 = (x1[indx_x] - x2[indx_x])**2

<Figure size 1920x1440 with 0 Axes>
```


3.55
3.50
3.45
3.40
3.35
3.30
3.25
3.20
Mean Squared Error
0
20
40
60
80
Number of points removed

In [423]:

```
# Points removed with aggressive cooling
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores = []
plt.figure(dpi = 300)
for counter in range(25):
    # storage
    paramets_all = []
    objective_results_all = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_all_removal = multirun_SA_point_removal(i
        paramets_all.append(best_parameters_found_all_removal[0])
        objective_results_all.append(best_parameters_found_all_removal[
    all_scores.append(objective_results_all)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_scores_all = []
variance_scores_all = []
for index in range(len(npoints)):
    current_score_count_all = np.array(all_scores)[:,index]
    means_scores_all.append(np.mean(current_score_count_all))
    variance_scores_all.append(statistics.variance(current_score_count_
ci_all = 1.96 * np.array(variance_scores_all)/25
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_all, linewidth = '1.2', color = 'red')
ax.fill_between(npoints, (np.array(means_scores_all)-ci_all), (np.array
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

<Figure size 1920x1440 with 0 Axes>
```

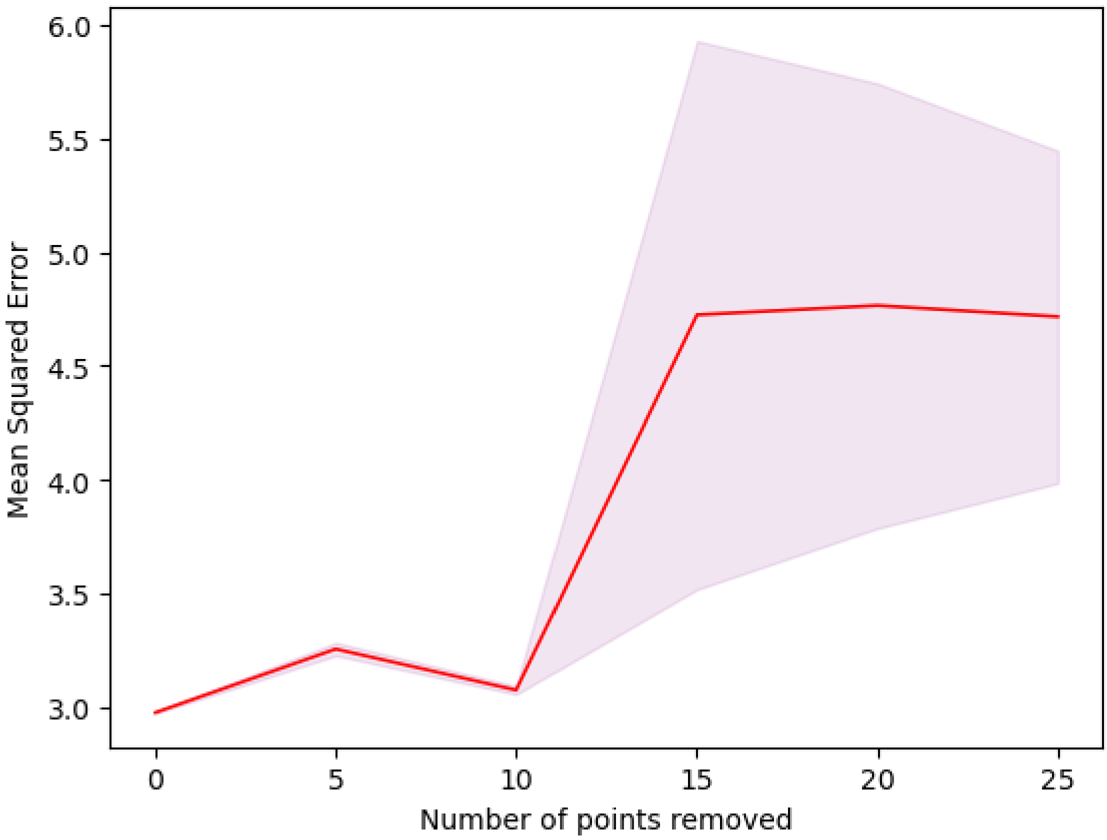


3.10
3.05
3.00
2.95
2.90
2.85
Mean Squared Error
0
20
40
60
80
Number of points removed

In [418]:

```
# Point extrema removed with aggressive cooling MSE2 function prey popu
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey = []
plt.figure(dpi = 300)
for counter in range(25):
    # storage
    paramets_prey = []
    objective_results_prey = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,30,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal = multirun_SA_point_removal(
        paramets_prey.append(best_parameters_found_prey_removal[0])
        objective_results_prey.append(best_parameters_found_prey_remova
    all_scores_prey.append(objective_results_prey)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_scores_prey = []
variance_scores_prey = []
for index in range(len(npoints)):
    current_score_count = np.array(all_scores_prey)[:,index]
    means_scores_prey.append(np.mean(current_score_count))
    variance_scores_prey.append(statistics.variance(current_score_count
ci = 1.96 * np.array(variance_scores_prey)/25
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey, linewidth = '1.2', color = 'red')
ax.fill_between(npoints, (np.array(means_scores_prey)-ci), (np.array(me
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: invalid value encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:11: Runtime
Warning: overflow encountered in square
  err1 = (x1[indx_x] - x2[indx_x])**2
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:12: Runtime
Warning: overflow encountered in square
  err2 = (y1[indx_y] - y2[indx_y])**2

<Figure size 1920x1440 with 0 Axes>
```

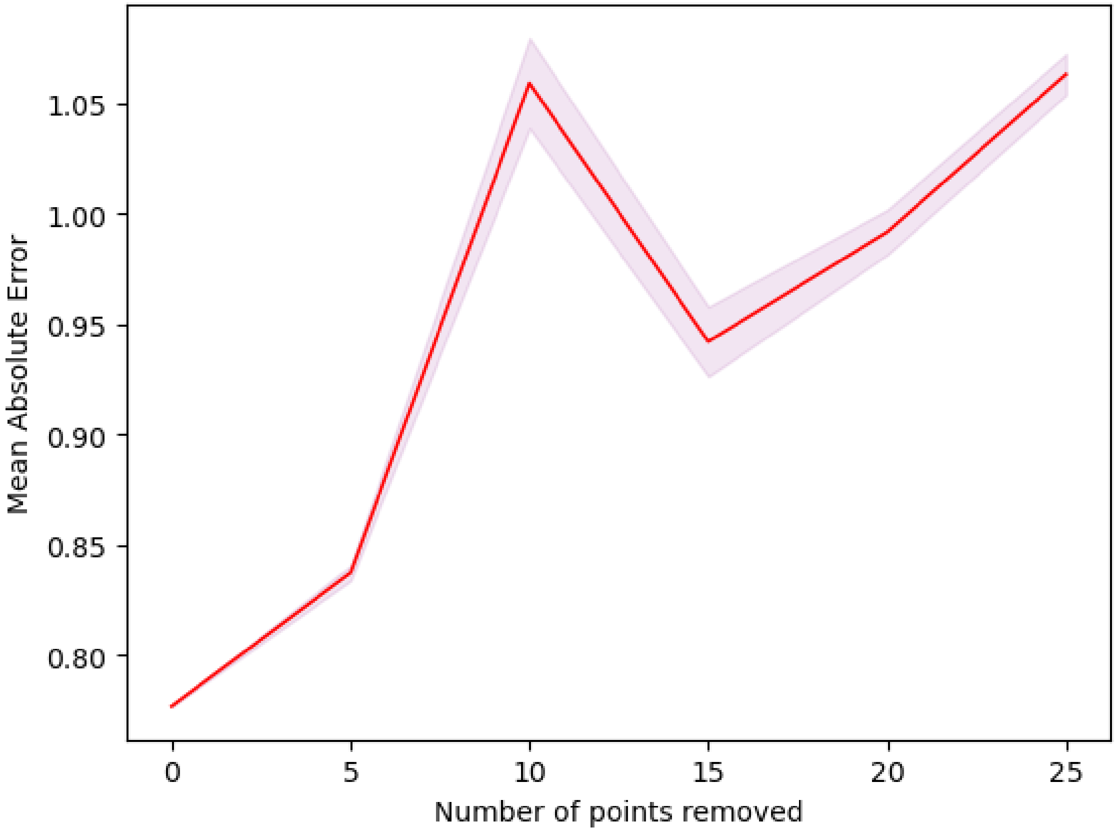


In [419]:

```
# Point extrema removed with aggressive cooling, prey population and MA
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey_MAE = []
for counter in range(25):
    # storage
    paramets_prey_MAE = []
    objective_results_prey_MAE = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,30,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal_MAE = multirun_SA_point_remo
        paramets_prey_MAE.append(best_parameters_found_prey_removal_MAE
        objective_results_prey_MAE.append(best_parameters_found_prey_re
    all_scores_prey_MAE.append(objective_results_prey_MAE)

means_scores_prey_MAE = []
variance_scores_prey_MAE = []
for index in range(len(npoints)):
    current_score_count_MAE = np.array(all_scores_prey_MAE)[:,index]
    means_scores_prey_MAE.append(np.mean(current_score_count_MAE))
    variance_scores_prey_MAE.append(statistics.variance(current_score_c
ci_MAE = 1.96 * np.array(variance_scores_prey_MAE)/25

plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey_MAE, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_prey_MAE)-ci_MAE), (np.
plt.xlabel('Number of points removed')
plt.ylabel('Mean Absolute Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: invalid value encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:35: Runtime
Warning: Mean of empty slice
  return np.nanmean([err])
```

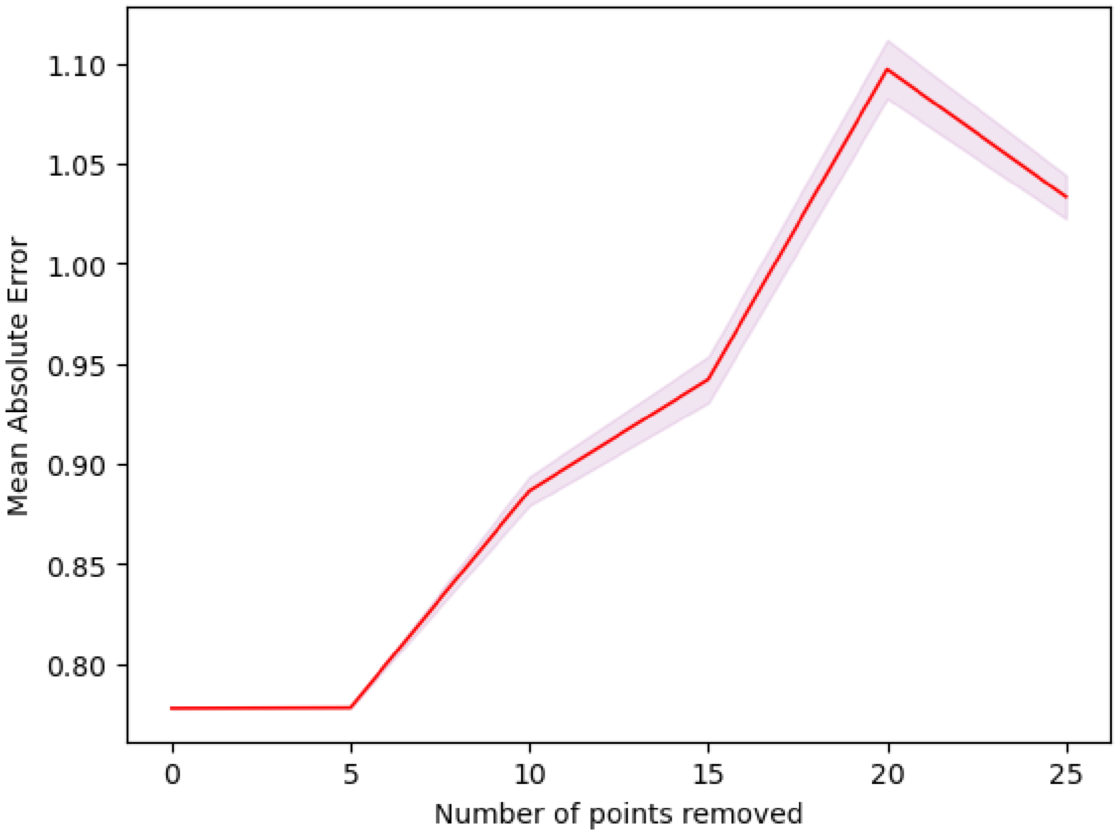
```
<Figure size 1920x1440 with 0 Axes>
```



In [420]:

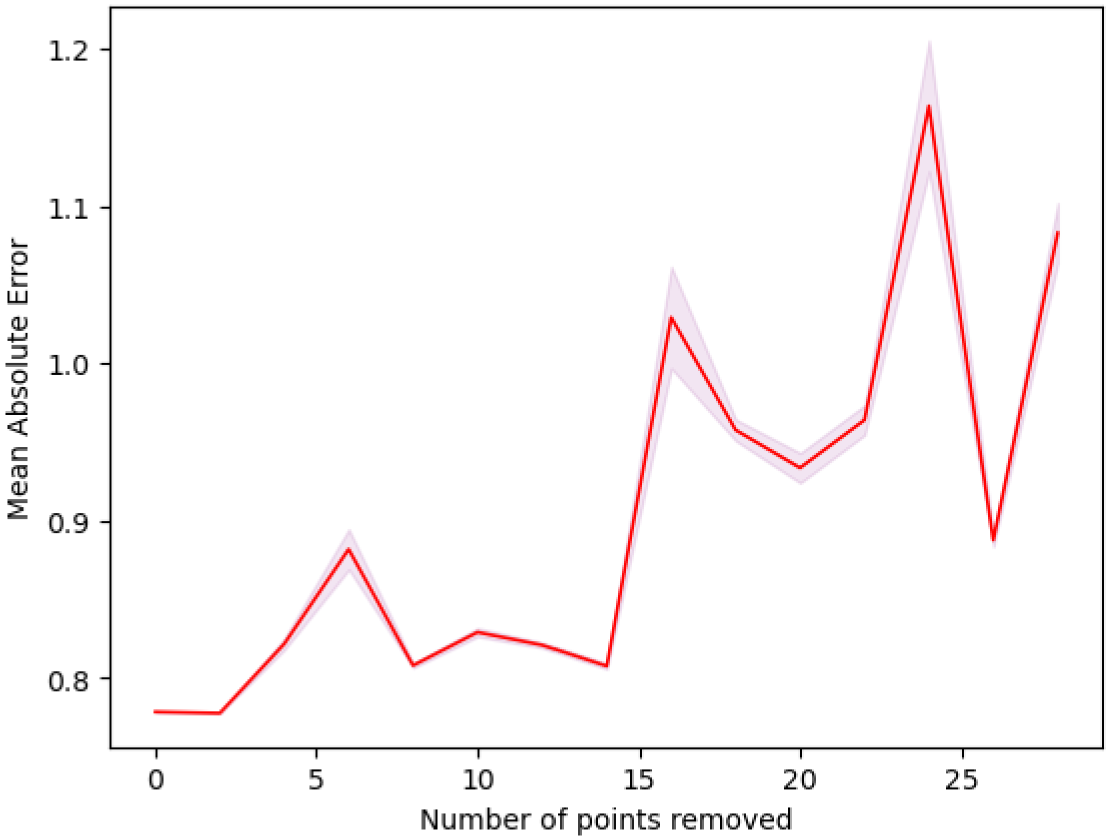
```
# Point extrema removed with not aggressive cooling, prey population ar
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.9 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey_MAE = []
for counter in range(25):
    # storage
    paramets_prey_MAE = []
    objective_results_prey_MAE = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,30,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal_MAE = multirun_SA_point_remo
        paramets_prey_MAE.append(best_parameters_found_prey_removal_MAE
        objective_results_prey_MAE.append(best_parameters_found_prey_re
    all_scores_prey_MAE.append(objective_results_prey_MAE)

means_scores_prey_MAE = []
variance_scores_prey_MAE = []
for index in range(len(npoints)):
    current_score_count_MAE = np.array(all_scores_prey_MAE)[:,index]
    means_scores_prey_MAE.append(np.mean(current_score_count_MAE))
    variance_scores_prey_MAE.append(statistics.variance(current_score_c
ci_MAE = 1.96 * np.array(variance_scores_prey_MAE)/25

plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey_MAE, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_prey_MAE)-ci_MAE), (np.
plt.xlabel('Number of points removed')
plt.ylabel('Mean Absolute Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\1517521670.py:4: Runtime
Warning: overflow encountered in scalar multiply
  dxdt = (alpha * x) - (beta * x * y)  # Prey ODE
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\1517521670.py:5: Runtime
Warning: overflow encountered in scalar multiply
  dydt = (delta * x * y) - (gamma * y)  # Predator ODE
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:35: Runtime
Warning: Mean of empty slice
  return np.nanmean([err])

<Figure size 1920x1440 with 0 Axes>
```


1.10
1.05
1.00
0.95
0.90
0.85
0.80
Mean Absolute Error
0
5
10
15
20
25
Number of points removed

In [428]:
```
# Point extrema removed with not aggressive cooling, prey population ar
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.9 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey_MAE = []
for counter in range(25):
    # storage
    paramets_prey_MAE = []
    objective_results_prey_MAE = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,30,2)
    for p_removed in npoints:
        best_parameters_found_prey_removal_MAE = multirun_SA_point_remo
        paramets_prey_MAE.append(best_parameters_found_prey_removal_MAE
        objective_results_prey_MAE.append(best_parameters_found_prey_re
    all_scores_prey_MAE.append(objective_results_prey_MAE)

means_scores_prey_MAE = []
variance_scores_prey_MAE = []
for index in range(len(npoints)):
    current_score_count_MAE = np.array(all_scores_prey_MAE)[:,index]
    means_scores_prey_MAE.append(np.mean(current_score_count_MAE))
    variance_scores_prey_MAE.append(statistics.variance(current_score_c
ci_MAE = 1.96 * np.array(variance_scores_prey_MAE)/25

plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey_MAE, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_prey_MAE)-ci_MAE), (np.
plt.xlabel('Number of points removed')
plt.ylabel('Mean Absolute Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:35: Runtime
Warning: Mean of empty slice
  return np.nanmean([err])
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\1517521670.py:4: Runtime
Warning: overflow encountered in scalar multiply
  dxdt = (alpha * x) - (beta * x * y)  # Prey ODE
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\1517521670.py:5: Runtime
Warning: overflow encountered in scalar multiply
  dydt = (delta * x * y) - (gamma * y)  # Predator ODE

<Figure size 1920x1440 with 0 Axes>
```

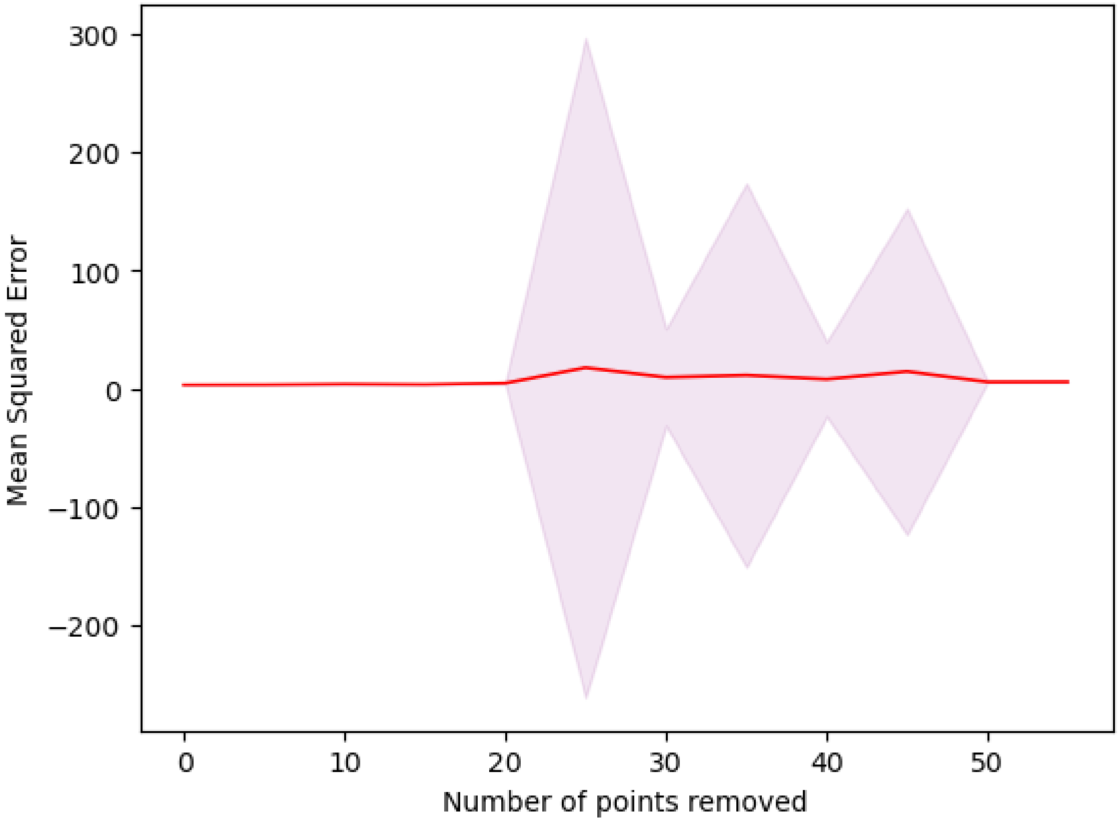

Mean Absolute Error
Number of points removed
1.2
1.1
1.0
0.9
0.8
0
5
10
15
20
25

In [421]:

```
# Point extrema removed with aggressive cooling for both species
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_predprey = []
for counter in range(25):
    # storage
    paramets_predprey = []
    objective_results_predprey = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,60,5)
    for p_removed in npoints:
        best_parameters_found_predprey_removal = multirun_SA_point_remc
        paramets_predprey.append(best_parameters_found_predprey_removal
        objective_results_predprey.append(best_parameters_found_predpre
    all_scores_predprey.append(objective_results_predprey)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_scores_predprey = []
variance_scores_predprey = []
for index in range(len(npoints)):
    current_score_count_predprey = np.array(all_scores_predprey)[:,inde
    means_scores_predprey.append(np.mean(current_score_count_predprey))
    variance_scores_predprey.append(statistics.variance(current_score_c
ci_predprey = 1.96 * np.array(variance_scores_predprey)/15
plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_predprey, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_predprey)-ci_predprey),
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

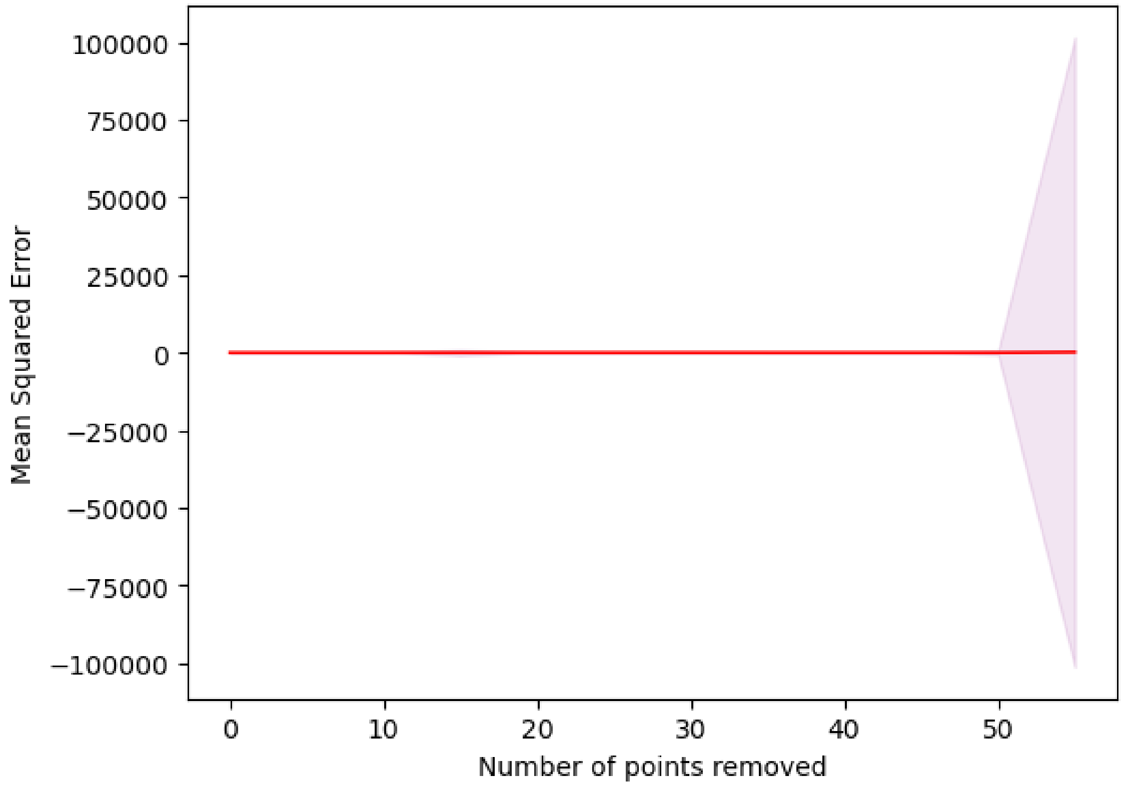
```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: invalid value encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:15: Runtime
Warning: Mean of empty slice
  return np.nanmean([err])
```

```
<Figure size 1920x1440 with 0 Axes>
```



In [422]:
```
# Point extrema removed with aggressive cooling for both species
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.9 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_predprey = []
for counter in range(25):
    # storage
    paramets_predprey = []
    objective_results_predprey = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,60,5)
    for p_removed in npoints:
        best_parameters_found_predprey_removal = multirun_SA_point_remo
        paramets_predprey.append(best_parameters_found_predprey_removal
        objective_results_predprey.append(best_parameters_found_predpre
    all_scores_predprey.append(objective_results_predprey)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_scores_predprey = []
variance_scores_predprey = []
for index in range(len(npoints)):
    current_score_count_predprey = np.array(all_scores_predprey)[:,inde
    means_scores_predprey.append(np.mean(current_score_count_predprey))
    variance_scores_predprey.append(statistics.variance(current_score_c
ci_predprey = 1.96 * np.array(variance_scores_predprey)/15
plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_predprey, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_predprey)-ci_predprey),
#plt.plot(npoints, means_scores_prey, linewidth = '1.2', color = 'red')
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

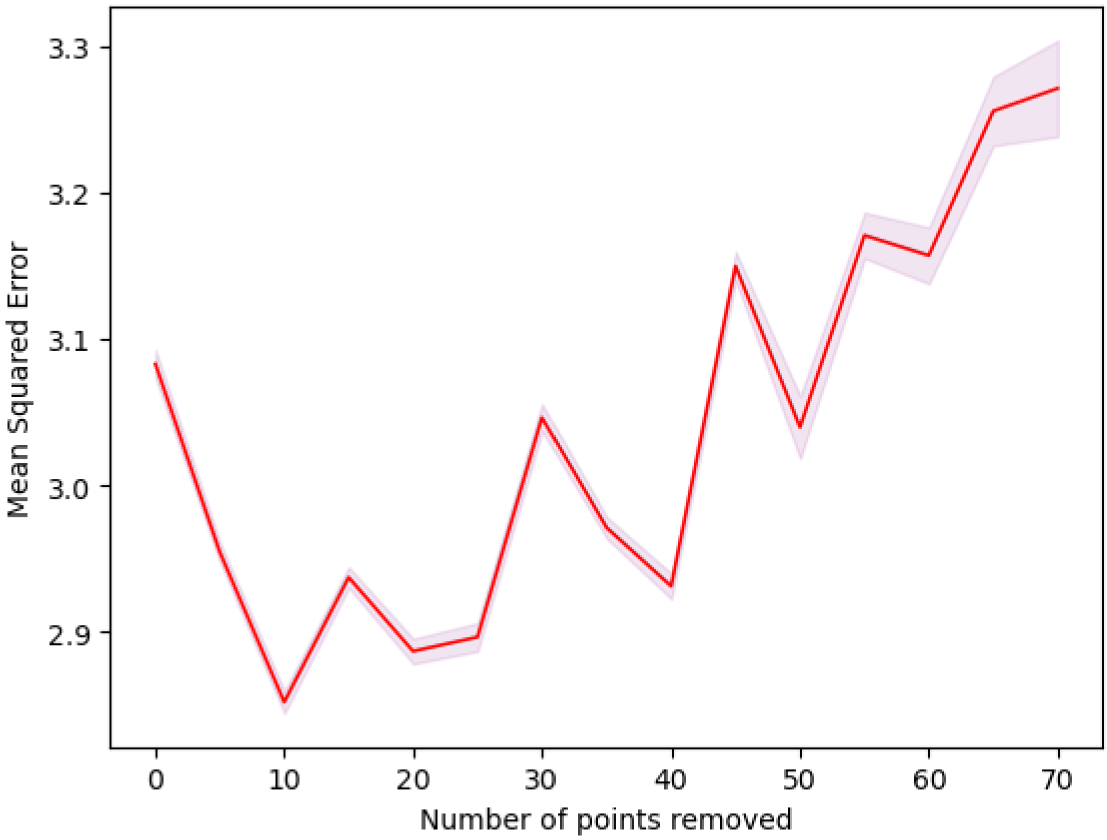
```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:15: RuntimeWarning: Mean of empty slice
  return np.nanmean([err])
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:11: RuntimeWarning: overflow encountered in square
  err1 = (x1[indx_x] - x2[indx_x])**2
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\528580857.py:12: RuntimeWarning: overflow encountered in square
  err2 = (y1[indx_y] - y2[indx_y])**2

<Figure size 1920x1440 with 0 Axes>
```


100000
75000
50000
25000
0
−25000
−50000
−75000
−100000
Mean Squared Error
0
10
20
30
40
50
Number of points removed

In [426]:

```
# Midpoint removal using MSE and aggressive cooling for the prey popula

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey_mid = []
for counter in range(25):
    # storage
    paramets_prey_mid = []
    objective_results_prey_mid = []
    # point removal loop (removing points at steps of 2)
    npoints = np.arange(0,75,5)
    for p_removed in npoints:
        best_parameters_found_prey_midremoval = multirun_SA_point_remov
        paramets_prey_mid.append(best_parameters_found_prey_midremoval[
        objective_results_prey_mid.append(best_parameters_found_prey_mi
    all_scores_prey_mid.append(objective_results_prey_mid)
means_scores_prey_mid = []
variance_scores_prey_mid = []
for index in range(len(npoints)):
    current_score_count_prey_mid = np.array(all_scores_prey_mid)[:,inde
    means_scores_prey_mid.append(np.mean(current_score_count_prey_mid))
    variance_scores_prey_mid.append(statistics.variance(current_score_c
ci_prey_mid = 1.96 * np.array(variance_scores_prey_mid)/25
plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_prey_mid, linewidth = '1.2', color = 'red'
ax.fill_between(npoints, (np.array(means_scores_prey_mid)-ci_prey_mid),
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

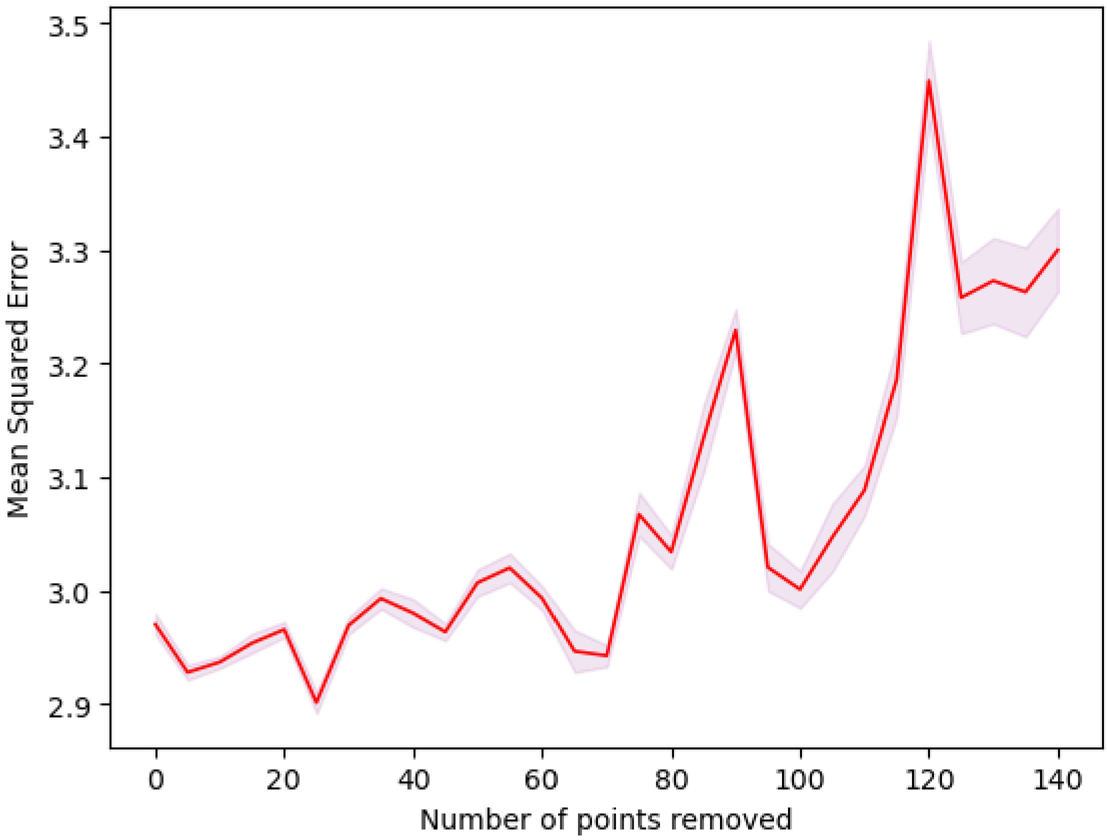
```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

<Figure size 1920x1440 with 0 Axes>
```


Mean Squared Error
Number of points removed
3.3
3.2
3.1
3.0
2.9
0
10
20
30
40
50
60
70

In [427]:

```
# Midpoint removal using MSE and not aggressive cooling for both popula

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_predprey_mid = []
for counter in range(25):
    # storage
    paramets_predprey_mid = []
    objective_results_predprey_mid = []
    # point removal loop
    npoints = np.arange(0,145,5)
    for p_removed in npoints:
        best_parameters_found_predprey_midremoval = multirun_SA_point_r
        paramets_predprey_mid.append(best_parameters_found_predprey_mic
        objective_results_predprey_mid.append(best_parameters_found_pre
    all_scores_predprey_mid.append(objective_results_predprey_mid)
means_scores_predprey_mid = []
variance_scores_predprey_mid = []
for index in range(len(npoints)):
    current_score_count_predprey_mid = np.array(all_scores_predprey_mic
    means_scores_predprey_mid.append(np.mean(current_score_count_predpr
    variance_scores_predprey_mid.append(statistics.variance(current_scc
ci_predprey_mid = 1.96 * np.array(variance_scores_predprey_mid)/25
plt.figure(dpi = 300)
fig, ax = plt.subplots()
ax.plot(npoints,means_scores_predprey_mid, linewidth = '1.2', color = '
ax.fill_between(npoints, (np.array(means_scores_predprey_mid)-ci_predpr
plt.xlabel('Number of points removed')
plt.ylabel('Mean Squared Error')
plt.show()
plt.close()
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: Runtim
eWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

<Figure size 1920x1440 with 0 Axes>
```


3.5
3.4
3.3
3.2
3.1
3.0
2.9
Mean Squared Error
0
20
40
60
80
100
120
140
Number of points removed

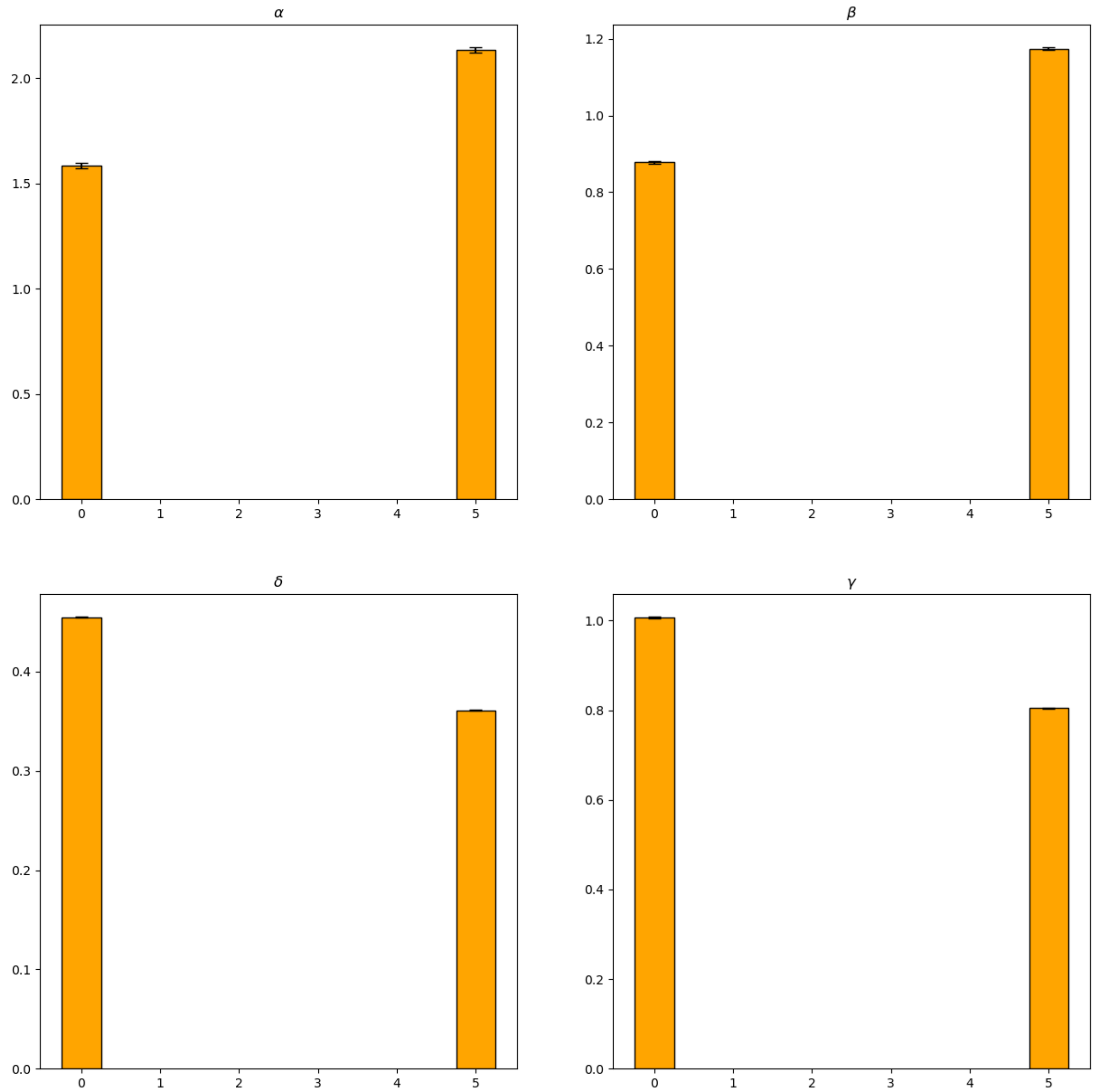
In [457]:
```
# Point extrema removed with aggressive cooling MSE2 function prey popu

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey = []
all_paramets_prey = []
for counter in range(25):
    # storage
    paramets_prey = []
    objective_results_prey = []
    # point removal loop
    npoints = np.arange(0,30,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal = multirun_SA_point_removal(
        paramets_prey.append(best_parameters_found_prey_removal[0])
        objective_results_prey.append(best_parameters_found_prey_remova
    all_scores_prey.append(objective_results_prey)
    all_paramets_prey.append(paramets_prey)
    #plt.plot(npoints ,objective_results_prey, linewidth = '0.6', color
means_paramets_prey = []


for index in range(len(npoints)):
    current_paramets_prey = np.array(all_paramets_prey)[:,index]
    means_paramets_prey.append([np.mean(current_paramets_prey[:,0]), np

alpha_all_means = np.array(means_paramets_prey)[:,0]
beta_all_means = np.array(means_paramets_prey)[:,1]
delta_all_means = np.array(means_paramets_prey)[:,2]
gamma_all_means = np.array(means_paramets_prey)[:,3]

variance_alpha_prey = statistics.variance(alpha_all_means)
variance_beta_prey = statistics.variance(beta_all_means)
variance_delta_prey = statistics.variance(delta_all_means)
variance_gamma_prey = statistics.variance(gamma_all_means)

ci_alpha_prey = 1.96 * np.array(variance_alpha_prey)/25
ci_beta_prey = 1.96 * np.array(variance_beta_prey)/25
ci_delta_prey = 1.96 * np.array(variance_delta_prey)/25
ci_gamma_prey = 1.96 *np.array(variance_gamma_prey)/25

print(beta_all_means, npoints)
plt.figure(dpi = 300)
fig, axes = plt.subplots(2, 2, figsize=(15, 15))

bar_width = 0.5
plt.subplot(221)
plt.title(r'$\alpha$')
plt.bar(npoints, alpha_all_means, yerr = ci_alpha_prey,color = "orange'
plt.subplot(222)
plt.title(r'$\beta$')
plt.bar(npoints, beta_all_means, yerr = ci_beta_prey,color = "orange",e
plt.subplot(223)
plt.title(r'$\delta$')
plt.bar(npoints, delta_all_means, yerr = ci_delta_prey,color = "orange'
```

```
plt.subplot(224)
plt.title(r'$\gamma$')
plt.bar(npoints, gamma_all_means, yerr = ci_gamma_prey,color = "orange'
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability

[0.87772397 1.17375944] [0 5]
```

Out[457]: <BarContainer object of 2 artists>

<Figure size 1920x1440 with 0 Axes>



In [ ]:

```
# Point extrema removed with aggressive cooling MSE2 function both popu

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey = []
all_paramets_prey = []
for counter in range(25):
    # storage
    paramets_prey = []
    objective_results_prey = []
    # point removal loop
    npoints = np.arange(0,60,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal = multirun_SA_point_removal(
        paramets_prey.append(best_parameters_found_prey_removal[0])
        objective_results_prey.append(best_parameters_found_prey_remova
    all_scores_prey.append(objective_results_prey)
    all_paramets_prey.append(paramets_prey)
means_paramets_prey = []


for index in range(len(npoints)):
    current_paramets_prey = np.array(all_paramets_prey)[:,index]
    means_paramets_prey.append([np.mean(current_paramets_prey[:,0]), np

alpha_all_means = np.array(means_paramets_prey)[:,0]
beta_all_means = np.array(means_paramets_prey)[:,1]
delta_all_means = np.array(means_paramets_prey)[:,2]
gamma_all_means = np.array(means_paramets_prey)[:,3]

variance_alpha_prey = statistics.variance(alpha_all_means)
variance_beta_prey = statistics.variance(beta_all_means)
variance_delta_prey = statistics.variance(delta_all_means)
variance_gamma_prey = statistics.variance(gamma_all_means)

ci_alpha_prey = 1.96 * np.array(variance_alpha_prey)/25
ci_beta_prey = 1.96 * np.array(variance_beta_prey)/25
ci_delta_prey = 1.96 * np.array(variance_delta_prey)/25
ci_gamma_prey = 1.96 *np.array(variance_gamma_prey)/25

print(beta_all_means, npoints)
plt.figure(dpi = 300)
fig, axes = plt.subplots(2, 2, figsize=(15, 15))

bar_width = 0.5
plt.subplot(221)
plt.title(r'$\alpha$')
plt.bar(npoints, alpha_all_means, yerr = ci_alpha_prey,color = "orange"
plt.subplot(222)
plt.title(r'$\beta$')
plt.bar(npoints, beta_all_means, yerr = ci_beta_prey,color = "orange",e
plt.subplot(223)
plt.title(r'$\delta$')
plt.bar(npoints, delta_all_means, yerr = ci_delta_prey,color = "orange"
plt.subplot(224)
```

```
plt.title(r'$\gamma$')
plt.bar(npoints, gamma_all_means, yerr = ci_gamma_prey,color = "orange'
```

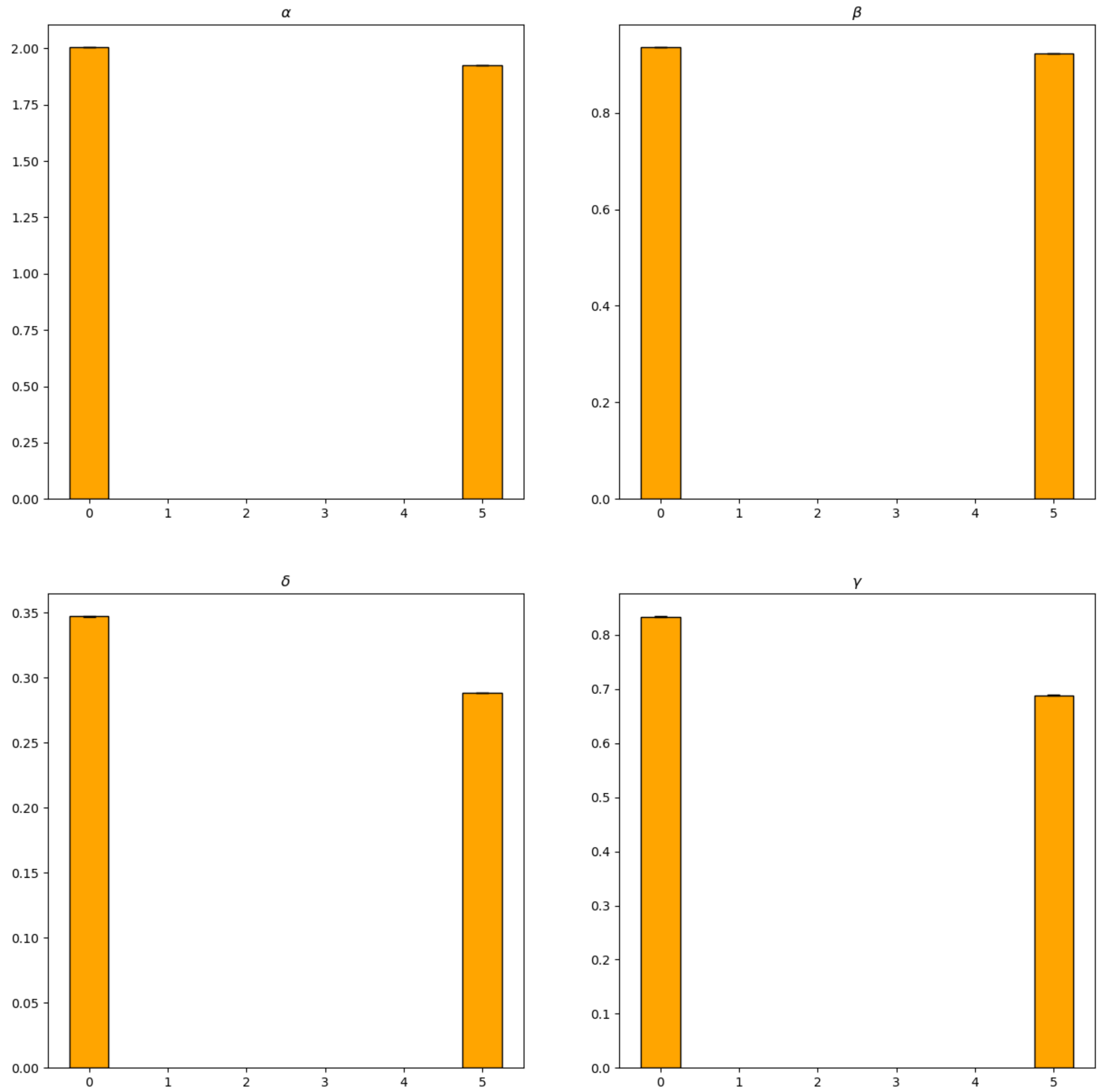
In [458]:
```
# Points removed randomly with aggressive cooling MSE2 function both pc

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores = []
all_paramets = []
for counter in range(25):
    # storage
    paramets = []
    objective_results = []
    # point removal loop
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_removal = multirun_SA_point_removal(itera
        paramets.append(best_parameters_found_removal[0])
        objective_results.append(best_parameters_found_removal[1])
    all_scores.append(objective_results)
    all_paramets.append(paramets)
means_paramets = []


for index in range(len(npoints)):
    current_paramets = np.array(all_paramets)[:,index]
    means_paramets.append([np.mean(current_paramets[:,0]), np.mean(curr

alpha_all_means = np.array(means_paramets)[:,0]
beta_all_means = np.array(means_paramets)[:,1]
delta_all_means = np.array(means_paramets)[:,2]
gamma_all_means = np.array(means_paramets)[:,3]

variance_alpha = statistics.variance(alpha_all_means)
variance_beta = statistics.variance(beta_all_means)
variance_delta = statistics.variance(delta_all_means)
variance_gamma = statistics.variance(gamma_all_means)

ci_alpha = 1.96 * np.array(variance_alpha)/25
ci_beta = 1.96 * np.array(variance_beta)/25
ci_delta = 1.96 * np.array(variance_delta)/25
ci_gamma = 1.96 *np.array(variance_gamma)/25

print(beta_all_means, npoints)
plt.figure(dpi = 300)
fig, axes = plt.subplots(2, 2, figsize=(15, 15))

bar_width = 0.5
plt.subplot(221)
plt.title(r'$\alpha$')
plt.bar(npoints, alpha_all_means, yerr = ci_alpha,color = "orange",ec =
plt.subplot(222)
plt.title(r'$\beta$')
plt.bar(npoints, beta_all_means, yerr = ci_beta,color = "orange",ec = '
plt.subplot(223)
plt.title(r'$\delta$')
plt.bar(npoints, delta_all_means, yerr = ci_delta,color = "orange",ec =
plt.subplot(224)
```

```
plt.title(r'$\gamma$')
plt.bar(npoints, gamma_all_means, yerr = ci_gamma,color = "orange",ec =
```

```
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability
C:\Users\kayad\AppData\Local\Temp\ipykernel_27100\3853094899.py:38: RuntimeWarning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptance probability

[0.93545137 0.92197714] [0 5]
```

Out[458]:

```
<BarContainer object of 2 artists>

<Figure size 1920x1440 with 0 Axes>
```



In [ ]:

```
# Random point removed with aggressive cooling MSE2 function prey popul

simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]

all_scores_prey = []
all_paramets_prey = []
for counter in range(25):
    # storage
    paramets_prey = []
    objective_results_prey = []
    # point removal loop
    npoints = np.arange(0,100,5)
    for p_removed in npoints:
        best_parameters_found_prey_removal = multirun_SA_point_removal(
        paramets_prey.append(best_parameters_found_prey_removal[0])
        objective_results_prey.append(best_parameters_found_prey_remova
    all_scores_prey.append(objective_results_prey)
    all_paramets_prey.append(paramets_prey)
means_paramets_prey = []


for index in range(len(npoints)):
    current_paramets_prey = np.array(all_paramets_prey)[:,index]
    means_paramets_prey.append([np.mean(current_paramets_prey[:,0]), np

alpha_all_means = np.array(means_paramets_prey)[:,0]
beta_all_means = np.array(means_paramets_prey)[:,1]
delta_all_means = np.array(means_paramets_prey)[:,2]
gamma_all_means = np.array(means_paramets_prey)[:,3]

variance_alpha_prey = statistics.variance(alpha_all_means)
variance_beta_prey = statistics.variance(beta_all_means)
variance_delta_prey = statistics.variance(delta_all_means)
variance_gamma_prey = statistics.variance(gamma_all_means)

ci_alpha_prey = 1.96 * np.array(variance_alpha_prey)/25
ci_beta_prey = 1.96 * np.array(variance_beta_prey)/25
ci_delta_prey = 1.96 * np.array(variance_delta_prey)/25
ci_gamma_prey = 1.96 *np.array(variance_gamma_prey)/25

print(beta_all_means, npoints)
plt.figure(dpi = 300)
fig, axes = plt.subplots(2, 2, figsize=(15, 15))

bar_width = 0.5
plt.subplot(221)
plt.title(r'$\alpha$')
plt.bar(npoints, alpha_all_means, yerr = ci_alpha_prey,color = "orange"
plt.subplot(222)
plt.title(r'$\beta$')
plt.bar(npoints, beta_all_means, yerr = ci_beta_prey,color = "orange",e
plt.subplot(223)
plt.title(r'$\delta$')
plt.bar(npoints, delta_all_means, yerr = ci_delta_prey,color = "orange"
plt.subplot(224)
```

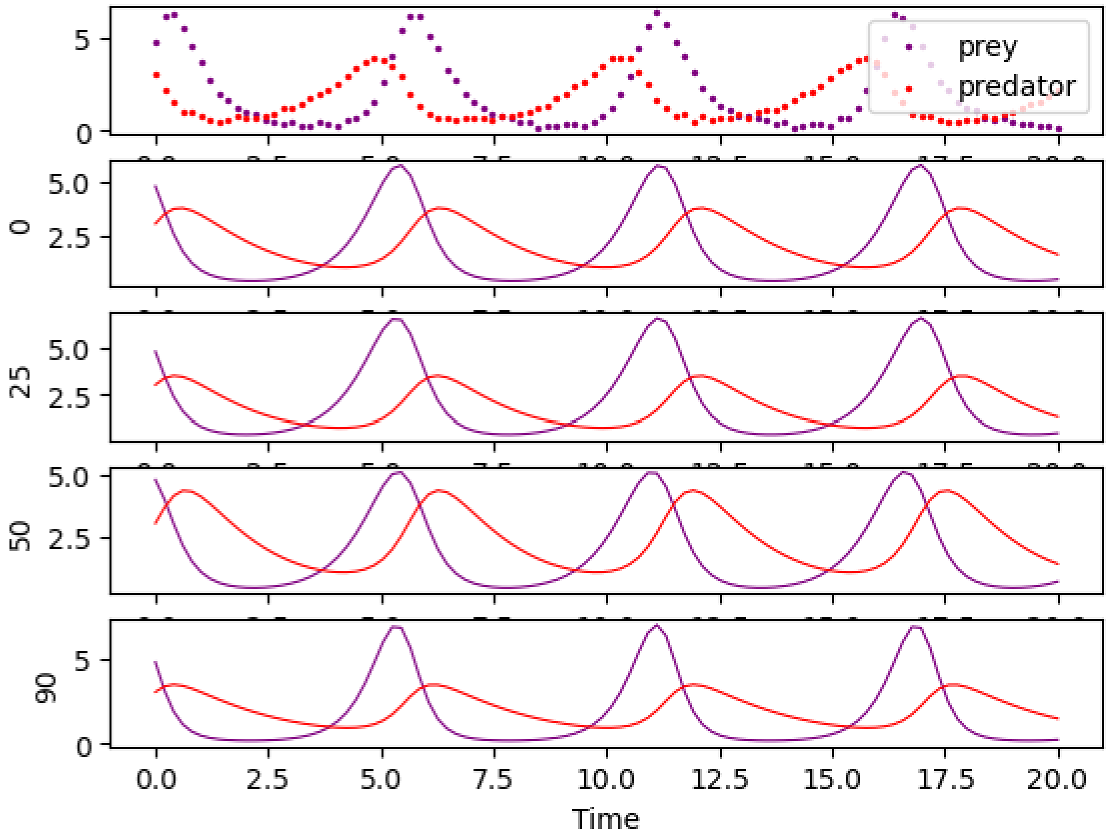
```
plt.title(r'$\gamma$')
plt.bar(npoints, gamma_all_means, yerr = ci_gamma_prey,color = "orange'
```

In [14]:

```
def MSE2(actual, predicted):
    '''Mean squared error'''
    x1 = actual[:, 0]
    y1 = actual[:, 1]

    #Getting useful indexes
    indx_x = np.where(~np.isnan(x1))
    indx_y = np.where(~np.isnan(y1))

    x2, y2 = predicted[:, 0], predicted[:, 1]
    err1 = (x1[indx_x] - x2[indx_x])**2
    err2 = (y1[indx_y] - y2[indx_y])**2
    err = np.concatenate([err1, err2])

    return np.nanmean(err)
```

In [20]:
```
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]
cooling_constant = 0.10
parameters =  [np.random.uniform(0,1), np.random.uniform(0,1), np.rando

Result_full = inferance_removal(initial_temp,cooling_constant, MSE2, si
Result_quarter = inferance_removal(initial_temp,cooling_constant, MSE2,
Result_half = inferance_removal(initial_temp,cooling_constant, MSE2, si
Result_90 = inferance_removal(initial_temp,cooling_constant, MSE2, simu

Integration_full = predator_prey_integration(time,inp[0],Result_full[0]
Integration_quarter = predator_prey_integration(time,inp[0],Result_quar
Integration_half = predator_prey_integration(time,inp[0],Result_half[0]
Integration_90 = predator_prey_integration(time,inp[0],Result_90[0])

plt.plot(dpi = 300, figsize = (20, 5))
plt.subplot(511)
plt.scatter(time, inp.T[0], color = 'purple', s = 2, label = 'prey')
plt.scatter(time, inp.T[1], color = 'red', s = 2, label = 'predator')
plt.legend()
plt.subplot(512)
plt.plot(time, Integration_full[:,0], color = 'purple', label = 'prey',
plt.plot(time, Integration_full[:,1], color = 'red', label = 'predator'
plt.ylabel('0')
plt.subplot(513)
plt.plot(time, Integration_quarter[:,0], color = 'purple', label = 'pre
plt.plot(time, Integration_quarter[:,1], color = 'red', label = 'predat
plt.ylabel('25')
plt.subplot(514)
plt.plot(time, Integration_half[:,0], color = 'purple', label = 'prey',
plt.plot(time, Integration_half[:,1], color = 'red', label = 'predator'
plt.ylabel('50')
plt.subplot(515)
plt.plot(time, Integration_90[:,0], color = 'purple', label = 'prey', l
plt.plot(time, Integration_90[:,1], color = 'red', label = 'predator',
plt.ylabel('90')
plt.xlabel('Time')
plt.show()
plt.close()

```

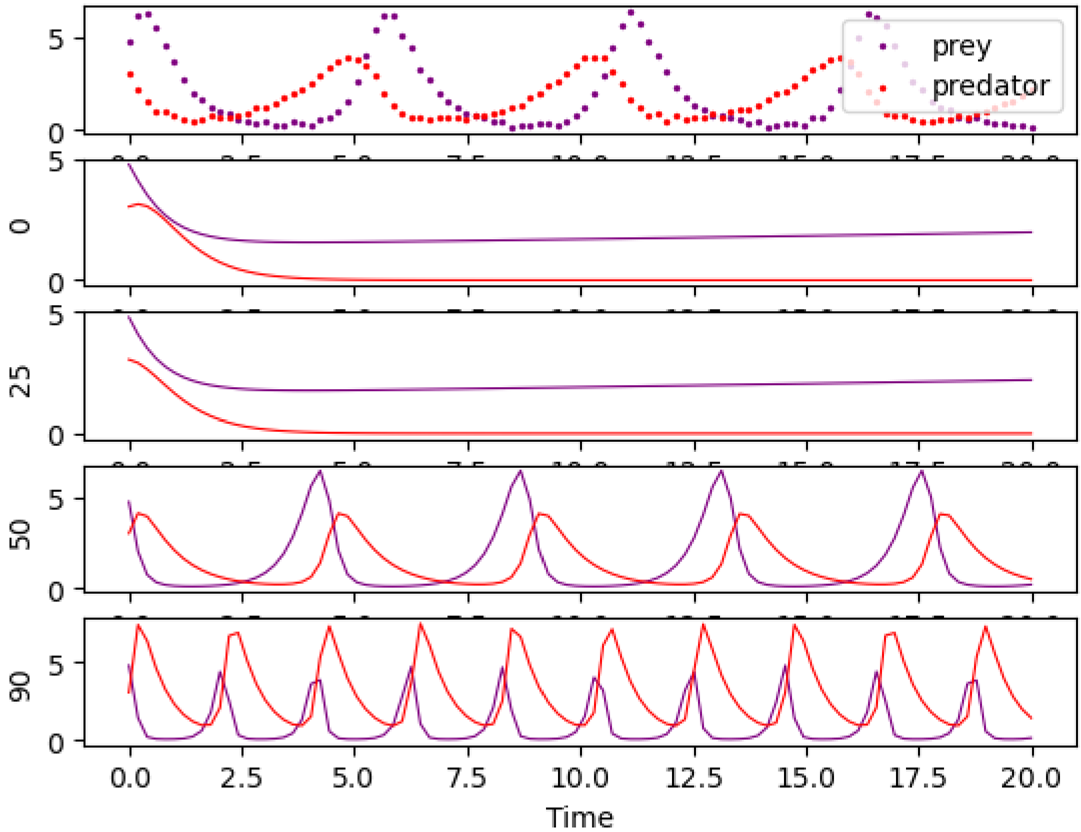
```
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\2635120008.py:22: Matplot
libDeprecationWarning: Auto-removal of overlapping axes is deprecated sinc
e 3.6 and will be removed two minor releases later; explicitly call ax.rem
ove() as needed.
  plt.subplot(511)
```



In [21]:

```
simulations = 2
iterations = 1
init_temp = 20
cooling = 0.1 # cooling strategy more aggressive
t = data[:,0]
time = t
inp = data[:,1:3]
cooling_constant = 0.10
parameters =  [np.random.uniform(0,1), np.random.uniform(0,1), np.rando

Result_full = inferance_removal(initial_temp,cooling_constant, MSE2, si
Result_quarter = inferance_removal(initial_temp,cooling_constant, MSE2,
Result_half = inferance_removal(initial_temp,cooling_constant, MSE2, si
Result_90 = inferance_removal(initial_temp,cooling_constant, MSE2, simu

Integration_full = predator_prey_integration(time,inp[0],Result_full[0]
Integration_quarter = predator_prey_integration(time,inp[0],Result_quar
Integration_half = predator_prey_integration(time,inp[0],Result_half[0]
Integration_90 = predator_prey_integration(time,inp[0],Result_90[0])

plt.plot(dpi = 300, figsize = (20, 5))
plt.subplot(511)
plt.scatter(time, inp.T[0], color = 'purple', s = 2, label = 'prey')
plt.scatter(time, inp.T[1], color = 'red', s = 2, label = 'predator')
plt.legend()
plt.subplot(512)
plt.plot(time, Integration_full[:,0], color = 'purple', label = 'prey',
plt.plot(time, Integration_full[:,1], color = 'red', label = 'predator'
plt.ylabel('0')
plt.subplot(513)
plt.plot(time, Integration_quarter[:,0], color = 'purple', label = 'pre
plt.plot(time, Integration_quarter[:,1], color = 'red', label = 'predat
plt.ylabel('25')
plt.subplot(514)
plt.plot(time, Integration_half[:,0], color = 'purple', label = 'prey',
plt.plot(time, Integration_half[:,1], color = 'red', label = 'predator'
plt.ylabel('50')
plt.subplot(515)
plt.plot(time, Integration_90[:,0], color = 'purple', label = 'prey', l
plt.plot(time, Integration_90[:,1], color = 'red', label = 'predator',
plt.ylabel('90')
plt.xlabel('Time')
plt.show()
plt.close()

```

```
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\1335953606.py:38: Runtime
Warning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Excess accuracy requested (tolerances to
o small). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
C:\Users\Aleks\AppData\Local\Temp\ipykernel_1540\631426890.py:22: Matplotl
ibDeprecationWarning: Auto-removal of overlapping axes is deprecated since
3.6 and will be removed two minor releases later; explicitly call ax.remov
e() as needed.
  plt.subplot(511)
```



In [ ]:

```
1
```

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.stats import norm
import pandas as pd
from scipy.integrate import odeint
import time
import statistics
import random
import scipy.stats

```

Opening predator-prey dataset

In [3]:
```
df = pd.read_csv('predator-prey-data.csv', index_col=False)
df.head()

```

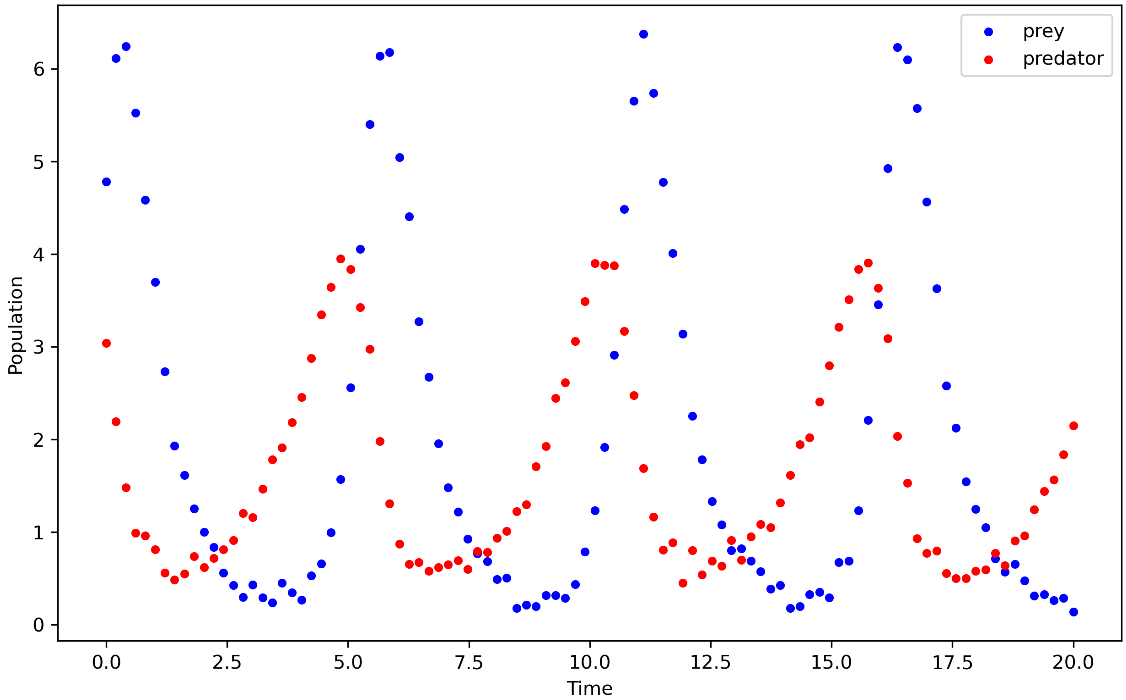
Out[3]:

	Unnamed: 0	t	x	y
0	0	0.000000	4.781635	3.035257
1	1	0.202020	6.114005	2.189746
2	2	0.404040	6.238361	1.478907
3	3	0.606061	5.520524	0.989836
4	4	0.808081	4.582546	0.957827

In [4]:

```
# Loading data into read-only numpy arrays
data = df[['t','x','y']].values
# data[1], data[2] = data[2].copy(), data[1].copy()
data.flags.writeable = False


# Plotting
plt.figure(dpi =300, figsize=(10, 6))
point_width = 13
# X should be prey
plt.scatter(data[:,0], data[:,1], label = 'prey', color = 'blue', s =pc
plt.scatter(data[:,0], data[:,2], label = 'predator', color = 'red', s=
plt.ylabel('Population')
plt.xlabel('Time')
plt.legend()

```

Out[4]: `<matplotlib.legend.Legend at 0x14c151ad390>`



Objective functions

Defining volterra equations function

In [5]:
```
def predator_prey_odes(initial_conditions,time ,alpha, beta, delta, gam
    x = initial_conditions[0]  # initial predator population
    y = initial_conditions[1]  # initial prey population
    dxdt = (alpha * x) - (beta * x * y)  # Predator ODE
    dydt = (delta * x * y) - (gamma * y)  # Predator ODE
    return [dxdt, dydt]

#Function that will return the data for predator and prey for a given s
def predator_prey_integration(time,initial_conditions,parameters):
    alpha,beta,delta,gamma = parameters
    #odeint is now used as part of this function which returns the # of
    results = odeint(predator_prey_odes,initial_conditions, time, args=
    predator_values,prey_values = results[:,0], results[:,1]
    return np.array([predator_values,prey_values]).T

```

In [ ]:
```



```

Defining objective functions

In [6]:

```
# modulo linear error
def MSE(actual, predicted):
    '''Mean squared error'''
    return np.mean((actual - predicted)**2)

def MSE2(actual, predicted):
    '''Mean squared error, handles nan values'''
    x1, y1 = actual[:, 0], actual[:, 1]

    # Getting useful indexes
    indx_x = np.where(~np.isnan(x1))
    indx_y = np.where(~np.isnan(y1))
    x2, y2 = predicted[:, 0], predicted[:, 1]

    err1 = (x1[indx_x] - x2[indx_x])**2
    err2 = (y1[indx_y] - y2[indx_y])**2

    # Concatenate the arrays before calculating the mean
    errors = np.concatenate([err1, err2])

    # Use np.nanmean to handle NaN values during the mean calculation
    return np.nanmean(errors)


def MAE(actual, predicted):
    '''Calculate Mean Absolute Error (MAE) for multidimensional data.''
    mae = np.mean(np.abs(actual - predicted))
    return mae

def MAE2(actual, predicted):
    '''Calculate Mean Absolute Error (MAE) for multidimensional data, h
    x1, y1 = actual[:, 0], actual[:, 1]

    # Getting useful indexes
    indx_x = np.where(~np.isnan(x1))
    indx_y = np.where(~np.isnan(y1))

    x2, y2 = predicted[:, 0], predicted[:, 1]

    err1 = np.abs(x1[indx_x] - x2[indx_x])
    err2 = np.abs(y1[indx_y] - y2[indx_y])

    mae = np.nanmean(np.concatenate([err1, err2]))

    return mae


```

Algorithms & Optimisation

Defining minimization algorithms

In [7]:

```

def random_walk(parameters, variance = 0.5):
    lst = [parameter + np.random.normal(0, 1) for parameter in paramete
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                while lst[indx] < 0:
                    lst[indx] = parameters[indx] + np.random.normal(0,
    return lst


def hill_climbing(data, time, initial_conditions, parameters, objective
    '''Tries to find the best solution using random walker'''
    # Initialize starting parameter state
    scores = []
    x_n = parameters
    all_scores = []

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est)
    scores.append(current_score)
    number_iterations= 1

    for k in range(max_iterations):
        # Generate a random walk for parameters
        x_n_1 = random_walk(x_n, variance)

        # Calculate the current and next estimations
        current_est = predator_prey_integration(time, initial_conditior
        new_estimation = predator_prey_integration(time, initial_condit

        new_score = objective(data, new_estimation)

        # If the next estimation is better, update the parameters
        if new_score < current_score:
            number_iterations = k
            current_score = new_score
            x_n = x_n_1
            scores.append(current_score)

    return x_n, scores, number_iterations
```

In [8]:
```
def simulated_annealing(initial_temp,cooling_constant, data, time, init

    temp = initial_temp #Scaling factor for random movement. We square 
    start = parameters #Initial starting parameters
    x_n = start
    scores = [] #A score is just the value of the objective function ev

    current_est = predator_prey_integration(time, initial_conditions, x
    current_score = objective(data, current_est) #The current value of 
    scores.append(current_score) #Keeping track of the values of the ob

    #cur = function(x) #The function value of the current x solution
    history = [x_n] #Stores previously searched x values

    for i in range (max_iterations):
        proposal = random_walk(x_n) #A new proposal for the parameters 
        new_est = predator_prey_integration(time, initial_conditions, p
        new_score = objective(data, new_est) #Calculate new value of ob

        delta = new_score - current_score #Difference in objective func

        #if proposal < 0 or proposal > 1:
           #proposal = x_n # Reject proposal by setting it equal to pre

        acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate

        #if delta < 0:
           #x_n = proposal ##Accept proposal
            #current_score = new_score

        if np.random.rand() < acceptance_probability: #else if it is nc
            x_n = proposal #Accept proposal
            current_score = new_score

        scores.append(current_score)
        temp = cooling_constant**i * initial_temp #Cool temperature
        #print(temp)
        history.append(x_n) #Add to history

    return x_n, scores



```

Multiple run algorithms

In [9]:
```
def uniform_draw_g(lower_bound, upper_bound):
    while True:
        yield np.random.uniform(lower_bound, upper_bound)

def multiple_runs_annealing(initial_temp,cooling_constant,input_data,t,

    mse_total_list = []
    all_all_best = []

    for i in range(n_runs):

        x_best, scores = simulated_annealing(initial_temp,cooling_const
        all_all_best.append(x_best)

        x = predator_prey_integration(t,initial_conditions,x_best)
        mse_prey = MSE(data[:,1],x[:,0])
        mse_predator = MSE(data[:,2],x[:,1])
        mse_total = mse_prey + mse_predator

        mse_total_list.append(mse_total) #Add total MSE for this simula

    return np.array(all_all_best) , mse_total_list



def multi_run_hill_climbing(data, objective, nruns = 50, nsamples=100,
    initial_conditions = data[0][1:3]
    time = data[:,0]

    # Defining generators for variables
    alpha = uniform_draw_g(0,1)
    beta = uniform_draw_g(0,1)
    delta = uniform_draw_g(0,1)
    gamma = uniform_draw_g(0,1)

    # Lists for storing values
    parameter_list = []
    best = []
    best_score = float('inf')
    best_param = None
    num_iterations = []

    # Running simulation for
    for __ in range(nruns):

        parameters = [next(alpha), next(beta), next(delta), next(gamma)
        params, score, iterations = hill_climbing(data[:,1:3], time, in
        parameter_list.append(params)
        num_iterations.append(iterations)
        scores.append(score)

        #Saving best parameter combination
        if score[-1] < best_score:
            best_score = score[-1]
            best_param = params

    parameter_list = np.array(parameter_list)

    return parameter_list, best_param, scores, best_score, num_iteratic
```

```
60
```

Plotting hill climbing

In [10]:

```python
input_data = data[:,1:3]
# t =
initial_conditions = [input_data[0][0], input_data[0][1]]

alpha = np.random.uniform(0.5, 2)
beta = np.random.uniform(0.5, 2)
delta = np.random.uniform(0.5, 2)
gamma = np.random.uniform(0.5, 2)
parameters = [alpha, beta, delta, gamma]

# Using MSEx
x_best, scores, num_iterations = hill_climbing(input_data, data[:,0], i
print(x_best,scores,num_iterations)
```

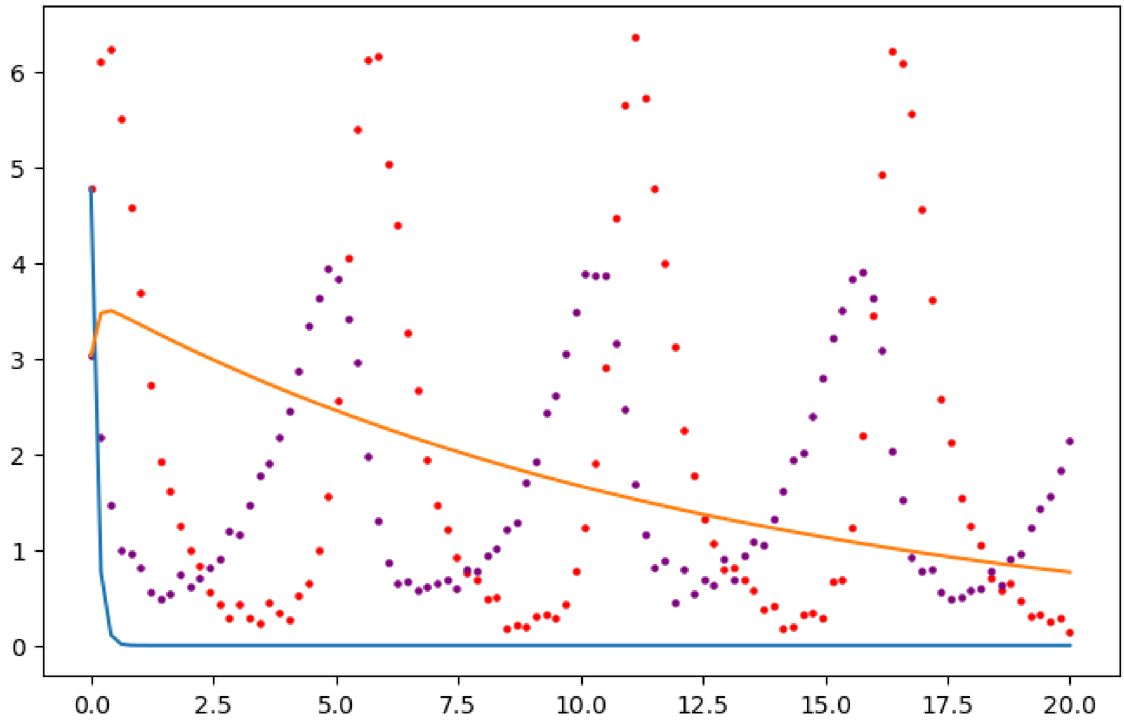
```
[2.058470826384955, 3.3348226913782497, 0.33391386324627437, 0.07775331273
010042] [1.7841476511911036, 1.7630633552849264, 1.7463166480090968, 1.741
6628363579707, 1.7024628624472102, 1.6549539797197672, 1.541264871748595]
16
```

Plotting hill climbing results

In [11]:

```
# t, x ,y = data
initial_conditions = [input_data[0][0], input_data[0][1]]
t = data[:,0]

parameters = x_best
# Using MSE
x = predator_prey_integration(t,initial_conditions,parameters)

# Increase the figure size
plt.figure(figsize=(8, 5))

plt.plot(t, x[:,0])
plt.plot(t, x[:,1])

plt.scatter(t, data[:,1], color= 'red', s =5)
plt.scatter(t, data[:,2], color= 'purple', s=5)

plt.figure(figsize=(10, 8))
```

Out[11]: <Figure size 1000x800 with 0 Axes>



<Figure size 1000x800 with 0 Axes>

Running simulation for different random walker variance

In [ ]:
```
# parameter_list = np.array(parameter_list)
# # Create a figure with 3x3 subplotshttp://localhost:8888/notebooks/De
# fig, axes = plt.subplots(3, 3, figsize=(12, 12), sharex=True)

# # Plot histograms on each subplot using for loops with the same color
# color = 'blue'
# titles = ['variance = 0.1', 'variance=0.25', 'variance=0.5']
# x_titles = ['alpha', 'beta', 'delta', 'omega']

# for i in range(3):
#     for j in range(3):
#         ax = axes[i, j]
#         ax.hist(parameter_list[j][:,i])
#         ax.set_xlabel(x_titles[i])
#         ax.set_ylabel('Frequency')
#         ax.set_title(titles[j])

# # Adjust layout to prevent overlapping
# plt.tight_layout()

# # Show the plot
# plt.show()

```

Running multi run for hill climbing

In [12]:
```

# We save the parameter estimation we will use as ground truth for test
parameter_list, reference_param, scores, reference_score, num_iteration

# Integrating with best guess
results = predator_prey_integration(t,initial_conditions,reference_para

# Increase the figure size
plt.figure(figsize=(8, 5))

plt.plot(data[:,0], results[:,0])
plt.plot(data[:,0], results[:,1])

plt.scatter(t, data[:,1], color= 'red', s =5)
plt.scatter(t, data[:,2], color= 'purple', s=5)

plt.show()

```

```
C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Excess work done on this call (perhaps w
rong Dfun type). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
```

```
---------------------------------------------------------------------------
KeyboardInterrupt                         Traceback (most recent call last)
Cell In[12], line 2
      1 # We save the parameter estimation we will use as ground truth for testing
----> 2 parameter_list, reference_param, scores, reference_score, num_iterations = multi_run_hill_climbing(data, MSE,nruns = 200)
      4 # Integrating with best guess
      5 results = predator_prey_integration(t,initial_conditions,reference_param)

Cell In[9], line 47, in multi_run_hill_climbing(data, objective, nruns, nsamples, variance)
     44 for __ in range(nruns):
     46     parameters = [next(alpha), next(beta), next(delta), next(gamma)]
---> 47     params, score, iterations = hill_climbing(data[:,1:3], time, initial_conditions, parameters, objective, max_iterations=nsamples,variance=variance)
     48     parameter_list.append(params)
     49     num_iterations.append(iterations)

Cell In[7], line 30, in hill_climbing(data, time, initial_conditions, parameters, objective, max_iterations, variance)
     28 # Calculate the current and next estimations
     29 current_est = predator_prey_integration(time, initial_conditions, x_n)
---> 30 new_estimation = predator_prey_integration(time, initial_conditions, x_n_1)
     32 new_score = objective(data, new_estimation)
     34 # If the next estimation is better, update the parameters

Cell In[5], line 12, in predator_prey_integration(time, initial_conditions, parameters)
     10 alpha,beta,delta,gamma = parameters
     11 #odeint is now used as part of this function which returns the # of infected in the model
---> 12 results = odeint(predator_prey_odes,initial_conditions, time, args=(alpha,beta,delta,gamma))
     13 predator_values,prey_values = results[:,0], results[:,1]
     14 return np.array([predator_values,prey_values]).T

File ~\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_odepack_py.py:242, in odeint(func, y0, t, args, Dfun, col_deriv, full_output, ml, mu, rtol, atol, tcrit, h0, hmax, hmin, ixpr, mxstep, mxhnil, mxordn, mxords, printmessg, tfirst)
    240 t = copy(t)
    241 y0 = copy(y0)
--> 242 output = _odepack.odeint(func, y0, t, args, Dfun, col_deriv, ml, mu,
    243                          full_output, rtol, atol, tcrit, h0, hmax, hmin,
    244                          ixpr, mxstep, mxhnil, mxordn, mxords,
    245                          int(bool(tfirst)))
    246 if output[-1] < 0:
    247     warning_msg = _msgs[output[-1]] + " Run with full_output = 1 to get quantitative information."
```

```
KeyboardInterrupt:
```

Kaya's code section: Points removal

In [13]:

```python
def point_removal(time, input_data, points_removed, Focus = 'both'):
    '''removes points randomly'''

    #We set the seed for removing points
    random.seed(123)

    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # initialize set up for removing points randomly given the bounds
    removal_options = np.arange(0,len(time))

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(removal_options, k = points

    # remove points based on choices for points to be removed
    if Focus == 'both':
        for i in removed_points_indices:
            prey[i] = None
            predator[i] = None

    elif Focus == 'prey':
        for i in removed_points_indices:
            prey[i] = None

    elif Focus == 'predator':
        for i in removed_points_indices:
            predator[i] = None

    return np.array([time, prey, predator]).T


```

In [14]:
```
def extrema_removal(time, input_data, points_removed, Focus = 'both'):
    '''Removes points in extrema'''
    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # Calculate mean and variance to set regions for data
    mean_prey_population, mean_predator_population = np.mean(prey), np.
    variance_prey, variance_predator = statistics.variance(prey), stati

    # set upper bound and lower bound for point removals
    ub_prey, lb_prey = mean_prey_population + 1.645*variance_prey/len(t
    ub_predator, lb_predator = mean_predator_population + 1.645*varianc

    # initialize set up for removing points randomly given the bounds
    prey_options = []
    predator_options = []
    # enumerate through list of stored points
    for index, prey_count in enumerate(prey):
        # check if they are in specified region
        if prey_count > ub_prey or prey_count < lb_prey:
            prey_options.append([index, prey_count, predator[index]])
    for index, predator_count in enumerate(predator):
        if predator_count > ub_predator or predator_count < lb_predator
            predator_options.append([index, prey[index], predator_count

    # remove points from list depending on which focus is set
    removal_options = []
    if Focus == 'both':
        removal_options = removal_options + prey_options + predator_opt
    elif Focus == 'prey':
        removal_options = removal_options + prey_options
    elif Focus == 'predator':
        removal_options = removal_options + predator_options
    else:
        print('Error: Removal option not known. Try either both, prey,

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(np.array(removal_options).T

    # turn the list into integers so we can remove them based on the in
    integer_array = []
    for counter in range(len(removed_points_indices)):
        integer_array.append(int(removed_points_indices[counter]))

    # update the lists based on points we wanted to remove
    if Focus == 'both':
        for i in integer_array:
            prey[i] = None
            predator[i] = None

    elif Focus == 'prey':
        for i in integer_array:
            prey[i] = None

    elif Focus == 'predator':
        for i in integer_array:
            predator[i] = None

```

```
    return np.array(time), np.array(prey), np.array(predator)

# extrema_removal(t, input_data, 5, Focus = 'both')
```

In [15]:
```
def midpoint_removal(time, input_data, points_removed, Focus = 'both'):
    '''Removes points close to the mean'''
    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # Calculate mean and variance to set regions for data
    mean_prey_population, mean_predator_population = np.mean(prey), np.
    variance_prey, variance_predator = statistics.variance(prey), stati

    # set upper bound and lower bound for point removals
    ub_prey, lb_prey = mean_prey_population + 1.645*variance_prey/len(t
    ub_predator, lb_predator = mean_predator_population + 1.645*varianc

    # initialize set up for removing points randomly given the bounds
    prey_options = []
    predator_options = []
    # enumerate through list of stored points
    for index, prey_count in enumerate(prey):
        # check if they are in specified region
        if prey_count <= ub_prey or prey_count >= lb_prey:
            prey_options.append([index, prey_count, predator[index]])
    for index, predator_count in enumerate(predator):
        if predator_count <= ub_predator or predator_count >= lb_predat
            predator_options.append([index, prey[index], predator_count

    # remove points from list depending on which focus is set
    removal_options = []
    if Focus == 'both':
        removal_options = removal_options + prey_options + predator_opt
    elif Focus == 'prey':
        removal_options = removal_options + prey_options
    elif Focus == 'predator':
        removal_options = removal_options + predator_options
    else:
        print('Error: Removal option not known. Try either both, prey,

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(np.array(removal_options).T

    # turn the list into integers so we can remove them based on the ir
    integer_array = []
    for counter in range(len(removed_points_indices)):
        integer_array.append(int(removed_points_indices[counter]))

    # update the lists based on points we wanted to remove
    if Focus == 'both':
        for i in integer_array:
            prey[i] = None
            predator[i] = None

    elif Focus == 'prey':
        for i in integer_array:
            prey[i] = None

    elif Focus == 'predator':
        for i in integer_array:
            predator[i] = None

```

```
    return np.array([time, prey, predator]).T

```

In [ ]:

```
# 1. Run multi run for different size datasets save best parameters
# 2.Calculate MSE for each run for best parameters
# 2. Do this for 2x, one only for predator, other for prey
# 4. Plot error relative to best solution of y axis
# 5. On x axis should be relative number points

```

Hypothesis testing random removal points (Aleks section)

Duplicating code for the functions I use in case they are different

In [ ]:

```
def random_walk(parameters, variance = 0.5):
    lst = [parameter + np.random.normal(0, 1) for parameter in paramet
    # Ensure all elements are positive
    while any(x <= 0 for x in lst):
        for indx in range(len(lst)):
            if lst[indx] <= 0:
                while lst[indx] < 0:
                    lst[indx] = parameters[indx] + np.random.normal(0,
    return lst


def hill_climbing(data, time, initial_conditions, parameters, objectiv
    '''Tries to find the best solution using random walker'''
    # Initialize starting parameter state
    scores = []
    x_n = parameters
    all_scores = []

    current_est = predator_prey_integration(time, initial_conditions, 
    current_score = objective(data, current_est)
    scores.append(current_score)
    number_iterations= 1

    for k in range(max_iterations):
        # Generate a random walk for parameters
        x_n_1 = random_walk(x_n, variance)

        # Calculate the current and next estimations
        current_est = predator_prey_integration(time, initial_conditio
        new_estimation = predator_prey_integration(time, initial_condi

        new_score = objective(data, new_estimation)

        # If the next estimation is better, update the parameters
        if new_score < current_score:
            number_iterations = k
            current_score = new_score
            x_n = x_n_1
            scores.append(current_score)

    return x_n, scores, number_iterations

def simulated_annealing(initial_temp,cooling_constant, data, time, ini

    temp = initial_temp #Scaling factor for random movement. We square
    start = parameters #Initial starting parameters
    x_n = start
    scores = [] #A score is just the value of the objective function e

    current_est = predator_prey_integration(time, initial_conditions, 
    current_score = objective(data, current_est) #The current value of
    scores.append(current_score) #Keeping track of the values of the o

    #cur = function(x) #The function value of the current x solution
    history = [x_n] #Stores previously searched x values

    for i in range (max_iterations):
        proposal = random_walk(x_n) #A new proposal for the parameters
        new_est = predator_prey_integration(time, initial_conditions, 
        new_score = objective(data, new_est) #Calculate new value of o

```

```
        delta = new_score - current_score #Difference in objective fun

        #if proposal < 0 or proposal > 1:
           #proposal = x_n # Reject proposal by setting it equal to pr

        acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculat

        #if delta < 0:
           #x_n = proposal ##Accept proposal
            #current_score = new_score

        if np.random.rand() < acceptance_probability: #else if it is n
            x_n = proposal #Accept proposal
            current_score = new_score

        scores.append(current_score)
        temp = cooling_constant**i * initial_temp #Cool temperature
        #print(temp)
        history.append(x_n) #Add to history

    return x_n, scores


def uniform_draw_g(lower_bound, upper_bound):
    while True:
        yield np.random.uniform(lower_bound, upper_bound)

def multiple_runs_annealing(initial_temp,cooling_constant,input_data,t

    mse_total_list = []
    all_all_best = []

    for i in range(n_runs):

        x_best, scores = simulated_annealing(initial_temp,cooling_cons
        all_all_best.append(x_best)

        x = predator_prey_integration(t,initial_conditions,x_best)
        mse_prey = MSE(data[:,1],x[:,0])
        mse_predator = MSE(data[:,2],x[:,1])
        mse_total = mse_prey + mse_predator

        mse_total_list.append(mse_total) #Add total MSE for this simul

    return np.array(all_all_best) , mse_total_list



def multi_run_hill_climbing(data, objective, nruns = 50, nsamples=100,
    initial_conditions = data[0][1:3]
    time = data[:,0]

    # Defining generators for variables
    alpha = uniform_draw_g(0,1)
    beta = uniform_draw_g(0,1)
    delta = uniform_draw_g(0,1)
    gamma = uniform_draw_g(0,1)

    # Lists for storing values
    parameter_list = []
    best = []
```

```
    best_score = float('inf')
    best_param = None
    num_iterations = []

    # Running simulation for
    for __ in range(nruns):

        parameters = [next(alpha), next(beta), next(delta), next(gamma
        params, score, iterations = hill_climbing(data[:,1:3], time, i
        parameter_list.append(params)
        num_iterations.append(iterations)
        scores.append(score)

        #Saving best parameter combination
        if score[-1] < best_score:
            best_score = score[-1]
            best_param = params

    parameter_list = np.array(parameter_list)

    return parameter_list, best_param, scores, best_score, num_iterati


def point_removal(time, input_data, points_removed, Focus = 'both'):
    '''removes points randomly'''

    #We set the seed for removing points
    random.seed(123)

    prey = input_data.T[0].copy()
    predator = input_data.T[1].copy()

    # initialize set up for removing points randomly given the bounds
    removal_options = np.arange(0,len(time))

    # choose points to be removed randomly
    if points_removed > len(removal_options):
        points_removed = len(removal_options)
        print('WARNING: Maximum number of points that can be removed ha
    removed_points_indices = random.choices(removal_options, k = point

    # remove points based on choices for points to be removed
    if Focus == 'both':
        for i in removed_points_indices:
            prey[i] = None
            predator[i] = None

    elif Focus == 'prey':
        for i in removed_points_indices:
            prey[i] = None

    elif Focus == 'predator':
        for i in removed_points_indices:
            predator[i] = None

    return np.array([time, prey, predator]).T
```

Getting distribution of averages of best guesses for hill climbing (reference dataset)

In [22]:
```
# We get the reference distribution for testing

# Timing your code
start_time = time.time()

# Reference distribution of averages
ref_average1 = []
for k in range(50):
    parameter_list, best_param, scores, best_score, num_iterations = mu
    # Appending average
    ref_average1.append(np.mean(parameter_list, axis=0))

ref_average1 = np.array(ref_average1)

end_time = time.time()

# Calculating and printing the total time
total_time = end_time - start_time
print(f"Total time taken: {total_time} seconds")

# param_distribution, reference_param, scores, reference_score, num_ite
```

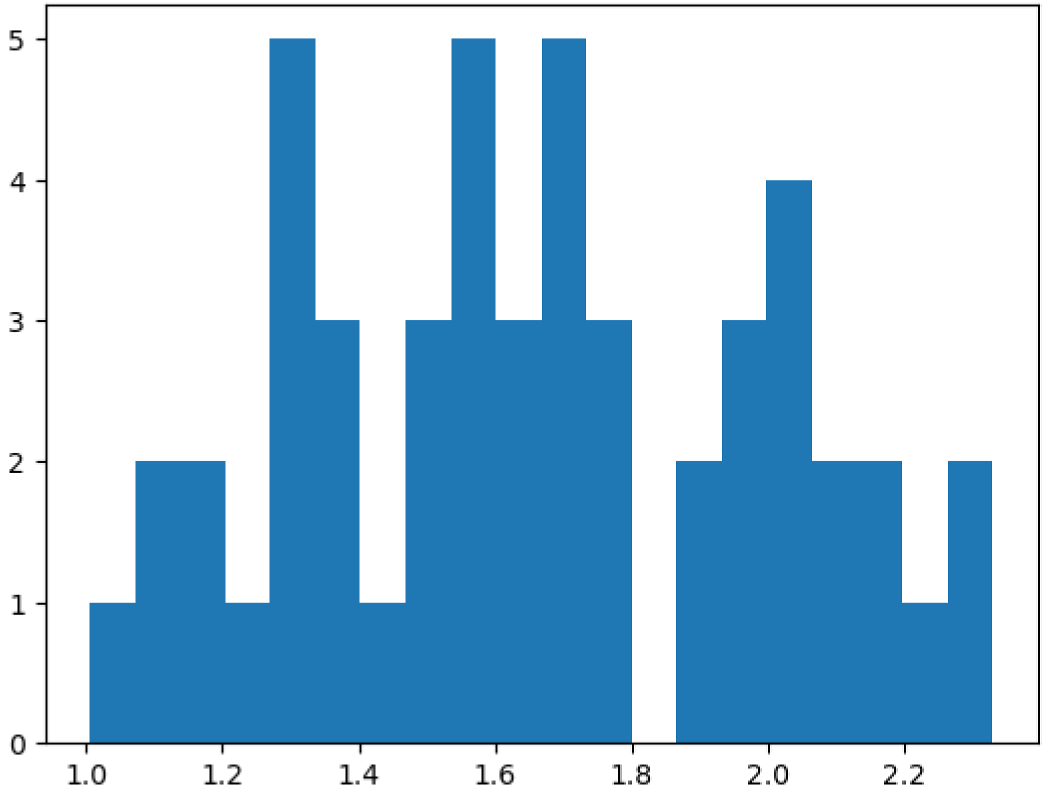
```
Total time taken: 439.93707609176636 seconds
```

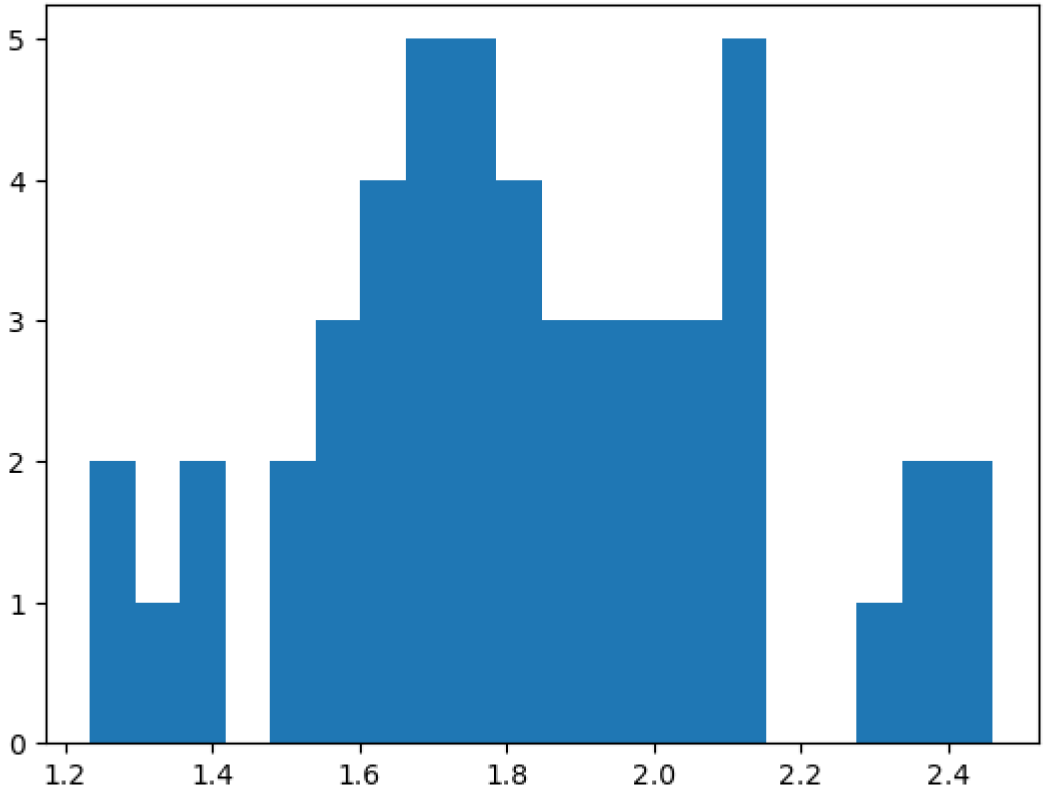
In [ ]:
```

```

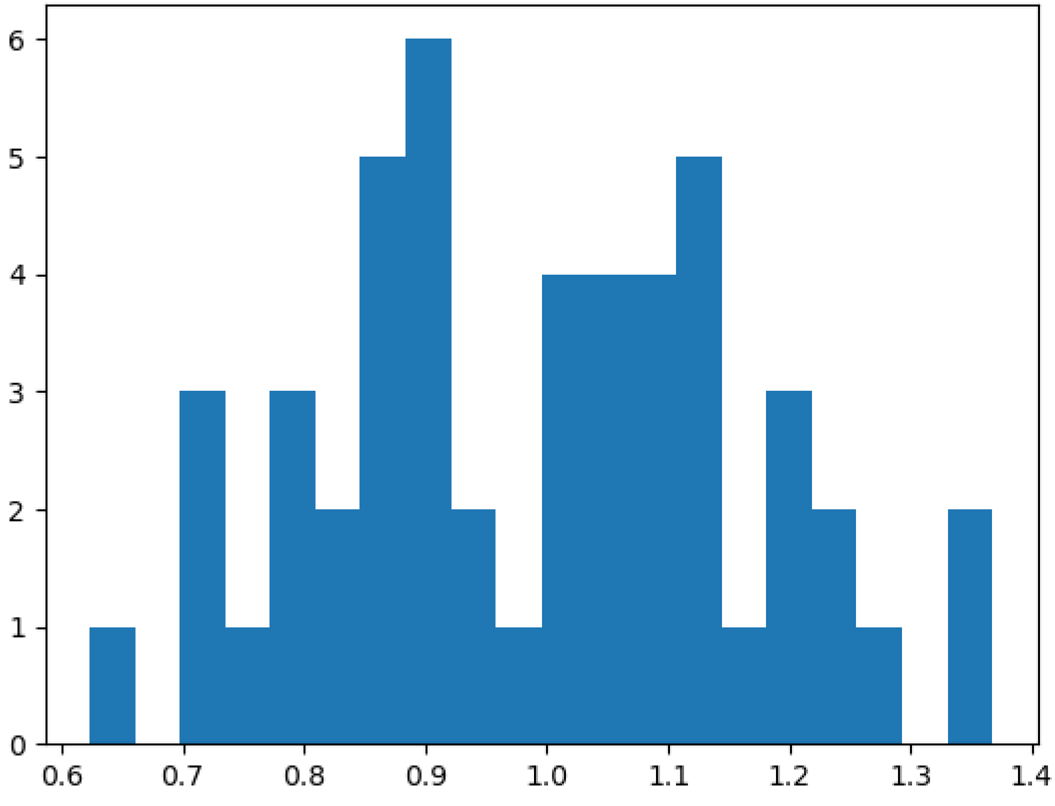
These histograms plots are optional (I dont think im adding them to the report)

In [24]:

```
# num_iterations
# print(ref_average)
# for k in range(3):
#         plt.hist(ref_average1[:,k], bins = 20)
#         plt.show()

# print(np.var(ref_average1,axis=0))
```








```
[0.1170307  0.08449044 0.02953349 0.11417836]
```

In [25]:
```
# # print(param_distribution)
# plt.axvline(x=reference_param[0], color='r', linestyle='--', label='V
# plt.hist(param_distribution[:,0], bins =30)
```

```
---------------------------------------------------------------------------
-
NameError                                 Traceback (most recent call las
t)
Cell In[25], line 2
      1 # print(param_distribution)
----> 2 plt.axvline(x=reference_param[0], color='r', linestyle='--', label
='Vertical Line at x=2.5')
      3 plt.hist(param_distribution[:,0], bins =30)

NameError: name 'reference_param' is not defined
```

Running welch test between reference distribution of averages and incomplete time series (hill climbing)

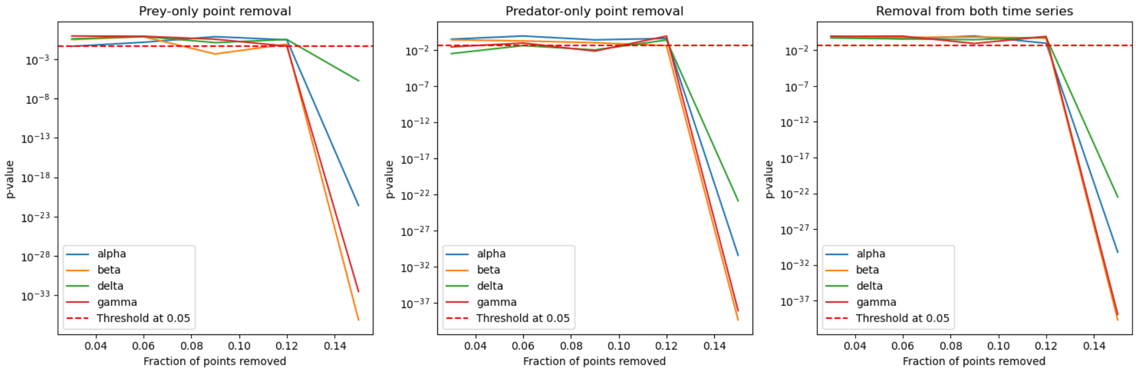
In [27]:
```
def random_point_ttests(data,ref_distribution, points_removed, focus_ch
    '''runs welch test for multi run of hill climbing for every paramet
    param_distribution = ref_distribution
#     focus_choices = ['prey', 'predator', 'both']
#     focus_choices = ['prey', 'predator', 'both']
    scores = [[],[]]
    p_values = {'prey': [], 'predator': [], 'both': []}

    for indx, choice in enumerate(focus_choices):
        print(choice)
        for npoints in points_removed:
            print(npoints)
    #         print(f"Points removed: {npoints}")
            limited_data = point_removal(data[:,0], data[:,1:3], npoint
            #Getting distribution of averages
            average_distribution = []
            for k in range(30):
                parameter_list, best_param, scores, best_score, num_ite
                #Appending average
                average_distribution.append(np.mean(parameter_list, axi

            average_distribution = np.array(average_distribution)
            t_stat1, p_value1 = scipy.stats.ttest_ind(ref_distribution[
            t_stat2, p_value2 = scipy.stats.ttest_ind(ref_distribution[
            t_stat3, p_value3 = scipy.stats.ttest_ind(ref_distribution[
            t_stat3, p_value4 = scipy.stats.ttest_ind(ref_distribution[
            p_values[choice].append([p_value1, p_value2, p_value3, p_va

    return p_values


```

In [28]:
```python
start_time = time.time()
p_values_hill_climbing =random_point_ttests(data,ref_average1, np.arang

end_time = time.time()

# Calculating and printing the total time
total_time = end_time - start_time
print(f"Total time taken: {total_time} seconds")
```

```
prey
3
6
9
12
15

C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Excess accuracy requested (tolerances to
o small). Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)

predator
3
6
9
12
15

C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Illegal input detected (internal error).
Run with full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)
C:\Users\Aleks\AppData\Local\anaconda3\Lib\site-packages\scipy\integrate\_
odepack_py.py:248: ODEintWarning: Run terminated (internal error). Run wit
h full_output = 1 to get quantitative information.
  warnings.warn(warning_msg, ODEintWarning)

both
3
6
9
12
15
Total time taken: 1060.7844800949097 seconds
```

Visualizing p-values from welch test for hill climbing

In [43]:
```

# Fraction points removed
fraction_points = np.arange(3,16,3) / 100
p_values_prey = np.array(p_values_hill_climbing['prey'])
p_values_predator = np.array(p_values_hill_climbing['predator'])
p_values_both = np.array(p_values_hill_climbing['both'])

# Creating subplots
fig, axes = plt.subplots(1, 3, figsize=(15, 5))

# Plotting p-values when only prey points are removed
axes[0].plot(fraction_points, p_values_prey[:, 0], label='alpha')
axes[0].plot(fraction_points, p_values_prey[:, 1], label='beta')
axes[0].plot(fraction_points, p_values_prey[:, 2], label='delta')
axes[0].plot(fraction_points, p_values_prey[:, 3], label='gamma')
axes[0].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[0].set_ylabel('p-value')
axes[0].set_xlabel('Fraction of points removed')
axes[0].set_yscale('log')
axes[0].set_title('Prey-only point removal')  # Add title to the first
axes[0].legend()

# Plotting p-values when only predator points are removed
axes[1].plot(fraction_points, p_values_predator[:, 0], label='alpha')
axes[1].plot(fraction_points, p_values_predator[:, 1], label='beta')
axes[1].plot(fraction_points, p_values_predator[:, 2], label='delta')
axes[1].plot(fraction_points, p_values_predator[:, 3], label='gamma')
axes[1].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[1].set_ylabel('p-value')
axes[1].set_xlabel('Fraction of points removed')
axes[1].set_yscale('log')
axes[1].set_title('Predator-only point removal')
axes[1].legend()

# Plotting p-values when both prey and predator points are removed
axes[2].plot(fraction_points, p_values_both[:, 0], label='alpha')
axes[2].plot(fraction_points, p_values_both[:, 1], label='beta')
axes[2].plot(fraction_points, p_values_both[:, 2], label='delta')
axes[2].plot(fraction_points, p_values_both[:, 3], label='gamma')
axes[2].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[2].set_ylabel('p-value')
axes[2].set_xlabel('Fraction of points removed')
axes[2].set_yscale('log')
axes[2].set_title('Removal from both time series')
axes[2].legend()

# Adjusting layout
plt.tight_layout()
plt.savefig('welch_tests_hill_climbing', dpi = 300)
plt.show()

```



Prey-only point removal
Predator-only point removal
Removal from both time series
p-value
Fraction of points removed
alpha
beta
delta
gamma
Threshold at 0.05

Getting distribution of averages of best guesses for simulated annealing (reference dataset)

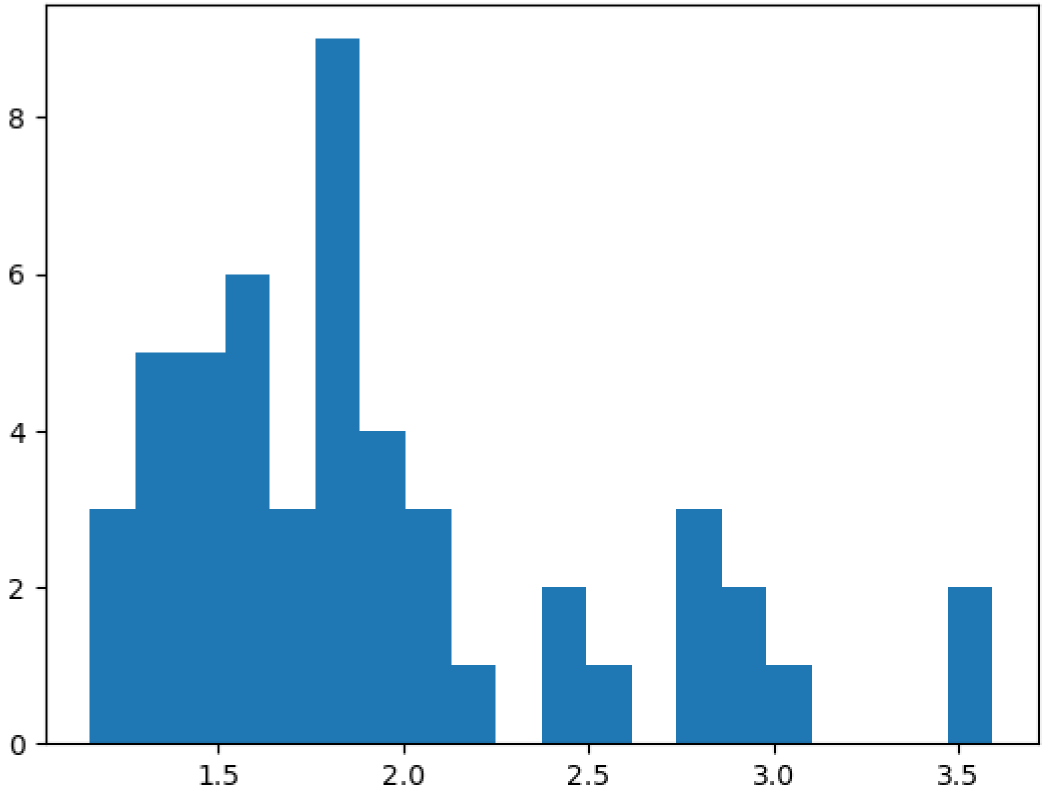
In [40]:

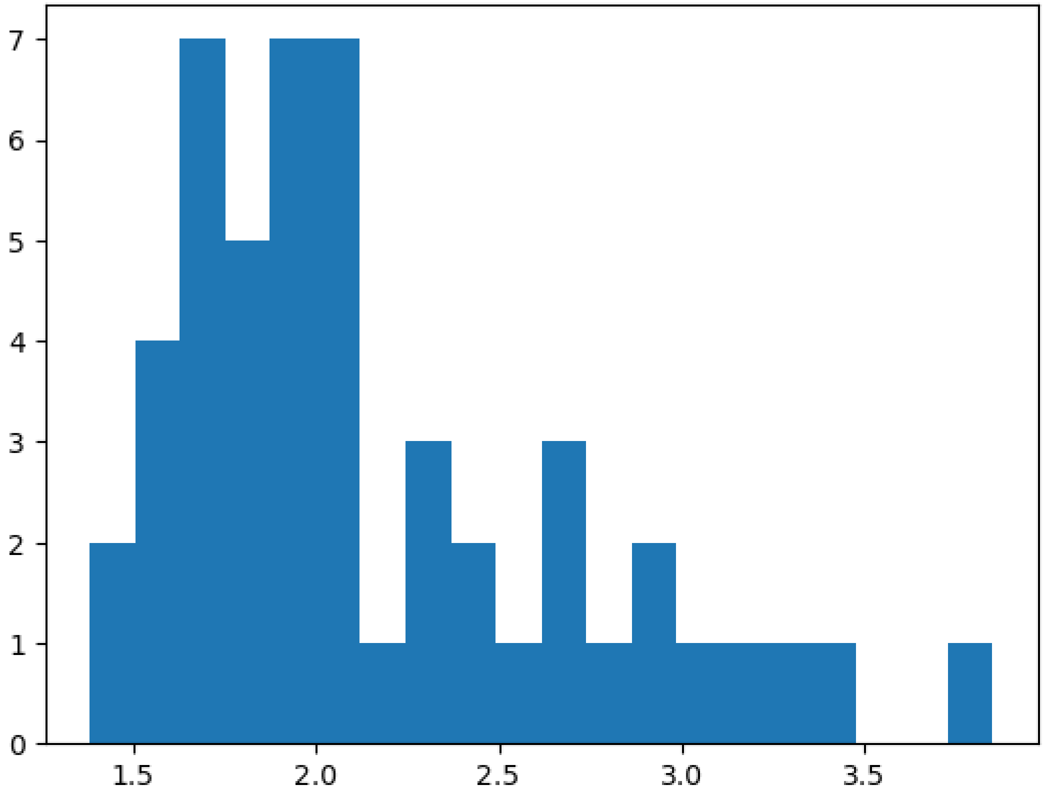
```
# We get the reference distribution for testing

# Timing your code
start_time = time.time()

initial_temp = 20
cooling_constant = 0.10

#Taking random draw for initial parameters (initial guess)
alpha = np.random.uniform(0,1)
beta = np.random.uniform(0,1)
delta = np.random.uniform(0,1)
gamma = np.random.uniform(0,1)
parameters = [alpha, beta, delta, gamma]
parameters = [alpha, beta, delta, gamma]

# Reference distribution of averages
ref_average2 = []
for k in range(50):
#     parameter_list, best_param, scores, best_score, num_iterations =
    parameter_list, scores= multiple_runs_annealing(initial_temp,coolir
    # Appending average
    ref_average2.append(np.mean(parameter_list, axis=0))

ref_average2 = np.array(ref_average2)
end_time = time.time()

# Calculating and printing the total time
total_time = end_time - start_time
print(f"Total time taken: {total_time} seconds")
```

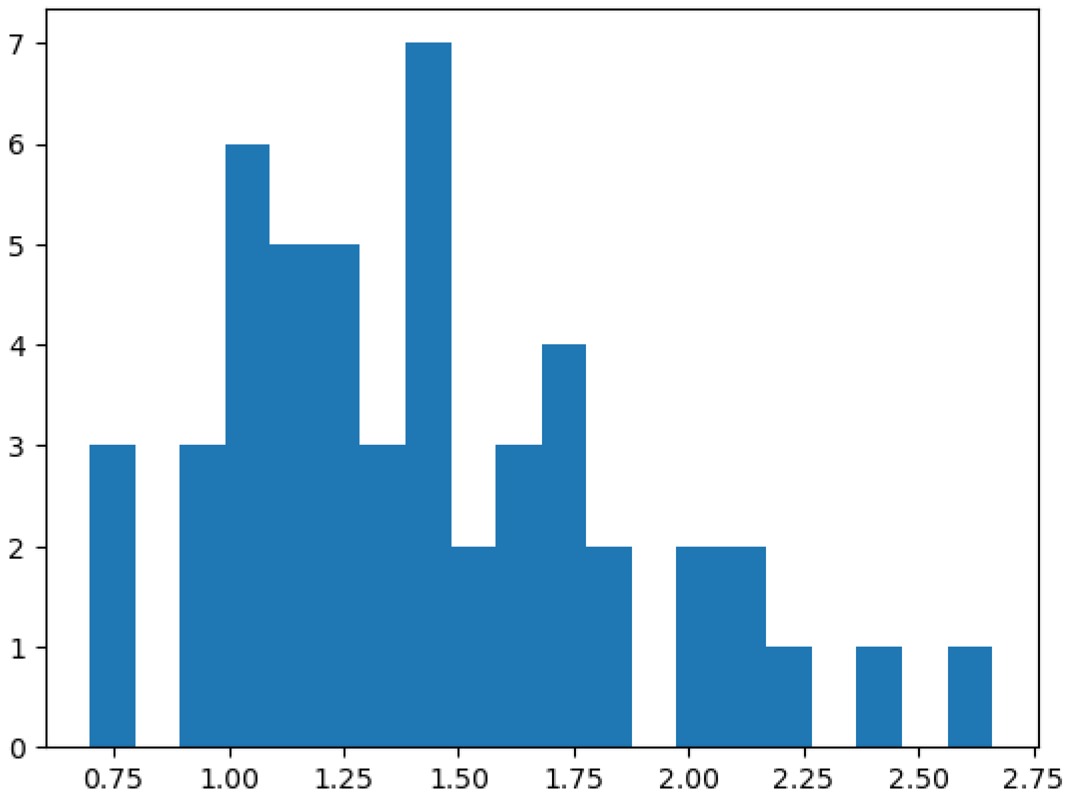
```
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

Total time taken: 1028.2772996425629 seconds
```

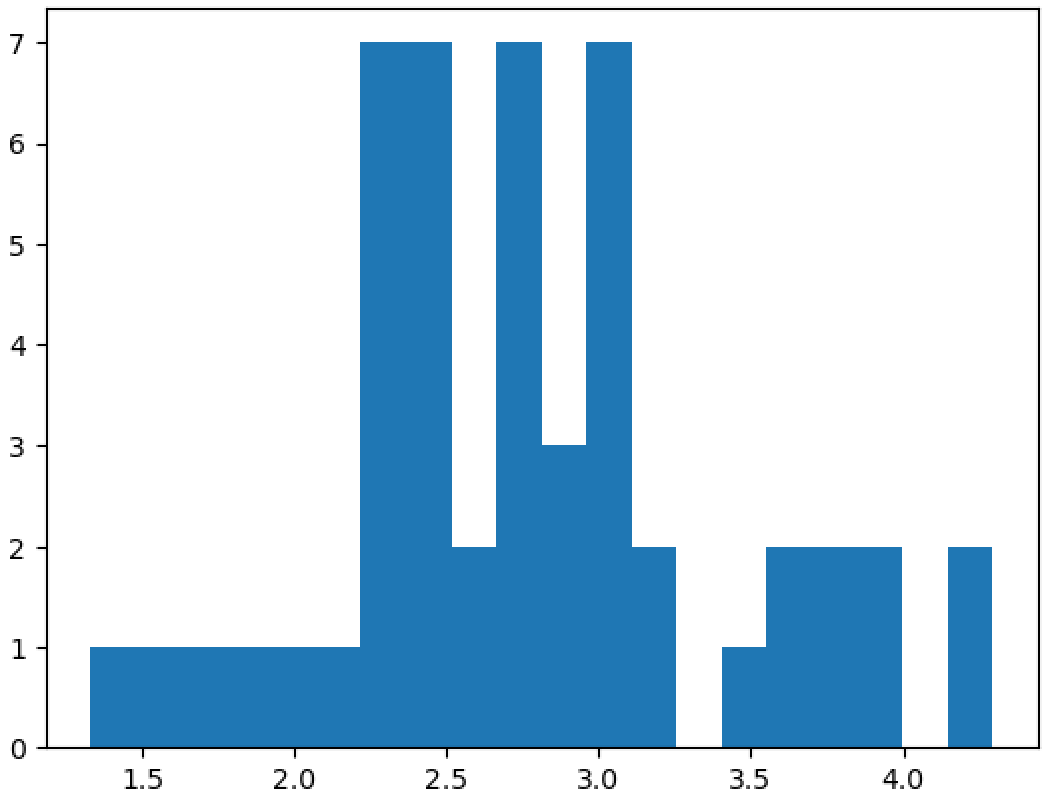
In [41]:
```
# print(np.var(ref_average1,axis=0))
print(np.var(ref_average2,axis=0))

for k in range(4):
        plt.hist(ref_average2[:,k], bins = 20)
        plt.show()

```

```
[0.35481283 0.29947082 0.18320262 0.4135741 ]
```






0
1
2
3
4
5
6
7
0.75
1.00
1.25
1.50
1.75
2.00
2.25
2.50
2.75


0
1
2
3
4
5
6
7
1.5
2.0
2.5
3.0
3.5
4.0

In [20]:

```
def random_point_ttests2(data,ref_distribution, points_removed, focus_c
    '''runs welch test for multi run of simulated annealing for every p
    param_distribution = ref_distribution
#     focus_choices = ['prey', 'predator', 'both']
#     focus_choices = ['prey', 'predator', 'both']
    scores = [[],[]]
    p_values = {'prey': [], 'predator': [], 'both': []}
    initial_temp = 20
    cooling_constant = 0.10

    for indx, choice in enumerate(focus_choices):
        print(choice)
        #We Iteratively increase the amount of points we remove
        for npoints in points_removed:
            print(f"points: {npoints}")
    #         print(f"Points removed: {npoints}")
            limited_data = point_removal(data[:,0], data[:,1:3], npoint
            #Getting distribution of averages
            average_distribution = []
            for k in range(30):
                parameter_list, best_score = multiple_runs_annealing(ir
                #Appending average
                average_distribution.append(np.mean(parameter_list, axi

            average_distribution = np.array(average_distribution)
            t_stat1, p_value1 = scipy.stats.ttest_ind(ref_distribution[
            t_stat2, p_value2 = scipy.stats.ttest_ind(ref_distribution[
            t_stat3, p_value3 = scipy.stats.ttest_ind(ref_distribution[
            t_stat3, p_value4 = scipy.stats.ttest_ind(ref_distribution[
            p_values[choice].append([p_value1, p_value2, p_value3, p_va

    return p_values
```

In [44]:
```
start_time = time.time()

# Calculating p-values for t-test
points_removed_annealing = np.arange(3,16,3)
p_values_annealing = random_point_ttests2(data,ref_average2,points_remo

end_time = time.time()
# Calculating and printing the total time
total_time = end_time - start_time
print(f"Total time taken: {total_time/60} min")
```

```
prey
points: 3

C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: overflow encountered in exp
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: overflow encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: divide by zero encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability

points: 6
points: 9
points: 12
points: 15

C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\951072704.py:25: RuntimeWa
rning: invalid value encountered in scalar divide
  acceptance_probability = min(np.exp(-(delta/temp)),1)#Calculate acceptan
ce probability
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\264107711.py:4: RuntimeWar
ning: overflow encountered in scalar multiply
  dxdt = (alpha * x) - (beta * x * y)  # Predator ODE
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\264107711.py:5: RuntimeWar
ning: overflow encountered in scalar multiply
  dydt = (delta * x * y) - (gamma * y)  # Predator ODE
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\2008888099.py:4: RuntimeWa
rning: overflow encountered in square
  return np.mean((actual - predicted)**2)
C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\2008888099.py:15: RuntimeW
arning: overflow encountered in square
  err1 = (x1[indx_x] - x2[indx_x])**2

predator
points: 3
points: 6
points: 9
points: 12
points: 15

C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\2008888099.py:16: RuntimeW
arning: overflow encountered in square
  err2 = (y1[indx_y] - y2[indx_y])**2
```

```
both
points: 3
points: 6
points: 9
points: 12
points: 15

C:\Users\Aleks\AppData\Local\Temp\ipykernel_764\264107711.py:4: RuntimeWar
ning: invalid value encountered in scalar subtract
  dxdt = (alpha * x) - (beta * x * y)  # Predator ODE

Total time taken: 63.41379015445709 min
```

In [46]:
```python

# Fraction points removed

# Fraction points removed
fraction_points = np.arange(3,16,3) / 100
p_values_prey = np.array(p_values_annealing['prey'])
p_values_predator = np.array(p_values_annealing['predator'])
p_values_both = np.array(p_values_annealing['both'])

# Creating subplots
fig, axes = plt.subplots(1, 3, figsize=(15, 5))

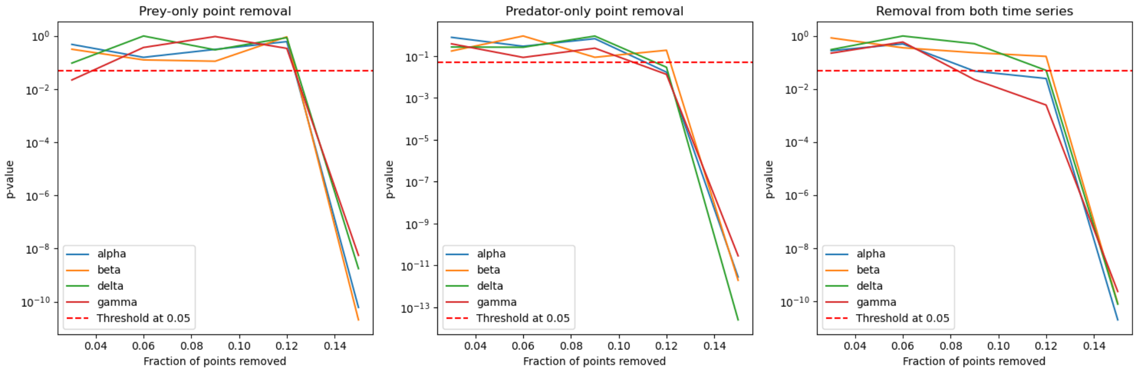
# Plotting p-values when only prey points are removed
axes[0].plot(fraction_points, p_values_prey[:, 0], label='alpha')
axes[0].plot(fraction_points, p_values_prey[:, 1], label='beta')
axes[0].plot(fraction_points, p_values_prey[:, 2], label='delta')
axes[0].plot(fraction_points, p_values_prey[:, 3], label='gamma')
axes[0].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[0].set_ylabel('p-value')
axes[0].set_xlabel('Fraction of points removed')
axes[0].set_yscale('log')
axes[0].set_title('Prey-only point removal')  # Add title to the first
axes[0].legend()

# Plotting p-values when only predator points are removed
axes[1].plot(fraction_points, p_values_predator[:, 0], label='alpha')
axes[1].plot(fraction_points, p_values_predator[:, 1], label='beta')
axes[1].plot(fraction_points, p_values_predator[:, 2], label='delta')
axes[1].plot(fraction_points, p_values_predator[:, 3], label='gamma')
axes[1].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[1].set_ylabel('p-value')
axes[1].set_xlabel('Fraction of points removed')
axes[1].set_yscale('log')
axes[1].set_title('Predator-only point removal')
axes[1].legend()

# Plotting p-values when both prey and predator points are removed
axes[2].plot(fraction_points, p_values_both[:, 0], label='alpha')
axes[2].plot(fraction_points, p_values_both[:, 1], label='beta')
axes[2].plot(fraction_points, p_values_both[:, 2], label='delta')
axes[2].plot(fraction_points, p_values_both[:, 3], label='gamma')
axes[2].axhline(y=0.05, color='r', linestyle='--', label='Threshold at
axes[2].set_ylabel('p-value')
axes[2].set_xlabel('Fraction of points removed')
axes[2].set_yscale('log')
axes[2].set_title('Removal from both time series')
axes[2].legend()

plt.savefig('welch_test_annealing', dpi=300)

# Adjusting layout
plt.tight_layout()
plt.show()
```



Prey-only point removal
Predator-only point removal
Removal from both time series
p-value
Fraction of points removed
alpha
beta
delta
gamma
Threshold at 0.05

In [ ]:
```
1
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