Homework 2: Climate Change (not done yet)

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▶ 详细信息

In this problem, you will attempt to study the relationship between average global temperature and several other factors. The file climate_change_1.csv contains climate data from May 1983 to December 2008. The available variables include:
`Year`: the observation year.

`Month`: the observation month.

`Temp`: the difference in degrees Celsius between the average global temperature in that period and a reference value. This data comes from the Climatic Research Unit at the University of East Anglia .
`CO2`, `N2O`, `CH4`, `CFC.11`, `CFC.12`: atmospheric concentrations of carbon dioxide (CO_2), nitrous oxide (N_2O), methane (CH_4), trichlorofluoromethane (CCl_3Fcommonly referred to as $CFC-11$) and dichlorodifluoromethane (CCl_2F_2; commonly referred to as $CFC-12$), respectively. This data comes from the ESRL/NOAA Global Monitoring Division.

`CO2`, `N2O` and `CH4` are expressed in ppmv (parts per million by volume -- i.e., *397 ppmv of CO2 means that CO2 constitutes 397 millionths of the total volume of the atmosphere*)

`CFC.11` and `CFC.12` are expressed in ppbv (parts per billion by volume).
`Aerosols`: the mean stratospheric aerosol optical depth at 550 nm. This variable is linked to volcanoes, as volcanic eruptions result in new particles being added to the atmosphere, which affect how much of the sun's energy is reflected back into space. This data is from the Godard Institute for Space Studies at NASA.

`TSI`: the total solar irradiance (TSI) in W/m2 (the rate at which the sun's energy is deposited per unit area). Due to sunspots and other solar phenomena, the amount of energy that is given off by the sun varies substantially with time. This data is from the SOLARIS-HEPPA project website.

`MEI`: multivariate El Nino Southern Oscillation index (MEI), a measure of the strength of the El Nino/La Nina-Southern Oscillation (a weather effect in the Pacific Ocean that affects global temperatures). This data comes from the ESRL/NOAA Physical Sciences Division.

Preparation

Import data

```
import pandas as pd
df1 = pd.read_csv('./data/climate_change_1.csv')
df2 = pd.read_csv('./data/climate_change_2.csv')
```

Exploration and cleaning

Data structure

```
df1.head().round()
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	Temp
0	1983	5	3.0	346.0	1639.0	304.0	191.0	350.0	1366.0	0.0	0.0
1	1983	6	2.0	346.0	1634.0	304.0	192.0	352.0	1366.0	0.0	0.0
2	1983	7	2.0	344.0	1633.0	304.0	193.0	354.0	1366.0	0.0	0.0
3	1983	8	1.0	342.0	1631.0	304.0	194.0	356.0	1366.0	0.0	0.0
4	1983	9	0.0	340.0	1648.0	304.0	194.0	357.0	1366.0	0.0	0.0

```
df2.head().round(2)
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
0	1983	5	2.56	345.96	1638.59	303.68	191.32	350.11	1366.10	0.09	2.64	0.11
1	1983	6	2.17	345.52	1633.71	303.75	192.06	351.85	1366.12	0.08	2.63	0.12
2	1983	7	1.74	344.15	1633.22	303.80	192.82	353.72	1366.28	0.07	2.63	0.14
3	1983	8	1.13	342.25	1631.35	303.84	193.60	355.63	1366.42	0.07	2.63	0.18
4	1983	9	0.43	340.17	1648.40	303.90	194.39	357.46	1366.23	0.06	2.65	0.15

Statistics

The most significant difference is the variable `NO`. Then explore **basic statistics** with round three:

```
df1.describe().round(3)
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	Temp
count	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000
mean	1995.662	6.552	0.276	363.227	1749.825	312.392	251.973	497.525	1366.071	0.017	0.257
std	7.423	3.447	0.938	12.647	46.052	5.225	20.232	57.827	0.400	0.029	0.179
min	1983.000	1.000	-1.635	340.170	1629.890	303.677	191.324	350.113	1365.426	0.002	-0.282
25%	1989.000	4.000	-0.399	353.020	1722.182	308.112	246.296	472.411	1365.717	0.003	0.122
50%	1996.000	7.000	0.238	361.735	1764.040	311.507	258.344	528.356	1365.981	0.006	0.248
75%	2002.000	10.000	0.830	373.455	1786.885	316.979	267.031	540.524	1366.363	0.013	0.407
max	2008.000	12.000	3.001	388.500	1814.180	322.182	271.494	543.813	1367.316	0.149	0.739

```
df2.describe().round(3)
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
count	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000	308.000
mean	1995.662	6.552	0.276	363.227	1749.825	312.392	251.973	497.525	1366.071	0.017	2.750	0.257
std	7.423	3.447	0.938	12.647	46.052	5.225	20.232	57.827	0.400	0.029	0.046	0.179
min	1983.000	1.000	-1.635	340.170	1629.890	303.677	191.324	350.113	1365.426	0.002	2.630	-0.282
25%	1989.000	4.000	-0.399	353.020	1722.182	308.112	246.296	472.411	1365.717	0.003	2.722	0.122
50%	1996.000	7.000	0.238	361.735	1764.040	311.507	258.344	528.356	1365.981	0.006	2.764	0.248
75%	2002.000	10.000	0.830	373.455	1786.885	316.979	267.031	540.524	1366.363	0.013	2.787	0.407
max	2008.000	12.000	3.001	388.500	1814.180	322.182	271.494	543.813	1367.316	0.149	2.814	0.739

Missing data

```
df1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 308 entries, 0 to 307
Data columns (total 11 columns):
Year         308 non-null int64
Month        308 non-null int64
MEI          308 non-null float64
CO2          308 non-null float64
CH4          308 non-null float64
N2O          308 non-null float64
CFC-11       308 non-null float64
CFC-12       308 non-null float64
TSI          308 non-null float64
Aerosols     308 non-null float64
Temp         308 non-null float64
dtypes: float64(9), int64(2)
memory usage: 26.6 KB
```

```
df2.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 308 entries, 0 to 307
Data columns (total 12 columns):
Year         308 non-null int64
Month        308 non-null int64
MEI          308 non-null float64
CO2          308 non-null float64
CH4          308 non-null float64
N2O          308 non-null float64
CFC-11       308 non-null float64
CFC-12       308 non-null float64
TSI          308 non-null float64
Aerosols     308 non-null float64
NO           308 non-null float64
Temp         308 non-null float64
dtypes: float64(10), int64(2)
memory usage: 29.0 KB
```

No missing data were found, then continue.

Duplication

```
print('Duplicated rows:', len(df1[df1.duplicated()]), ', then continue.')
```

```
Duplicated rows: 0 , then continue.
```

Outliers

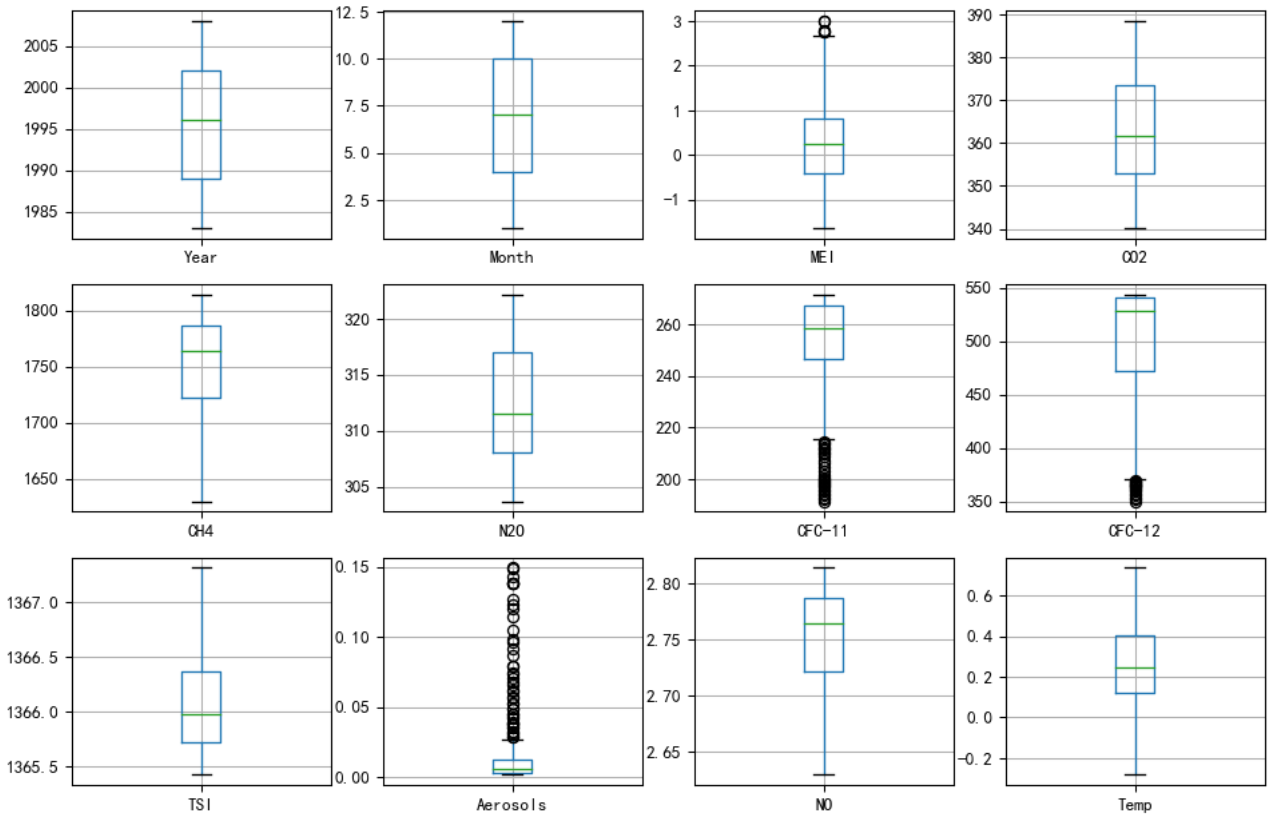
Conduct a boxploting to find out outliers in DF1 and DF2:

```
import sys
import seaborn as sns
import matplotlib.pyplot as plt
fig1 = plt.figure(figsize=(12,8), dpi=96)
for i in range(1, len(df1.columns) + 1):
    fig1.add_subplot(3, 4, i)
    df1.iloc[:, [i-1]].boxplot()
```

```
range(1, len(df2.columns) + 1)
```

```
range(1, 13)
```

```
fig2 = plt.figure(figsize=(12,8), dpi=96)
for i in range(1, len(df2.columns) + 1):
    fig2.add_subplot(3, 4, i)
    df2.iloc[:, [i-1]].boxplot()
```



Check outliers:

```
import ipywidgets as widgets
z_slider = widgets.FloatSlider(
    value=2.9,
    min=2,
    max=3.5,
    step=0.1,
    description='Threshold:',
    disabled=False,
    continuous_update=True,
    orientation='horizontal',
    readout=True,
    readout_format='.1f',
)
z_slider
```

```
FloatSlider(value=2.9, description='Threshold:', max=3.5, min=2.0, readout_format='.1f')
```

```
from scipy import stats
import numpy as np
z = np.abs(stats.zscore(df1['MEI']))
outlier_index = np.where(z > z_slider.value)[0]
print('Threshhold:', z_slider.value)
print('Index:', outlier_index)
print('Outlier:', [df1['MEI'][i] for i in outlier_index])
```

```
Threshhold: 2.9
Index: [171 172]
Outlier: [3.0010000000000003, 3.0]
```

Since rare outliers, ignore at preparation step and continue.

Correlation

Find and plot highly correlated variables (r>0.6 in df1, plotting r>0.5):

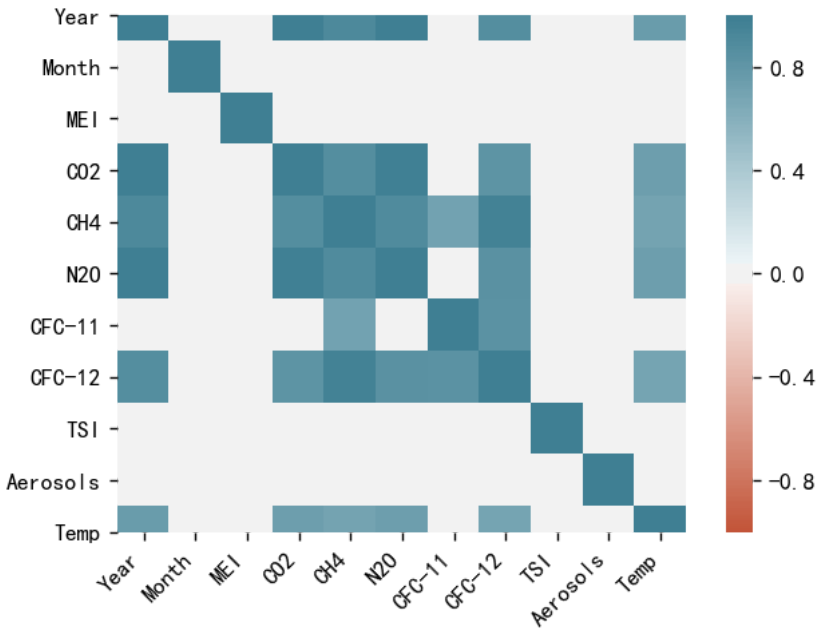
```
corr = df1.corr()
high_corr = corr[np.abs(corr) > 0.5].fillna(0)
corr[np.abs(corr) > 0.6].fillna('')
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	Temp
Year	1			0.985379	0.910563	0.99485		0.870067			0.755731
Month		1									
MEI			1								
CO2	0.985379			1	0.872253	0.981135		0.82321			0.748505
CH4	0.910563			0.872253	1	0.894409	0.713504	0.958237			0.699697
N2O	0.99485			0.981135	0.894409	1		0.839295			0.743242
CFC-11					0.713504		1	0.831381			
CFC-12	0.870067			0.82321	0.958237	0.839295	0.831381	1			0.688944
TSI									1		
Aerosols										1	
Temp	0.755731			0.748505	0.699697	0.743242		0.688944			1

```
plt.figure(dpi=128)
ax = sns.heatmap(
    high_corr,
    vmin=-1, vmax=1, center=0,
    cmap=sns.diverging_palette(20, 220, n=200),
    square=True
)
ax.set_xticklabels(
    ax.get_xticklabels(),
    rotation=45,
    horizontalalignment='right'
);
```



Similarly, correlation in df1:

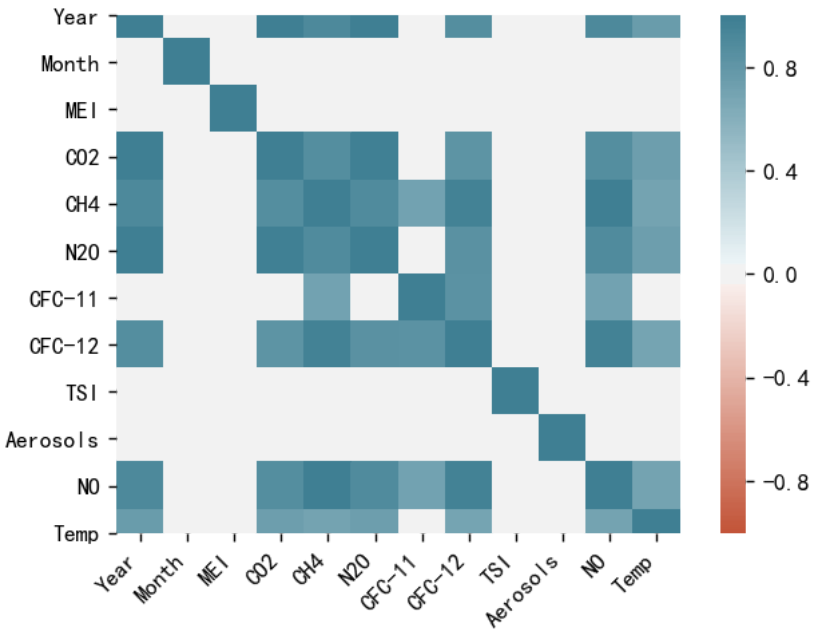
```
corr = df2.corr()
high_corr = corr[np.abs(corr) > 0.5].fillna(0)
corr[np.abs(corr) > 0.6].fillna('')
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
Year	1			0.985379	0.910563	0.99485		0.870067			0.910563	0.755731
Month		1										
MEI			1									
CO2	0.985379			1	0.872253	0.981135		0.82321			0.872253	0.748505
CH4	0.910563			0.872253	1	0.894409	0.713504	0.958237			1	0.699697
N2O	0.99485			0.981135	0.894409	1		0.839295			0.894409	0.743242
CFC-11					0.713504		1	0.831381			0.713504	
CFC-12	0.870067			0.82321	0.958237	0.839295	0.831381	1			0.958237	0.688944
TSI									1			
Aerosols										1		
NO	0.910563			0.872253	1	0.894409	0.713504	0.958237			1	0.699697
Temp	0.755731			0.748505	0.699697	0.743242		0.688944			0.699697	1

```
plt.figure(dpi=128)
ax = sns.heatmap(
    high_corr,
    vmin=-1, vmax=1, center=0,
    cmap=sns.diverging_palette(20, 220, n=200),
    square=True
)
ax.set_xticklabels(
    ax.get_xticklabels(),
    rotation=45,
    horizontalalignment='right'
);
```



Potential redundant variables found, however, now the data is prepared for analyzing.

Problem 1 — First Model

We are interested in how changes in these variables affect future temperatures, as well as how well these variables explain temperature changes so far. To do this, first read the dataset climate_change_1.csv into Python or Matlab.

Then, split the data into a training set, consisting of all the observations up to and including 2006, and a testing set consisting of the remaining years. A training set refers to the data that will be used to build the model, and a testing set refers to the data we will use to test our predictive ability.

After seeing the problem, your classmate Alice immediately argues that we can apply a linear regression model. Though being a little doubtful, you decide to have a try. To solve the linear regression problem, you recall the linear regression has a closed form solution:
$\theta = (X^T X)^{-1} X^T Y$

Read and split

Though data have been prepared in section *Data Preparation*, dataset df1 has been imported again here following problem description.

Read the dataset:

```
# loaded in exploration

# import pandas as pd
# df1 = pd.read_csv('../data/climate_change_1.csv').iloc[:,2:]
```

Split into training set and testing set:

```
# Df1 trainset
df1_train = df1[df1['Year']<=2006].iloc[:,2:]
# Check the result
df1_train.iloc[[0, 1,-2, -1],:]
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	Temp
0	2.556	345.96	1638.59	303.677	191.324	350.113	1366.1024	0.0863	0.109
1	2.167	345.52	1633.71	303.746	192.057	351.848	1366.1208	0.0794	0.118
282	1.292	380.18	1791.91	320.321	248.605	539.500	1365.7039	0.0049	0.440
283	0.951	381.79	1795.04	320.451	248.480	539.377	1365.7087	0.0054	0.518

```
# Df1 testet
df1_test = df1[df1['Year']>2006].iloc[:,2:]
# Check the result
df1_test.iloc[[0, 1,-2, -1],:]
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	Temp
284	0.974	382.93	1799.66	320.561	248.372	539.206	1365.7173	0.0054	0.601
285	0.510	383.81	1803.08	320.571	248.264	538.973	1365.7145	0.0051	0.498
306	-0.621	384.13	1812.37	322.013	244.225	534.906	1365.7065	0.0048	0.394
307	-0.666	385.56	1812.88	322.182	244.204	535.005	1365.6926	0.0046	0.330

1. Closed form function

Implement a function `closed_form_1` *that computes this closed form solution given the features X, labels y (using Python or Matlab).*

Given a pandas `Dataframe`, the features X is the dataframe excluding taget y, then:

```
import numpy as np  # matrix, vector, and linear algebra support
from numpy.linalg import inv  # matrix inversion


def closed_form_1(X: np.ndarray, y: np.ndarray) -> np.matrix:
    """
    To calculate OLS theta(s) given X, y in ndarrays.

    Parameters:
    ----------
        X: features, IV.
        y: taget variable, DV.
    Return:
    ----------
        theta: coefficients
    """

    X = np.column_stack((np.ones(len(X)), X))  # add x0 = 1 to matrix X
    theta = inv(X.T @ X) @ X.T @ y
    #theta = theta[1:].reshape((1,10))
    return theta


def closed_form_df(df: pd.core.frame.DataFrame, column: int = 8) -> np.matrix:
    """
    To calculate OLS theta(s) given data in a DataFrame.

    Parameters:
    ----------
        df: a DataFrame of data including both IV X and DV y.
        column = 8: index number of clomn where DV y lies. The default value is 8.

    Return:
    ----------
        theta: coefficients
    """

    X = df.drop(df.columns[column], axis=1).to_numpy()  # X: the features
    X = np.column_stack((np.ones(len(X)), X))  # add x0 = 1 to matrix X
    y = df.iloc[:, [column]].to_numpy(
    )  # y: the results, lower case to emphasize the difference
    theta = inv(X.T @ X) @ X.T @ y
    #theta = theta[1:].reshape((1,10))
    return theta
```

Test `closed_form_1` and `closed_form_df` on df1:

```
df1_train.drop(df1_train.columns[8], axis=1).head(3)
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols
0	2.556	345.96	1638.59	303.677	191.324	350.113	1366.1024	0.0863
1	2.167	345.52	1633.71	303.746	192.057	351.848	1366.1208	0.0794
2	1.741	344.15	1633.22	303.795	192.818	353.725	1366.2850	0.0731

```
# Given X, and y in numpy arrays
X = df1_train.drop(df1_train.columns[8], axis=1).to_numpy() # X: the features
y = df1_train.iloc[:, [8]].to_numpy()                       # y: the results, lower case to emphasize the difference
X_test = df1_test.drop(df1_train.columns[8], axis=1).to_numpy()
y_test = df1_test.iloc[:, [8]].to_numpy()
theta = closed_form_1(X, y)
theta.flatten()
```

```
array([-1.24594260e+02,  6.42053134e-02,  6.45735927e-03,  1.24041896e-04,
       -1.65280032e-02, -6.63048889e-03,  3.80810324e-03,  9.31410835e-02,
       -1.53761324e+00])
```

```
# Given a DataFrame
theta = closed_form_df(df1_train).reshape((1,9))
theta.flatten()
```

```
array([-1.24594260e+02,  6.42053134e-02,  6.45735927e-03,  1.24041896e-04,
       -1.65280032e-02, -6.63048889e-03,  3.80810324e-03,  9.31410835e-02,
       -1.53761324e+00])
```

Using *scipy* to check the result:

```
from sklearn.linear_model import LinearRegression as lm
l=lm().fit(X, y)
l.coef_.flatten()
```

```
array([ 6.42053134e-02,  6.45735927e-03,  1.24041896e-04, -1.65280033e-02,
       -6.63048889e-03,  3.80810324e-03,  9.31410835e-02, -1.53761324e+00])
```

Works fine (some differences due to SVD used in *sklearn.LinearRegression*).

2. Fomula and R squre

Write down the mathematical formula for the linear model and evaluate the model R squre on the training set and the testing set.

```
df1_train.columns
```

```
Index(['MEI', 'CO2', 'CH4', 'N2O', 'CFC-11', 'CFC-12', 'TSI', 'Aerosols',
       'Temp'],
      dtype='object')
```

Formula of this model(`round(5)`)

$\hat{Temp} = -124.594 + 0.06421 * MEI + 0.00646 * CO_2 + 0.00012 * CH_4 - 0.01653 * N_2O - 0.00663 * CFC11 + 0.00381 * CFC12 + 0.09314 * TSI - 1.53761 * Aerosol$

Formula of R-squred

R-squared measures model fitting and can be calculated as: $R^2 = \frac{var(X\hat{\beta})}{var(y)} = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$

```
def predict(X: np.ndarray, theta: np.ndarray) -> np.ndarray:
    """
    To predict y given X and theta.

    Parameters:
    ----------

        X: features, IV.
        theta: coefficients.

    Return:
    ----------
        y_hat: predicted value.
    """

    X = np.column_stack((np.ones(len(X)), X))  # add x0 = 1 to matrix X
    # theta = theta.reshape((1, len(theta)))
    y_hat = np.sum(X @ theta, axis=1)
    return (y_hat)

```

Define a `score` function to calculate R^2:

```
def score(y: np.ndarray, y_hat: np.ndarray) -> float:
    """
    To calculate OLS R^2 given data in ndarrays.

    Parameters:
```

```
    ----------
        y: actual labels.
        y_hat: predicted values.

    Return:
    ----------
        SST: R^2 caculated based on y and y_hat.
    """

    mean = y.mean()
    TSS = np.sum(np.square(y_hat - mean))
    ESS = np.sum(np.square(y - mean))
    SST = TSS / ESS
    return SST
```

On training set:

```
X = df1_train.drop(df1_train.columns[8], axis=1).to_numpy()
y = df1_train.iloc[:, [8]].to_numpy()
rsquare_train = score(y, predict(X, closed_form_1(X, y)))
print("R2:", rsquare_train)

# Use *scipy* to check the result:
l=lm().fit(X, y)
print("R2 by scipy:", l.score(X, y))
```

```
R2: 0.7508932770388383
R2 by scipy: 0.7508932770523428
```

On testing set:

```
rsquare_test = score(y_test, predict(X_test, closed_form_1(X, y)))
print("R2:", rsquare_test)
```

```
R2: 0.22517701916249677
```

Works fine.

Evaluation

Based on the formula above, R-squred can be applied in Python to evaluate previous model. On training set: R^2 is 0.75089, while on testing set, R^2 is 0.22518.

*** *However, for a multi-variable linear model, $R^2_{adjusted}$ may be a better indicator because the original R^2 is sensitive to the number of features.*

3. Significant variables

Which variables are significant in the model?

```
import statsmodels.api as sm

# set an alpha
alpha = 0.05

X2 = sm.add_constant(X)
l = sm.OLS(y, X2).fit()
pvalues = l.summary2().tables[1]['P>|t|']
labels =  ['x0: constant'] + ["x" + str(i+1) + ": " + df1_train.columns[i] for i in range(len(df1_train.columns)-1)]
variables = pd.DataFrame(np.concatenate([pd.DataFrame(labels), pd.DataFrame(pvalues)], axis=1))
variables.columns = ['Variable', 'pvalues']

# print significant variables
variables[variables.pvalues < alpha]
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Variable	pvalues
0	x0: constant	1.43105e-09
1	x1: MEI	4.89889e-20
2	x2: CO2	0.00505252
5	x5: CFC-11	5.95729e-05
6	x6: CFC-12	0.00020972
7	x7: TSI	1.09594e-09
8	x8: Aerosols	5.41127e-12

That's to say, significant(alpha=0.05) varibles are:

```
[i for i in variables[variables.pvalues < alpha].Variable.to_numpy()]
```

```
['x0: constant',
 'x1: MEI',
 'x2: CO2',
 'x5: CFC-11',
 'x6: CFC-12',
 'x7: TSI',
 'x8: Aerosols']
```

4. Necessary conditions and application

Write down the necessary conditions for using the closed form solution. And you can apply it to the dataset climate_change_2.csv, explain the solution is unreasonable.

Necessary conditions
$X^T X$ must be invertible.

```
df2.head(3)
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	Year	Month	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
0	1983	5	2.556	345.96	1638.59	303.677	191.324	350.113	1366.1024	0.0863	2.63859	0.109
1	1983	6	2.167	345.52	1633.71	303.746	192.057	351.848	1366.1208	0.0794	2.63371	0.118
2	1983	7	1.741	344.15	1633.22	303.795	192.818	353.725	1366.2850	0.0731	2.63322	0.137

```
# Df2 trainset
df2_train = df2[df2['Year']<=2006].iloc[:,2:]
# Check the result
df2_train.iloc[[0, 1,-2, -1],:]
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
0	2.556	345.96	1638.59	303.677	191.324	350.113	1366.1024	0.0863	2.63859	0.109
1	2.167	345.52	1633.71	303.746	192.057	351.848	1366.1208	0.0794	2.63371	0.118
282	1.292	380.18	1791.91	320.321	248.605	539.500	1365.7039	0.0049	2.79191	0.440
283	0.951	381.79	1795.04	320.451	248.480	539.377	1365.7087	0.0054	2.79504	0.518

```
# Df2 testet
df2_test = df2[df2['Year']>2006].iloc[:,2:]
# Check the result
df2_test.iloc[[0, 1,-2, -1],:]
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	MEI	CO2	CH4	N2O	CFC-11	CFC-12	TSI	Aerosols	NO	Temp
284	0.974	382.93	1799.66	320.561	248.372	539.206	1365.7173	0.0054	2.79966	0.601
285	0.510	383.81	1803.08	320.571	248.264	538.973	1365.7145	0.0051	2.80308	0.498
306	-0.621	384.13	1812.37	322.013	244.225	534.906	1365.7065	0.0048	2.81237	0.394
307	-0.666	385.56	1812.88	322.182	244.204	535.005	1365.6926	0.0046	2.81288	0.330

```
# Given X, and y in numpy arrays
X_2 = df2_train.drop(df2_train.columns[9], axis=1).to_numpy() # X: the features
y_2 = df2_train.iloc[:, [9]].to_numpy()                       # y: the results, lower case to emphasize the difference
X_2_test = df2_test.drop(df2_test.columns[9], axis=1).to_numpy()
y_2_test = df2_test.iloc[:, [9]].to_numpy()
theta = closed_form_1(X_2, y_2)
theta.flatten()
```

```
array([-1.18459383e+02,  6.41762745e-02,  6.48209178e-03,  6.24389931e-03,
       -1.65280032e-02, -6.63048889e-03,  3.80810324e-03,  9.31410835e-02,
       -1.53761324e+00, -6.12593018e+00])
```

Why unreasonable:
Because $X^T X$ is non-invertible.

According to Andrew NG,

> When implementing the normal equation in octave we want to use the `pinv` function rather than `inv`. The 'pinv' function will give you a value of \thetaθ even if $X^T X$ is not invertible.
> If $X^T X$ is noninvertible, the common causes might be having :
>
> - **Redundant features**, where two features are very closely related (i.e. they are linearly dependent)
> - **Too many features** (e.g. m ≤ n). In this case, delete some features or use "regularization" (to be explained in a later lesson).
>
> Solutions to the above problems include deleting a feature that is linearly dependent with another or deleting one or more features when there are too many features.

In this case, many variables (as mentioned in the first section exploration) are highly correlated.

Problem 2 — Regularization

Regularization is a method to boost robustness of model, including L1 regularization and L_2 regularization.

1. Loss function

Please write down the loss function for linear model with L1 regularization, L2 regularization, respectively.

L1， Lasso Regression: $J(\theta) = \frac{1}{2m}[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}|\theta_j|]$

L2, Ridge Regression: $J(\theta) = \frac{1}{2m}[\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^{n}\theta_j^2]$

2. Compute and regularization

The closed form solution for linear model with L2 regularization: $\theta = (\mathbf{X}^\mathbf{T}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\mathbf{T}\mathbf{Y}$ *where I is the identity matrix. Write a function closed_form_2 that computes this closed form solution given the features X, labels Y and the regularization parameter λ (using Python or Matlab).*

```
def closed_form_2(X: np.ndarray, y: np.ndarray, lambd: float) -> np.ndarray:
    """
    To calculate OLS theta(s) given X, y in ndarrays.

    Parameters:
    ----------
        X: features, IV.
        y: taget variable, DV.
        lambd: regularization parameter
    Return:
    ----------
        theta: coefficients
    """

    X = np.concatenate([np.ones((len(X), 1)), X], axis=1)  # add x0 = 1 to matrix X
    I = np.identity(len(X[0]))
    theta = inv(X.T @ X + lambd * I) @ (X.T @ y)
    return theta
```

3. Comparison

Compare the two solutions in problem 1 and problem 2 and explain the reason why linear model with L2 regularization is robust. (using climate_change_1.csv)

```
X_train = df1_train.drop(df1_train.columns[8], axis=1).to_numpy()
y_train = df1_train.iloc[:, [8]].to_numpy()
theta_0 = closed_form_1(X_train, y_train)
theta_0.flatten()
```

```
array([-1.24594260e+02,  6.42053134e-02,  6.45735927e-03,  1.24041896e-04,
       -1.65280032e-02, -6.63048889e-03,  3.80810324e-03,  9.31410835e-02,
       -1.53761324e+00])
```

```
theta_2 = closed_form_2(X_train, y_train, 0.5)
theta_2.flatten()
```

```
array([-4.68953239e-03,  4.55768014e-02,  7.80443532e-03,  1.95701031e-04,
       -1.64893727e-02, -6.38359095e-03,  3.74766007e-03,  1.44919104e-03,
       -3.65599605e-01])
```

```
rsquare_test_theta_0 = score(y_test, predict(X_test, theta_0))
rsquare_test_theta_2 = score(y_test, predict(X_test, theta_2))
print("R2:", rsquare_test_theta_0, rsquare_test_theta_2)
```

```
R2: 0.225177019162496 77 0.8022366128860432
```

Obviously, theta_2, which is the result of ridge regression, is much better due to the lower effect of redundant variables.

4. Change λ

You can change the regularization parameter λ to get different solutions for this problem. Suppose we set λ = 10, 1, 0.1, 0.01, 0.001, and please evaluate the model R^2 *on the training set and the testing set.*

```
from sklearn.metrics import mean_squared_error as mse

# Define constants
X_train = df1_train.drop(df1_train.columns[8], axis=1).to_numpy()
y_train = df1_train.iloc[:, [8]].to_numpy()
X_test = df1_test.drop(df1_test.columns[8], axis=1).to_numpy()
y_test = df1_test.iloc[:, [8]].to_numpy()
lambds = [10.00, 1.000, 0.10, 0.01, 0.001]

print("R scores comparison")
# print("λ          Training R2          Testing R2          Testing MSE")
print("λ          Training R2          Testing R2")
for lambd in lambds:
```

```
    theta = closed_form_2(X_train, y_train, lambd)
    rsquare_train = score(y_train, predict(X_train, theta))
    rsquare_test = score(y_test, predict(X_test, theta))
    # meanse = mse(y_test, predict(X_test, theta))
    # print(lambd, "       ", rsquare_train.round(5), "            ", rsquare_test.round(5), "            ", meanse.round(5))
    print(lambd, "       ", rsquare_train.round(5), "           ", rsquare_test.round(5))
```

```
R scores comparison
λ          Training R2          Testing R2
10.0         0.67461             0.94087
1.0         0.67947             0.84675
0.1         0.69447             0.67329
0.01         0.71165             0.58528
0.001         0.71483             0.56252
```

Finally, please decide the best regularization parameter λ. (Note that: As a qualified data analyst, you must know how to choose model parameters, please learn about cross validation methods.)

```
from sklearn.model_selection import KFold
from sklearn.linear_model import Ridge
from sklearn.model_selection import GridSearchCV

def cross_validation(X, y):
    """
    Using k-fold to get optimal value of lambda based on R-squared.

    Parameters:
    ----------
        X: features, IV.
        y: taget variable, DV.
    Return:
    ----------
        alpha: learning rate
    """
    kfold = KFold(n_splits=10).split(X, y)
    model = Ridge(normalize=True)  # Normalization returns better result
    lambdas = [10, 1, 0.1, 0.01, 0.001]
    grid_param = {"alpha": lambdas}
    grid = GridSearchCV(estimator=model,
                        param_grid=grid_param,
                        cv=kfold,
                        scoring="r2")
    grid.fit(X, y)
    alpha = grid.best_params_['alpha']
    return alpha


print('Optimal lamba should be ', cross_validation(X_train, y_train))
```

```
Optimal lamba should be  0.1
```

```
C:\Users\oyrx\Anaconda3\lib\site-packages\sklearn\model_selection\_search.py:814: DeprecationWarning: The default of the `iid` parameter will change from True to False in version 0.22 and will be removed in 0.24. This will change numeric results when test-set sizes are unequal.
  DeprecationWarning)
```

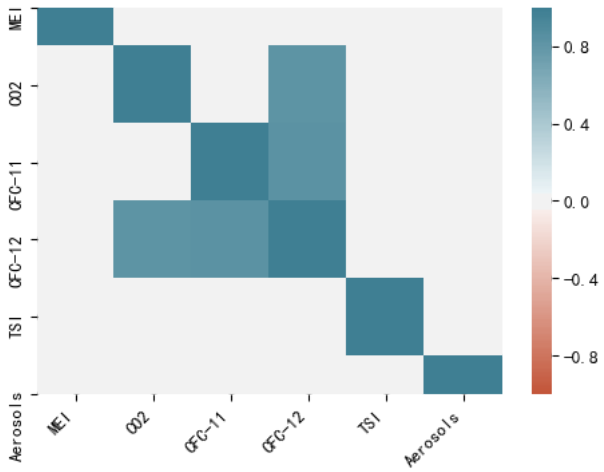
Problem 3 — Feature Selection

1. Lesser variables

From Problem 1, you can know which variables are significant, therefore you can use less variables to train model. For example, remove highly correlated and redundant features. You can propose a workflow to select feature.

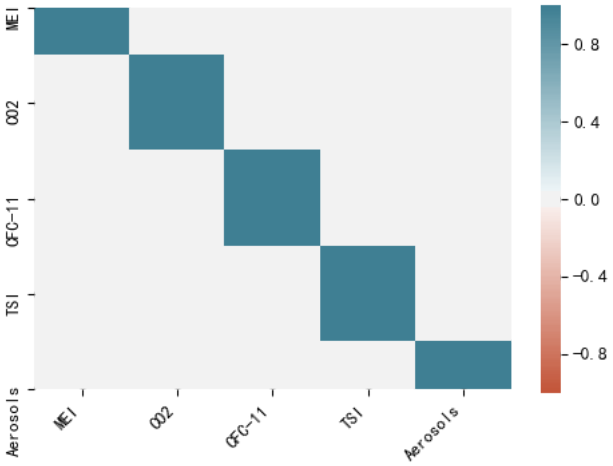
As mentioned in the first section and known siginificant variables(MEI, CO2, CDC-11, CDC-12, TST, Aerocols), a new correlation matrix can be introduced:

```
corr = df1[['MEI', 'CO2', 'CFC-11', 'CFC-12', 'TSI', 'Aerosols' ]].corr()
high_corr = corr[np.abs(corr) > 0.5].fillna(0)
corr[np.abs(corr) > 0.6].fillna('')
plt.figure(dpi=96)
ax = sns.heatmap(
    high_corr,
    vmin=-1, vmax=1, center=0,
    cmap=sns.diverging_palette(20, 220, n=200),
    square=True
)
ax.set_xticklabels(
    ax.get_xticklabels(),
    rotation=45,
    horizontalalignment='right'
);
```



Thus, CFC-12 should also be removed(r>0.6) then we have:

```
corr = df1[['MEI', 'CO2', 'CFC-11', 'TSI', 'Aerosols' ]].corr()
high_corr = corr[np.abs(corr) > 0.5].fillna(0)
corr[np.abs(corr) > 0.6].fillna('')
plt.figure(dpi=96)
ax = sns.heatmap(
    high_corr,
    vmin=-1, vmax=1, center=0,
    cmap=sns.diverging_palette(20, 220, n=200),
    square=True
)
ax.set_xticklabels(
    ax.get_xticklabels(),
    rotation=45,
    horizontalalignment='right'
);
```



Now no redundant variables left.

2. A better model

Train a better model than the model in Problem 2.

```
X_lesser = df1_train[['MEI', 'CO2', 'CFC-11', 'TSI', 'Aerosols' ]].to_numpy() # X: the features
y_lesser = df1_train.iloc[:, [8]].to_numpy()                                  # y: the results, lower case to emphasize the difference
X_test = df1_test[['MEI', 'CO2', 'CFC-11', 'TSI', 'Aerosols' ]].to_numpy()
y_test = df1_test.iloc[:, [8]].to_numpy()

#theta_lesser = closed_form_1(X_lesser, y_lesser)
theta_lesser = closed_form_2(X_lesser, y_train, cross_validation(X_lesser,y_lesser))
theta_lesser = np.array(theta_lesser)
formula = [str(theta_lesser.round(5).tolist()[i][0]) + ' * x' + str(i) + ' + ' for i in range(0, len(theta_lesser.round(5).tolist()))]
print('Thus our better model is: \ny = '+ ' '.join(formula).replace(' * x0', '')[:-3])
```

```
Thus our better model is:
y = -0.02465 +  0.04909 * x1 +  0.0118 * x2 +  2e-05 * x3 +  -0.00293 * x4 +  -0.88807 * x5
```

```
C:\Users\oyrx\Anaconda3\lib\site-packages\sklearn\model_selection\_search.py:814: DeprecationWarning: The default of the `iid` parameter will change from True to False in version 0.22 and will be removed in 0.24. This will change numeric results when test-set sizes are unequal.
  DeprecationWarning)
```

Significance:

```
l = sm.OLS(y_lesser, X_lesser).fit()
pvalues = l.summary2().tables[1]['P>|t|']
pvalues < 0.05
```

```
x1     True
x2     True
x3    False
x4     True
x5     True
Name: P>|t|, dtype: bool
```

Then remove x3 based on the new result:

```
X_lesser = df1_train[['MEI', 'CO2', 'TSI', 'Aerosols' ]].to_numpy() # X: the features
y_lesser = df1_train.iloc[:, [8]].to_numpy()                        # y: the results, lower case to emphasize the difference
X_test = df1_test[['MEI', 'CO2', 'TSI', 'Aerosols' ]].to_numpy()
y_test = df1_test.iloc[:, [8]].to_numpy()

theta_lesser = closed_form_1(X_lesser, y_train)
theta_lesser = np.array(theta_lesser)
formula = [str(theta_lesser.round(5).tolist()[i][0]) + ' * x' + str(i) + ' + ' for i in range(0, len(theta_lesser.round(5).tolist()))]
print('Thus our better model is: \n\ny = '+ ' '.join(formula).replace(' * x0', '')[:-3])
```

```
Thus our better model is:

y = -118.60162 +  0.06204 * x1 +  0.01069 * x2 +  0.08418 * x3 +  -1.58444 * x4
```

```
l = sm.OLS(y_lesser, X_lesser).fit()
pvalues = l.summary2().tables[1]['P>|t|']
pvalues < 0.05
```

```
x1    True
x2    True
x3    True
x4    True
Name: P>|t|, dtype: bool
```

R2:

```
rsquare_train = score(y_lesser, predict(X_lesser, theta_lesser))
rsquare_test = score(y_test, predict(X_test, theta_lesser))
print(('R2\nTraining: {}\nTesting: {}').format(rsquare_train, rsquare_test))
```

```
R2
Training: 0.7336403428986276
Testing: 0.6328867941215394
```

Problem 4 — Gradient Descent

Gradient descent algorithm is an iterative process that takes us to the minimum of a function. Please write down the iterative expression for updating the solution of linear model and implement it using Python or Matlab in gradientDescent function.

Cost and gradient functions

```
def normalize(mtx: np.matrix, method="std"):
    """
    To normalize a matrix

    Parameters:
    ----------
        mtx: matrix
    Return:
```

```
    ----------
        normalized matrix
    """
    return (mtx - np.mean(mtx)) / np.std(mtx)  # Normalization for faster convergence

def costFunction(X: np.matrix, y: np.matrix, theta: np.ndarray) -> float:
    """
    To calculate cost given X, y, and theta in ndarrays.

    Parameters:
    ----------
        X: features, IV.
        y: taget variable, DV.
        theta: coefficients
    Return:
    ----------
        cost: calculated cost
    """
    # print(X.shape, np.array(theta).shape, y.shape) # for debugging

    m = len(y_train)  # no. of training samples
    temp = X @ theta - y
    return np.sum(np.power(temp, 2)) / (2 * m)


def gradientDescent(X: np.matrix,
                    y: np.matrix,
                    theta: np.ndarray,
                    alpha: float = 0.001,
                    iterations: int = 10000,
                    norm: bool = True) -> np.ndarray:
    """
    To find optimal theta given X, y, theta in ndarrays and alpha, iters in float.

    Parameters:
    ----------
        X: features, IV.
        y: taget variable, DV.
        theta: initial coefficients
        alpha: learning rate, default by 0.001
        iterations: an assigned number of iterations
        norm: nomalization or not, default by True
    Return:
    ----------
        theta: np.matrix, final theta
        J_history: np.ndarray, cost history
    """

    X = (X, normalize(X))[norm] # normalization
    # print(X.shape, np.array(theta).shape, y.shape)
    m = len(y)
    J_history = []
    _theta = theta.copy()
    for i in range(iterations):
        error = X.T @ (X @ _theta - y)
        _theta -= alpha * 1 / m * error
        J_history.append(costFunction(X, y, _theta))
    # print(_theta, J_history)
    return _theta, J_history
```

Datasets

```

features = ["MEI", "CO2", "CH4", "N2O", "CFC-11", "CFC-12", "TSI", "Aerosols"]  # Features
target = ["Temp"] # taget

# Splitting into training and testing
year = 2006  # Specific year for splitting
train, test= df1[df1['Year'] <= year], df1[df1['Year'] > year]
X_train, X_test = train.get(features), test.get(features)
X_train, X_test = np.column_stack((np.ones(len(X_train)), X_train)), np.column_stack((np.ones(len(X_test)), X_test))
y_train, y_test = train.get(target), test.get(target)
X_train, X_test, y_train, y_test = np.mat(X_train), np.mat(X_test), np.mat(y_train), np.mat(y_test)
```

Parameters

```
# Define parameters
alpha = 0.01  # Learning rate
iterations = 300000  # The number of iterations
```

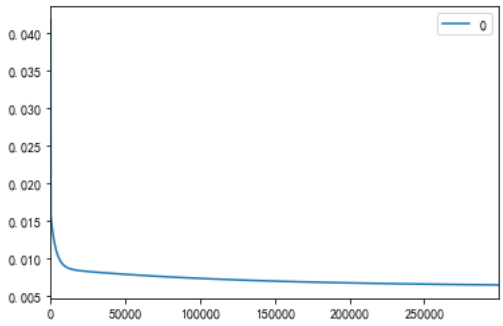
Run

```
# Initial
theta_init = np.zeros((X_train.shape[1], 1))
J_init = costFunction(X_train, y_train, theta_init)
print("Initial cost:", J_init.round(3))

## Gradient descent method (for normalized features)
result = gradientDescent(X_train, y_train, theta_init, alpha, iterations)
theta, J_history = result[0], pd.DataFrame(result[1])

J_history.plot.line()
J_final = float(J_history.round(3)[-1:][0])
print("Final cost:", J_final, "\nFinal theta(for normalized features):",
      [i[0] for i in theta.round(3)])
```

```
Initial cost: 0.047
Final cost: 0.006
Final theta(for normalized features): [0.205, 0.367, 1.474, 0.588, 0.584, -1.649, 1.033, -0.32, 0.201]
```



Compare with theta(s)=0

```
comparison = {'Init': [J_init.round(2)],
              'Final': [float(J_history[-1:][0])]}
pd.DataFrame(comparison).plot.bar()
```

```
<matplotlib.axes._subplots.AxesSubplot at 0x20767150e08>
```