In [32]:
```
import math
import numpy as np
import random
import matplotlib.pyplot as plt
```

题目2

模拟退火算法求解系统最低的能量态

对于系统初值的选取,这里随手选取了T=2000 算法流程大致如下:

```
1、初始化
    根据随机均匀分布生成系统的初始能量态;
    计算系统初值能量;
2、循环体
    while(冷却温度T>设定冷却停止温度Tf):
        for i=1 to N(单次冷却温度中最大迭代次数):
            给定温度生成符合要求的新状态;
            计算接受状态概率;
            生成随机数，判断状态转移并转移到下一个状态;
        T=alpha(冷却速率)*T
```

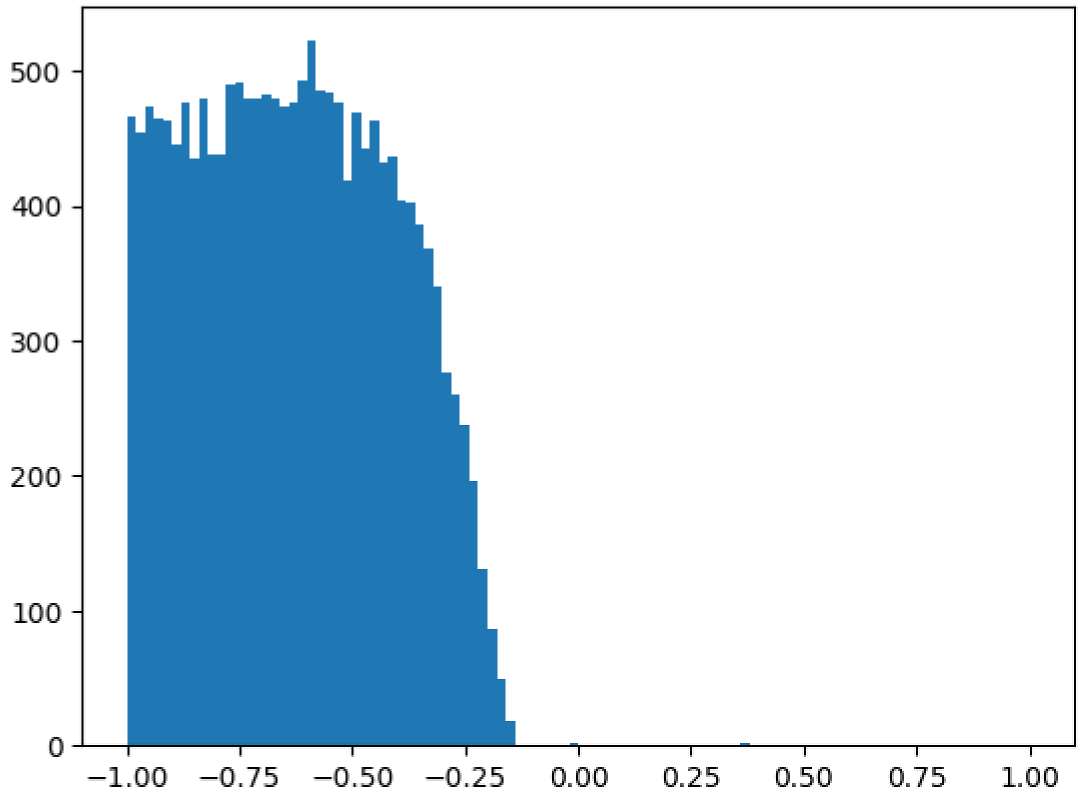
In [33]:
```
'''
Author: loyunemo 3210100968@zju.edu.cn
Date: 2023-11-26 16:43:25
LastEditors: loyunemo 3210100968@zju.edu.cn
LastEditTime: 2023-11-27 19:18:20
FilePath: \Repo_Computer_Simulation\Hw9\Hw9.ipynb
Description: 这是默认设置,请设置`customMade`, 打开koroFileHeader查看配置 进行设置: h
'''
def deltaE(r1,r2):
    r=abs(r1-r2)
    if r==0:
        return 0
    else:
        deltae=4000*(math.pow(0.1/r,12)-math.pow(0.1/r,6))
        return deltae
class system():
    def __init__(self):
        self.x_vector=np.random.uniform(-1,1,4)
        self.EnergySum=self.Energy()
    def Renew(self):
        self.x_vector=np.random.uniform(-1,1,4)
        self.EnergySum=self.Energy()
    def disturb(self,T,Iteration):
        for a in range(Iteration):
            disturb_place=random.randint(0,3)
            disturb_new=random.normalvariate(0,0.2)
            while(disturb_new>1 or disturb_new<-1):
                disturb_new=random.normalvariate(0,0.2)
            newx=np.copy(self.x_vector)
            newx[disturb_place]=disturb_new
            Energynew=0
            for t in range(newx.shape[0]):
                for u in range(t):
                    Energynew+=self.deltaE(newx[t],newx[u])
            h=min(1,math.exp(-(Energynew-self.EnergySum)/T))
            accept=random.uniform(0,1)
            if accept<h:
```

```
                self.x_vector=newx
                self.EnergySum=self.Energy()
    def Energy(self):
        Energysum=0
        for t in range(self.x_vector.shape[0]):
            for u in range(t):
                Energysum+=self.deltaE(self.x_vector[t],self.x_vector[u])
        return Energysum
    def deltaE(self,r1,r2):
        r=abs(r1-r2)
        deltae=4000*(math.pow(0.1/r,12)-math.pow(0.1/r,6))
        return deltae
    def Metropolis_Annealing(self,StartTemperature,CoolRate,maxIter,StopTemperature):
        T=StartTemperature
        while(T>=StopTemperature):
            self.disturb(T,maxIter)
            T=CoolRate*T
def Estimate():
    num=100000
    aver=np.zeros(num)

    for t in range(num):
        E1=random.normalvariate(0,0.2)
        while(E1>1 or E1<-1):
            E1=random.normalvariate(0,0.2)
        E2=random.normalvariate(0,0.2)
        while(E2>1 or E2<-1):
            E2=random.normalvariate(0,0.2)


        aver[t]=E1-E2
    EnergyEstimate=np.mean(aver)
    return EnergyEstimate
Eg1=system()
Eg1.Metropolis_Annealing(2000,0.89,400,0.04)
Eg2=system()
Eg2.Metropolis_Annealing(2000,0.89,400,0.08)
print("T_Stop=0.04: ",Eg1.EnergySum)
print("T_Stop=0.08: ",Eg2.EnergySum)
```

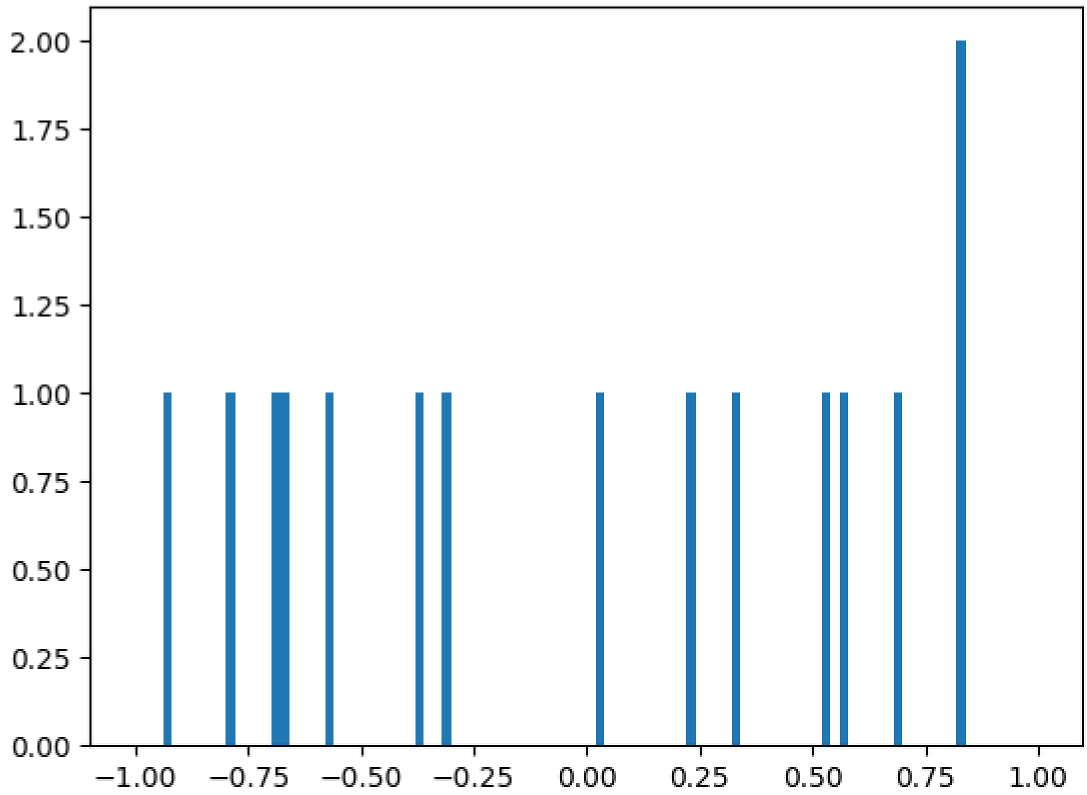
```
T_Stop=0.04:  -3064.9560290415675
T_Stop=0.08:  -3064.8909352570417
```

In [34]:

```
num=1000000
x=np.zeros(num)
for t in range(num):
    q=system()
    x[t]=q.EnergySum
plt.hist(x,100,[-1,1])
plt.show()
```



In [35]:
```
num=1000000
x=np.zeros(num)
for t in range(num):
    q=system()
    for z in range(q.x_vector.shape[0]):
        q.x_vector[z]=random.normalvariate(0,0.2)
        while(q.x_vector[z]>1 or q.x_vector[z]<-1):
            q.x_vector[z]=random.normalvariate(0,0.2)
    q.EnergySum=q.Energy()
    x[t]=q.EnergySum
plt.hist(x,100,[-1,1])
plt.show()
```



题目3

模拟退火求解旅行商问题, 首先需要对距离进行估计，估计退火初始温度T_0

In [36]:
```
CitiesMatrix=np.array([[12,12],[18,23],[24,21],[29,25],[31,52],[36,43],[37,14],[42,8
def dis_between(a,b):
    return np.sqrt(np.dot(a-b,a-b))
def discal(CitiesMatrix,rank):
    DisSum=0
    for t in range(rank.shape[0]-1):
        DisSum+=dis_between(CitiesMatrix[rank[t]],CitiesMatrix[rank[t+1]])
    return DisSum
Trialnum=10000
distance=0
for t in range(Trialnum):
# 随机打乱列表
    rank = np.array(list(range(0, 16)))
    random.shuffle(rank)
    distance+=discal(CitiesMatrix,rank)
ave_dis=distance/Trialnum
print(ave_dis)
```

573.0273425436

在这里E_0大约在571左右， 考虑： $0.99 = e^{-\frac{571}{T}}$ 计算得到： T=56814,取56000即可。

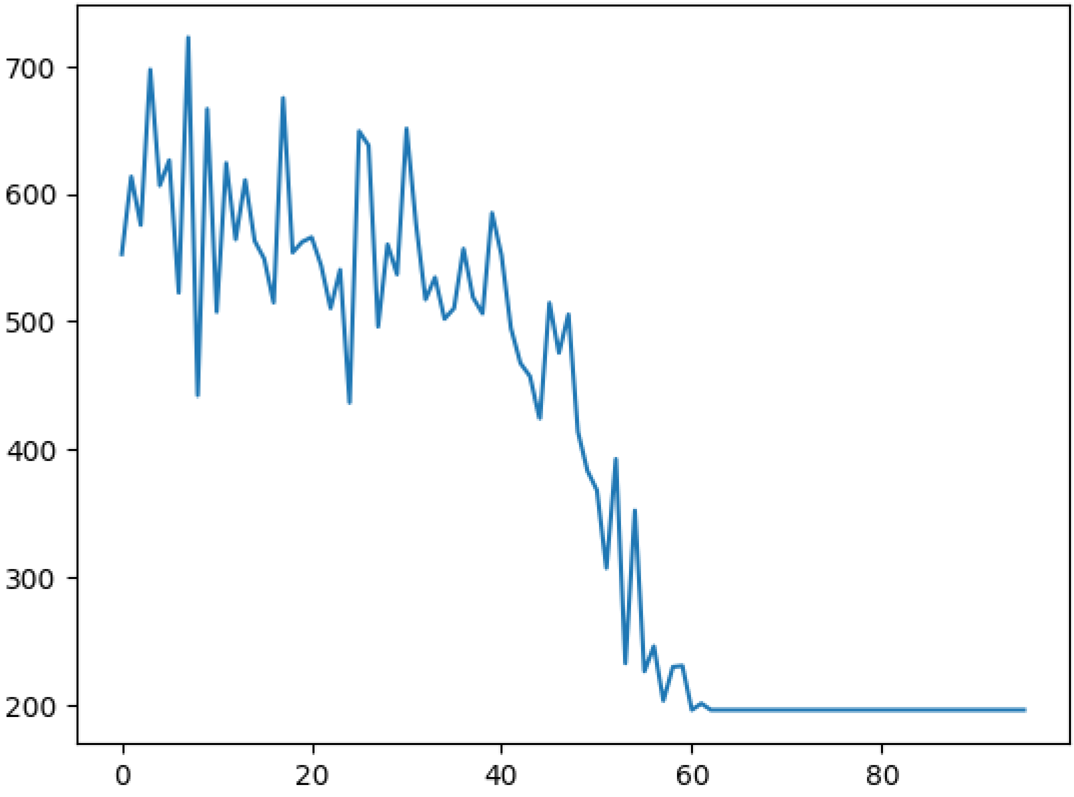
接下来根据模拟算法计算旅行商问题,每次随机选择路径进行逆转，根基Metropolis算法进行判断并接受

In [38]:
```
def TSP_TemperatureIteration(CitiesMatrix,rank,Iteration,T):
    ranknow=rank
    for t in range(Iteration):
        start=random.randint(0,15)
        end=random.randint(1,16)
        while(end<=start):
```

```
            end=random.randint(1,16)
        reverge=ranknow[start:end][::-1]
        ranknew=ranknow.copy()
        ranknew[start:end]=reverge
        dis=discal(CitiesMatrix,ranknew)
        h=min(1,math.exp(-(dis-discal(CitiesMatrix,ranknow))/T))
        u=random.uniform(0,1)
        if u<h:
            ranknow=ranknew
    return ranknow
def Simulate_Annealing_TSP(CitiesMatrix,StartTemperature,EndTemperature,Iteration,Co
    rank = np.array(list(range(0, 16)))
    random.shuffle(rank)
    T=StartTemperature
    while(T>=EndTemperature):
        #print("Temperature: ",T," Distance:",discal(CitiesMatrix,rank))
        rank=TSP_TemperatureIteration(CitiesMatrix,rank,Iteration,T)
        WriteList.append(rank)
        T*=CoolRate
    return rank
Writelist=[]
rankresult=Simulate_Annealing_TSP(CitiesMatrix,56000,0.01,1600,0.85,Writelist)
```

In [39]:
```
distancelist=np.zeros(len(Writelist))
for t in range(len(Writelist)):
    distancelist[t]=discal(CitiesMatrix,Writelist[t])
print(rankresult.tolist(),discal(CitiesMatrix,rankresult))
plt.plot(np.arange(0,len(Writelist)),distancelist)
plt.show()
```

```
[4, 5, 8, 9, 11, 14, 15, 13, 12, 10, 7, 6, 3, 2, 1, 0] 195.68923304678708
```

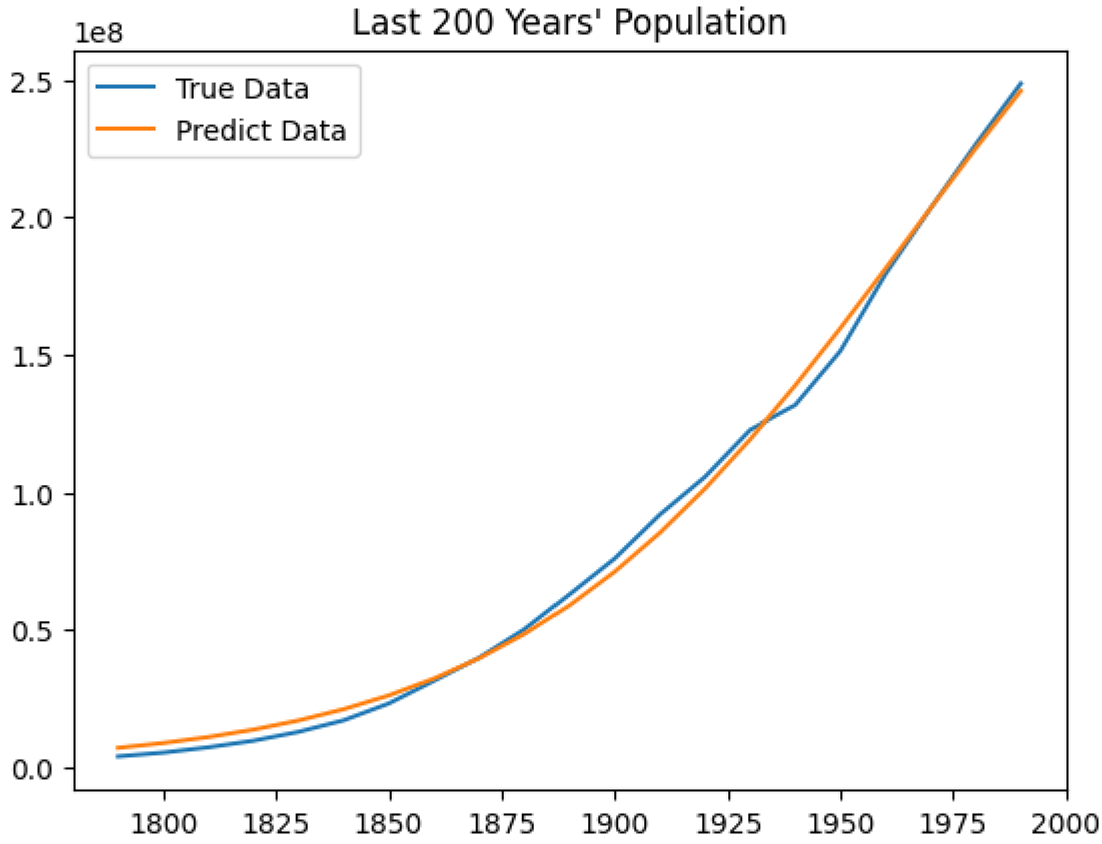


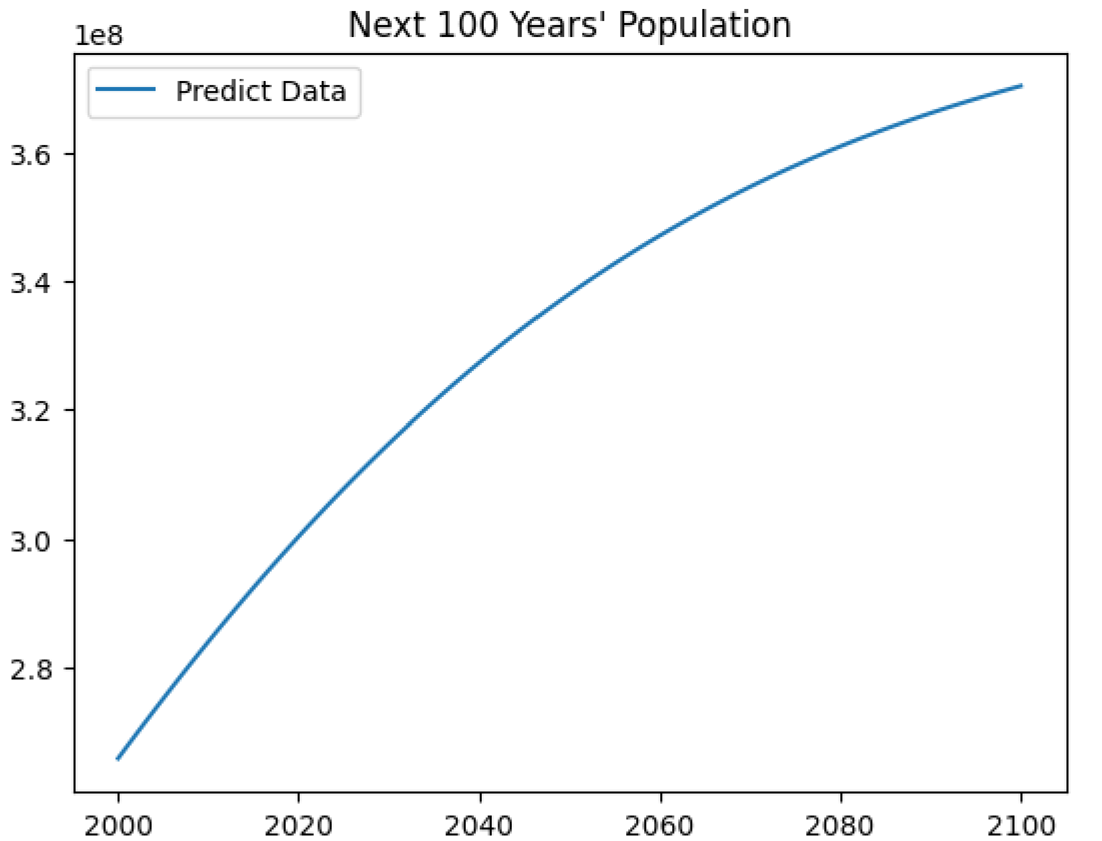
题目6

最小二乘法拟合人口数据

In [76]:
```
import numpy as np
from scipy.optimize import curve_fit
from scipy.optimize import least_squares
from scipy.optimize import leastsq
# 定义模型函数
import warnings

warnings.filterwarnings('ignore')
def model_function(params, t):

    A, r, K = params
    return A*K*np.exp(r*t)/(K+A*np.exp(r*t))

# 定义目标函数（残差平方和）
def objective_function(params, x, y_observed):
    return y_observed - model_function(params, x)

# 生成一些模拟数据

x_data = np.linspace(1790,1990,21).flatten()

y_data = np.array([3929214,5308483,7239881,9638453,12866020,17069453,23191876,314333
# 初始化参数猜测
initial_guess = [1.60826987e-11, 2.27034768e-02, 3.87967929e+08]

# 使用leastsq进行非线性最小二乘法拟合
optimized_params=leastsq(objective_function, initial_guess, args=(x_data, y_data))
#print(optimized_params)
for t in range(100):
    optimized_params=leastsq(objective_function, optimized_params[0], args=(x_data,

print("Optimized Parameters:", optimized_params)
predict=model_function(optimized_params[0],x_data)

plt.plot(x_data,y_data,label="True Data")
plt.plot(x_data,predict,label="Predict Data")
plt.title("Last 200 Years' Population")
plt.legend()
plt.show()
next=np.linspace(2000,2100,101)
predictnew=model_function(optimized_params[0],next)

plt.plot(next,predictnew,label="Predict Data")
plt.title("Next 100 Years' Population")
plt.legend()
plt.show()
```

```
Optimized Parameters: (array([1.60827563e-11, 2.27034749e-02, 3.87967978e+08]), 1)
```


Last 200 Years' Population
1e8
True Data
Predict Data
2.5
2.0
1.5
1.0
0.5
0.0
1800
1825
1850
1875
1900
1925
1950
1975
2000


Next 100 Years' Population
1e8
Predict Data
3.6
3.4
3.2
3.0
2.8
2000
2020
2040
2060
2080
2100