

Tutorial 2

Outline

- Simulated Annealing (for HW#2)
- Pandas
- Numba

Simulated Annealing

```
In [1]: import numpy as np
import matplotlib.pyplot as plt

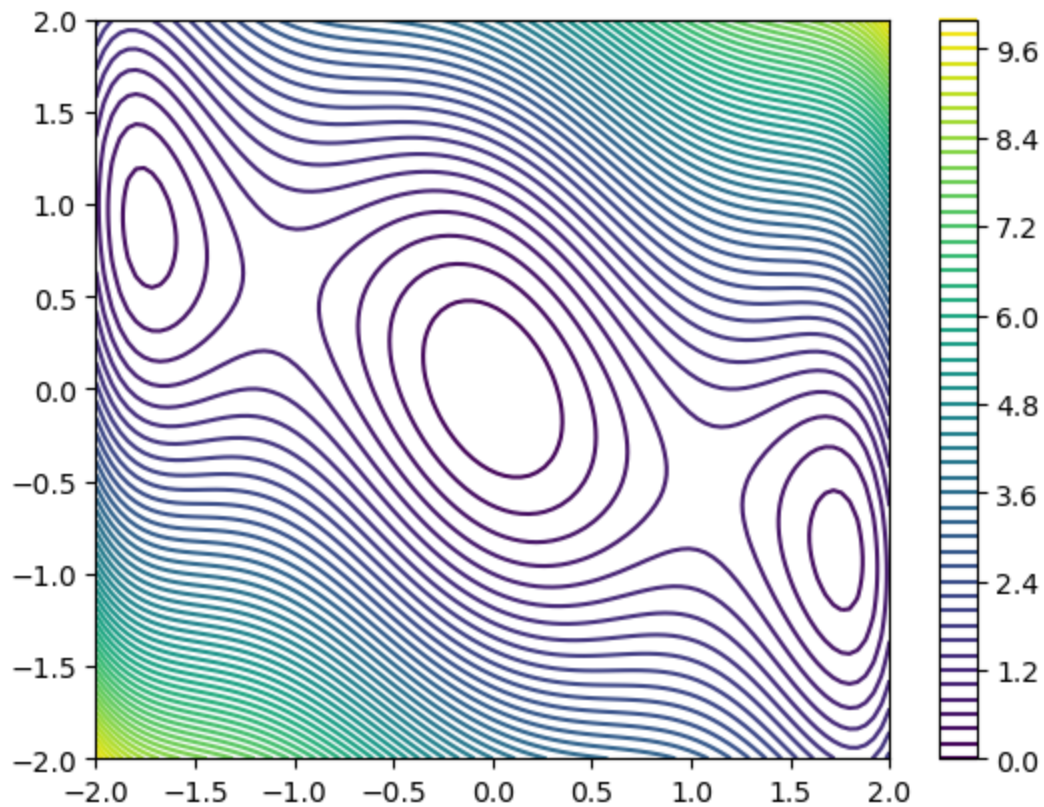
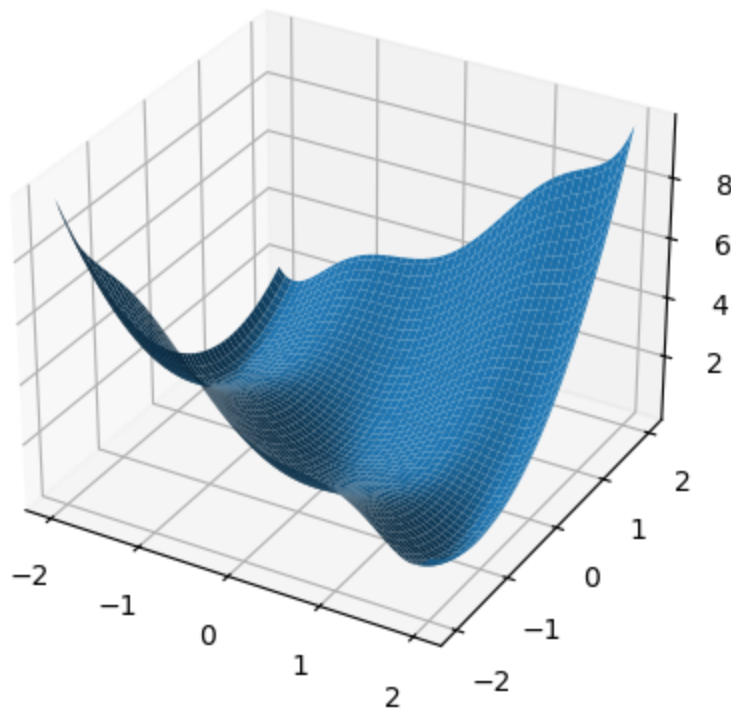
def Camel(X):
    x, y = X
    return 2 * x**2 - 1.05 * x**4 + x**6 / 6 + x * y + y**2


def plot_surface(func, x_min=-2, x_max=2, y_min=-2, y_max=2):
    a = np.linspace(x_min, x_max, 100)
    b = np.linspace(y_min, y_max, 100)
    x,y = np.meshgrid(a, b)
    z = func((x, y))
    fig = plt.figure()
    ax = fig.add_subplot(projection='3d')
    ax.plot_surface(x, y, z)

plot_surface(Camel)

def draw_path(func, path=None, x_min=-2, x_max=2, y_min=-2, y_max=2):
    a = np.linspace(x_min, x_max, 100)
    b = np.linspace(y_min, y_max, 100)
    x, y = np.meshgrid(a, b)
    z = func((x, y))
    fig, ax = plt.subplots()
    contour = ax.contour(x, y, z, 50)
    plt.colorbar(contour)
    if path:
        ax.plot(path[:, 0], path[:, 1], color='red')
        print(len(path))

draw_path(Camel)
```



 No description has been provided for this image

- Random Displacement:

$$X_{i+1} = X_i + \Delta * (2 * \text{URN} - 1)$$

- Metropolis Rule:

$$P(\text{accept}) = \exp\left(-\frac{\Delta E}{T}\right)$$

```
In [2]: def SA(solution, func, schedule, delta, boundary, n_iter, report_interval=None):
        """
        Simulated Annealing for minimization

        Parameters
        -----
        solution: np.ndarray
            Initial guess
        func: Callable
            Function to minimize
        schedule: np.ndarray
            An array of temperatures for simulated annealing
        delta: float
            Magnitude of random displacement
        boundary: tuple
            Boundary of the variables to minimize. (lowerbound,upperbound)
        n_iter: int
            Number of random displacement move in each temperature
        report_interval: int
            Number of temperature steps to report result

        Returns
        -----
        res: dict
            Minimized point and its evaluation value
        """

        best_solution = solution.copy()
        lowest_eval = func(best_solution)

        for idx, temp in enumerate(schedule):
            if report_interval is not None and ((idx + 1) % report_interval == 0 or idx
                msg = (
                    f"{idx + 1}/{len(schedule)}, Temp: {temp:.2f}, "
                    f"Best solution: {best_solution}, Value: {lowest_eval:.7f}"
                )
                print(msg)

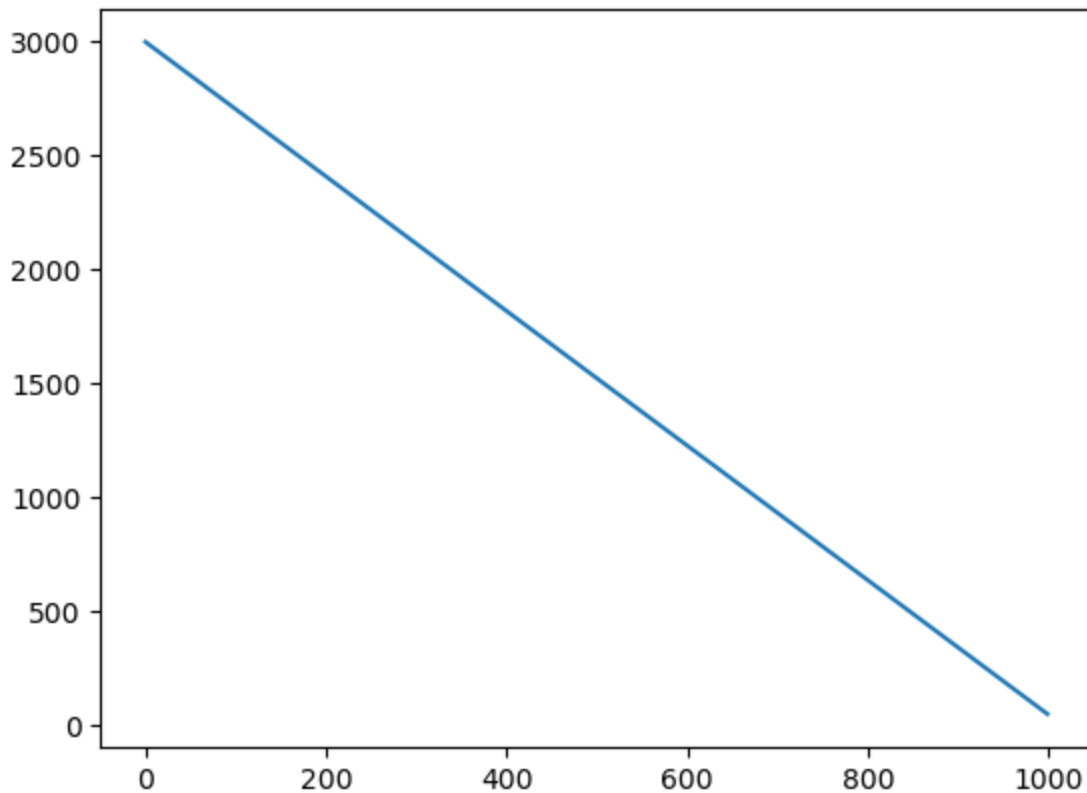
            for n in range(n_iter):
                trial = solution.copy()
                trial += delta * (2 * np.random.random(trial.shape) - 1)
                if np.all(trial >= boundary[0]) and np.all(trial <= boundary[1]):
                    # fill in acceptance criterion
                    if np.exp(-(func(trial) - func(solution)) / temp) > np.random.random():
                        solution = trial
                        if func(solution) < lowest_eval:
                            # update solution here
                            best_solution = solution.copy()
                            lowest_eval = func(best_solution)
```

```
return {"solution":best_solution, "evaluation":lowest_eval}
```

Try linear cooling

```
In [3]: linear_cooling = np.linspace(3000, 50, 1000)
plt.plot(linear_cooling)
```

```
Out[3]: [<matplotlib.lines.Line2D at 0x1a54d604710>]
```



```
In [4]: # Start from a point which is close to local minimum
starting_point = np.array([-1.7, 0.7])
SA(starting_point, Camel, linear_cooling, 0.1, (-2, 2), 5, 100)
```

```
1/1000, Temp: 3000.00, Best solution: [-1.7  0.7], Value: 0.3332232
100/1000, Temp: 2707.66, Best solution: [ 0.02742354 -0.38066902], Value: 0.1359731
200/1000, Temp: 2412.36, Best solution: [0.08827732 0.04828203], Value: 0.0221154
300/1000, Temp: 2117.07, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
400/1000, Temp: 1821.77, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
500/1000, Temp: 1526.48, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
600/1000, Temp: 1231.18, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
700/1000, Temp: 935.89, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
800/1000, Temp: 640.59, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
900/1000, Temp: 345.30, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
1000/1000, Temp: 50.00, Best solution: [ 0.01358763 -0.03255679], Value: 0.0009868
```

```
Out[4]: {'solution': array([ 0.01358763, -0.03255679]),
        'evaluation': 0.000986786501804797}
```

```
In [5]: # Local minimization methods fail to find the global minimum
from scipy.optimize import minimize
```

```
minimize(Camel, starting_point, method="BFGS")
```

```
Out[5]: message: Optimization terminated successfully.
        success: True
        status: 0
         fun: 0.298638442236861
          x: [-1.748e+00  8.738e-01]
         nit: 5
         jac: [ 3.129e-07 -7.451e-09]
        hess_inv: [[ 8.564e-02 -4.261e-02]
                  [-4.261e-02  5.250e-01]]
         nfev: 21
         njev: 7
```

Pandas

- [Documentation](#)

```
In [6]: import pandas as pd
```

```
C:\Users\artui\AppData\Local\Temp\ipykernel_12292\4080736814.py:1: DeprecationWarning:
Pyarrow will become a required dependency of pandas in the next major release of pan
das (pandas 3.0),
(to allow more performant data types, such as the Arrow string type, and better inte
roperability with other libraries)
but was not found to be installed on your system.
If this would cause problems for you,
please provide us feedback at https://github.com/pandas-dev/pandas/issues/54466
```

```
import pandas as pd
```

Read CSV file

```
In [7]: df = pd.read_csv("Datasets/titanic.csv")
        print(type(df))
        df
```

```
<class 'pandas.core.frame.DataFrame'>
```

Out[7]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.25
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.92
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.10
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.05
...
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.00
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.00
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	23.45
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.00
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.73

891 rows × 12 columns



```
In [8]: df.head(40)
```

Out[8]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	7
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8
5	6	0	3	Moran, Mr. James	male	NaN	0	0	330877	8
6	7	0	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	5
7	8	0	3	Palsson, Master. Gosta Leonard	male	2.0	3	1	349909	2
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Berg)	female	27.0	0	2	347742	1
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30
10	11	1	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549	16
11	12	1	1	Bonnell, Miss. Elizabeth	female	58.0	0	0	113783	26
12	13	0	3	Saunderscock, Mr. William Henry	male	20.0	0	0	A/5. 2151	8

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	
13	14	0	3	Andersson, Mr. Anders Johan	male	39.0	1	5	347082	3
14	15	0	3	Vestrom, Miss. Hulda Amanda Adolfina	female	14.0	0	0	350406	7
15	16	1	2	Hewlett, Mrs. (Mary D Kingcome)	female	55.0	0	0	248706	16
16	17	0	3	Rice, Master. Eugene	male	2.0	4	1	382652	29
17	18	1	2	Williams, Mr. Charles Eugene	male	NaN	0	0	244373	13
18	19	0	3	Vander Planke, Mrs. Julius (Emelia Maria Vande...	female	31.0	1	0	345763	18
19	20	1	3	Masselmani, Mrs. Fatima	female	NaN	0	0	2649	7
20	21	0	2	Fynney, Mr. Joseph J	male	35.0	0	0	239865	26
21	22	1	2	Beesley, Mr. Lawrence	male	34.0	0	0	248698	13
22	23	1	3	McGowan, Miss. Anna "Annie"	female	15.0	0	0	330923	8
23	24	1	1	Sloper, Mr. William Thompson	male	28.0	0	0	113788	35
24	25	0	3	Palsson, Miss. Torborg Danira	female	8.0	3	1	349909	27
25	26	1	3	Asplund, Mrs. Carl Oscar (Selma Augusta Emilia...	female	38.0	1	5	347077	37
26	27	0	3	Emir, Mr. Farred	male	NaN	0	0	2631	7

PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	
Chehab									
27	28	0	1	Fortune, Mr. Charles Alexander	male	19.0	3	2	19950 263
28	29	1	3	O'Dwyer, Miss. Ellen "Nellie"	female	NaN	0	0	330959 7
29	30	0	3	Todoroff, Mr. Lalio	male	NaN	0	0	349216 7
30	31	0	1	Uruchurtu, Don. Manuel E	male	40.0	0	0	PC 17601 27
31	32	1	1	Spencer, Mrs. William Augustus (Marie Eugenie)	female	NaN	1	0	PC 17569 146
32	33	1	3	Glynn, Miss. Mary Agatha	female	NaN	0	0	335677 7
33	34	0	2	Wheadon, Mr. Edward H	male	66.0	0	0	C.A. 24579 10
34	35	0	1	Meyer, Mr. Edgar Joseph	male	28.0	1	0	PC 17604 82
35	36	0	1	Holverson, Mr. Alexander Oskar	male	42.0	1	0	113789 52
36	37	1	3	Mamee, Mr. Hanna	male	NaN	0	0	2677 7
37	38	0	3	Cann, Mr. Ernest Charles	male	21.0	0	0	A./5. 2152 8
38	39	0	3	Vander Planke, Miss. Augusta Maria	female	18.0	2	0	345764 18
39	40	1	3	Nicola- Yarred, Miss. Jamila	female	14.0	1	0	2651 17

In [9]: `df.tail(10)`

Out[9]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	
881	882	0	3	Markun, Mr. Johann	male	33.0	0	0	349257	7.
882	883	0	3	Dahlberg, Miss. Gerda Ulrika	female	22.0	0	0	7552	10.
883	884	0	2	Banfield, Mr. Frederick James	male	28.0	0	0	C.A./SOTON 34068	10.
884	885	0	3	Sutehall, Mr. Henry Jr	male	25.0	0	0	SOTON/OQ 392076	7.
885	886	0	3	Rice, Mrs. William (Margaret Norton)	female	39.0	0	5	382652	29.
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	23.
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.

Drop columns

In [10]: `df2 = df.drop(['Cabin'], axis=1, inplace=True)`

Drop NaN values

Drop the rows where at least one element is missing

```
In [11]: df.dropna()
```

Out[11]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.25
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.92
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.10
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.05
...
885	886	0	3	Rice, Mrs. William (Margaret Norton)	female	39.0	0	5	382652	29.12
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.00
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.00
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.00
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.75

712 rows × 11 columns



Drop the columns where at least one element is missing.

```
In [12]: df.dropna(axis=1) # or axis='columns'
```

Out[12]:

	PassengerId	Survived	Pclass	Name	Sex	SibSp	Parch	Ticket	Fare
0	1	0	3	Braund, Mr. Owen Harris	male	1	0	A/5 21171	7.2500
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	1	0	PC 17599	71.2833
2	3	1	3	Heikkinen, Miss. Laina	female	0	0	STON/O2. 3101282	7.9250
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	1	0	113803	53.1000
4	5	0	3	Allen, Mr. William Henry	male	0	0	373450	8.0500
...
886	887	0	2	Montvila, Rev. Juozas	male	0	0	211536	13.0000
887	888	1	1	Graham, Miss. Margaret Edith	female	0	0	112053	30.0000
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	1	2	W./C. 6607	23.4500
889	890	1	1	Behr, Mr. Karl Howell	male	0	0	111369	30.0000
890	891	0	3	Dooley, Mr. Patrick	male	0	0	370376	7.7500

891 rows × 9 columns

Define in which columns to look for missing values.

```
In [13]: df.dropna(subset=['Age'])
```

Out[13]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.25
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.92
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.10
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.05
...
885	886	0	3	Rice, Mrs. William (Margaret Norton)	female	39.0	0	5	382652	29.12
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.00
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.00
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.00
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.75

714 rows × 11 columns



Indexing

```
In [14]: df.loc[0, "Pclass"]
```

```
Out[14]: 3
```

```
In [15]: df.iloc[0, 2]
```

```
Out[15]: 3
```

```
In [16]: df[['Pclass', 'Survived']]
```

```
Out[16]:
```

	Pclass	Survived
0	3	0
1	1	1
2	3	1
3	1	1
4	3	0
...
886	2	0
887	1	1
888	3	0
889	1	1
890	3	0

891 rows × 2 columns

```
In [17]: df[df['Survived'] == 1]
```

Out[17]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.92
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.10
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Berg)	female	27.0	0	2	347742	11.13
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30.07
...
875	876	1	3	Najib, Miss. Adele Kiamie "Jane"	female	15.0	0	0	2667	7.22
879	880	1	1	Potter, Mrs. Thomas Jr (Lily Alexenia Wilson)	female	56.0	0	1	11767	83.15
880	881	1	2	Shelley, Mrs. William (Imanita Parrish Hall)	female	25.0	0	1	230433	26.00
887	888	1	1	Graham, Miss.	female	19.0	0	0	112053	30.00

PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare
			Margaret Edith						
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369 30.00

342 rows × 11 columns

Other useful methods

Use `.values` attribute to get values in `numpy.ndarray`

In [18]: `df.values`

Out[18]: `array([[1, 0, 3, ..., 'A/5 21171', 7.25, 'S'],
[2, 1, 1, ..., 'PC 17599', 71.2833, 'C'],
[3, 1, 3, ..., 'STON/O2. 3101282', 7.925, 'S'],
...,
[889, 0, 3, ..., 'W./C. 6607', 23.45, 'S'],
[890, 1, 1, ..., '111369', 30.0, 'C'],
[891, 0, 3, ..., '370376', 7.75, 'Q']], dtype=object)`

Use `describe()` method to get statistics

In [19]: `df.describe()`

Out[19]:

	PassengerId	Survived	Pclass	Age	SibSp	Parch	Fare
count	891.000000	891.000000	891.000000	714.000000	891.000000	891.000000	891.000000
mean	446.000000	0.383838	2.308642	29.699118	0.523008	0.381594	32.204208
std	257.353842	0.486592	0.836071	14.526497	1.102743	0.806057	49.693429
min	1.000000	0.000000	1.000000	0.420000	0.000000	0.000000	0.000000
25%	223.500000	0.000000	2.000000	20.125000	0.000000	0.000000	7.910400
50%	446.000000	0.000000	3.000000	28.000000	0.000000	0.000000	14.454200
75%	668.500000	1.000000	3.000000	38.000000	1.000000	0.000000	31.000000
max	891.000000	1.000000	3.000000	80.000000	8.000000	6.000000	512.329200

Use `.index` or `.columns` get index/columns

In [20]: `for index in df.index:
print(index)`

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```
In [21]: for col in df.columns:  
         print(col)
```

PassengerId
Survived
Pclass
Name
Sex
Age
SibSp
Parch
Ticket
Fare
Embarked

Use `to_csv()` to export DataFrame

```
In [22]: df.to_csv("test_export.csv")
```

Use `sort_values()` method to sort the DataFrame according to values in one column.

```
In [23]: df.sort_values(by=["Age"], ascending=False)
```

Out[23]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	F
630	631	1	1	Barkworth, Mr. Algernon Henry Wilson	male	80.0	0	0	27042	30.00
851	852	0	3	Svensson, Mr. Johan	male	74.0	0	0	347060	7.73
493	494	0	1	Artagaveytia, Mr. Ramon	male	71.0	0	0	PC 17609	49.50
96	97	0	1	Goldschmidt, Mr. George B	male	71.0	0	0	PC 17754	34.61
116	117	0	3	Connors, Mr. Patrick	male	70.5	0	0	370369	7.73
...
859	860	0	3	Razi, Mr. Raihed	male	NaN	0	0	2629	7.26
863	864	0	3	Sage, Miss. Dorothy Edith "Dolly"	female	NaN	8	2	CA. 2343	69.50
868	869	0	3	van Melkebeke, Mr. Philemon	male	NaN	0	0	345777	9.50
878	879	0	3	Laleff, Mr. Kristo	male	NaN	0	0	349217	7.80
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	23.40

891 rows × 11 columns



Numba

Use `pip install numba` or `conda install numba -c conda-forge` to install numba package.

Numba is a package that help users to accelerate the code.

In [24]:

```
import numba
```

```
In [25]: def test():  
        i = 0  
        for a in range(100000):  
            i += a  
        return i  
  
        %timeit test()
```

4.98 ms \pm 219 μ s per loop (mean \pm std. dev. of 7 runs, 100 loops each)

```
In [26]: @numba.njit()  
        def test():  
            i = 0  
            for a in range(100000):  
                i += a  
            return i  
  
        %timeit test()
```

The slowest run took 65.00 times longer than the fastest. This could mean that an intermediate result is being cached.

1.1 μ s \pm 2.21 μ s per loop (mean \pm std. dev. of 7 runs, 1 loop each)