Chem 277B Spring 2024 Tutorial 2

Outline

- Notes on HW#1
- Simulated Annealing (for HW#2)
- Pandas
- Numba

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1. Notes on HW#1

- Prob 1b: number of steps in SD (in debugging output) are the number of *accepted* steps
- Prob 2: "formulate a stochastic_deriv that is the same norm as your gradient" means
  - generate a random array stochastic_deriv
  - rescale it so that norm(stochastic_deriv) = norm(deriv)
- Prob 2: clarification on stochastic_injection:
  - stochastic_injection controls the scale of stochasticity/randomness injected into the Gradient Descent algorithm.
  - When it is 0, direction = -deriv, corresponding to GD, and when it is > 0, the algorithm is SGD because the direction now has some randomness.
  - The scale of the randomness increases as you increase stochastic_injection.
  - With the above normalization, norm(stochastic_deriv) = norm(deriv), stochastic_injection=1 means that the random part has the same magnitude as the non-random part, i.e. the gradient.
- Prob 2: SGD often has a fixed step size which means it is not always the case.
  - HW1 asks you to implement SGD based on your steepest_descent code with step size update rule specified in 1b -> your step size should change in the same way each iteration for SGD.

2. Pandas

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

```
/var/folders/k8/mg372j_55z30k1z4y_8mb0w00000gn/T/ipykernel_50799/4080736814.
py:1: DeprecationWarning:
Pyarrow will become a required dependency of pandas in the next major releas
e of pandas (pandas 3.0),
(to allow more performant data types, such as the Arrow string type, and bet
ter interoperability 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/54
466

  import pandas as pd
```

Read CSV file

In [ ]:
```
df = pd.read_csv('titanic.csv')
print(type(df))
df
```

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

Out[ ]:

	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
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450
...	...	...	...	...	...	...	...	...	...
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376

891 rows × 12 columns

In [ ]:
```
df.head() # show the first entries
```

Out[ ]:

	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	
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	
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	5
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	

In [ ]:
```
df.tail() # show the last entries
```

Out[ ]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	1
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	3
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	2
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	3
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	

Drop columns

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

# df.drop(['Cabin'], axis=1, inplace=True) # modify original data frame
```

Drop NaN values

Drop the rows where at least one element is missing: a way to clean the data

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

Out[ ]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803
6	7	0	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463
10	11	1	3	Sandstrom, Miss. Marguerite Rut	female	4.0	1	1	PP 9549
11	12	1	1	Bonnell, Miss. Elizabeth	female	58.0	0	0	113783
...	...	...	...	...	...	...	...	...	...
871	872	1	1	Beckwith, Mrs. Richard Leonard (Sallie Monypeny)	female	47.0	1	1	11751
872	873	0	1	Carlsson, Mr. Frans Olof	male	33.0	0	0	695
879	880	1	1	Potter, Mrs. Thomas Jr (Lily Alexenia Wilson)	female	56.0	0	1	11767
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369

183 rows × 12 columns

Drop the columns where at least one element is missing.

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

Out[ ]:

	PassengerId	Survived	Pclass	Name	Sex	SibSp	Parch	Ticket	F
0	1	0	3	Braund, Mr. Owen Harris	male	1	0	A/5 21171	7.2
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	1	0	PC 17599	71.2
2	3	1	3	Heikkinen, Miss. Laina	female	0	0	STON/O2. 3101282	7.9
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	1	0	113803	53.1
4	5	0	3	Allen, Mr. William Henry	male	0	0	373450	8.0
...	...	...	...	...	...	...	...	...	
886	887	0	2	Montvila, Rev. Juozas	male	0	0	211536	13.0
887	888	1	1	Graham, Miss. Margaret Edith	female	0	0	112053	30.0
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	1	2	W./C. 6607	23.4
889	890	1	1	Behr, Mr. Karl Howell	male	0	0	111369	30.0
890	891	0	3	Dooley, Mr. Patrick	male	0	0	370376	7.7

891 rows × 9 columns

Define in which columns to look for missing values.

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

Out[ ]:

	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
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450
...	...	...	...	...	...	...	...	...	...
885	886	0	3	Rice, Mrs. William (Margaret Norton)	female	39.0	0	5	382652
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376

714 rows × 12 columns

Indexing

In [ ]:
```
df.loc[0, 'Pclass']
```

Out[ ]: 3

In [ ]:
```
df.iloc[0, 2] # replace col name with its loc
```

Out[ ]: 3

In [ ]:
```
df[['Pclass', 'Survived']] # pick cols of interest
```

Out[ ]:

	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 [ ]:
```
df[df['Survived'] == 1] # similar to numpy
```

Out[ ]:

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

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

342 rows × 12 columns

Other useful methods

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

In [ ]:
```
df.values
```

Out[ ]:
```
array([[1, 0, 3, ..., 7.25, nan, 'S'],
       [2, 1, 1, ..., 71.2833, 'C85', 'C'],
       [3, 1, 3, ..., 7.925, nan, 'S'],
       ...,
       [889, 0, 3, ..., 23.45, nan, 'S'],
       [890, 1, 1, ..., 30.0, 'C148', 'C'],
       [891, 0, 3, ..., 7.75, nan, 'Q']], dtype=object)
```

Use `describe()` method to get statistics of numeric columns

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

Out[ ]:

	PassengerId	Survived	Pclass	Age	SibSp	Parch	
count	891.000000	891.000000	891.000000	714.000000	891.000000	891.000000	89
mean	446.000000	0.383838	2.308642	29.699118	0.523008	0.381594	3
std	257.353842	0.486592	0.836071	14.526497	1.102743	0.806057	4
min	1.000000	0.000000	1.000000	0.420000	0.000000	0.000000	
25%	223.500000	0.000000	2.000000	20.125000	0.000000	0.000000	
50%	446.000000	0.000000	3.000000	28.000000	0.000000	0.000000	1
75%	668.500000	1.000000	3.000000	38.000000	1.000000	0.000000	3
max	891.000000	1.000000	3.000000	80.000000	8.000000	6.000000	51

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

In [ ]:
```
df.index

# for index in df.index:
# print(index)
```

Out[ ]:
```
RangeIndex(start=0, stop=891, step=1)
```

In [ ]:
```
df.columns
```

Out[ ]:
```
Index(['PassengerId', 'Survived', 'Pclass', 'Name', 'Sex', 'Age', 'SibSp',
       'Parch', 'Ticket', 'Fare', 'Cabin', 'Embarked'],
      dtype='object')
```

Use `to_csv()` to export DataFrame

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

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

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

Out[ ]:

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

891 rows × 12 columns

3. Numba

Use `pip install numba` to install numba package.

Numba is a package that help users to accelerate the code. (if HW#2 is running slowly)

In [ ]:
```
import numba
```

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

%timeit test()
```

```
2.42 ms ± 63.5 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

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

%timeit test()
```

```
The slowest run took 16.57 times longer than the fastest. This could mean th
at an intermediate result is being cached.
280 ns ± 448 ns per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

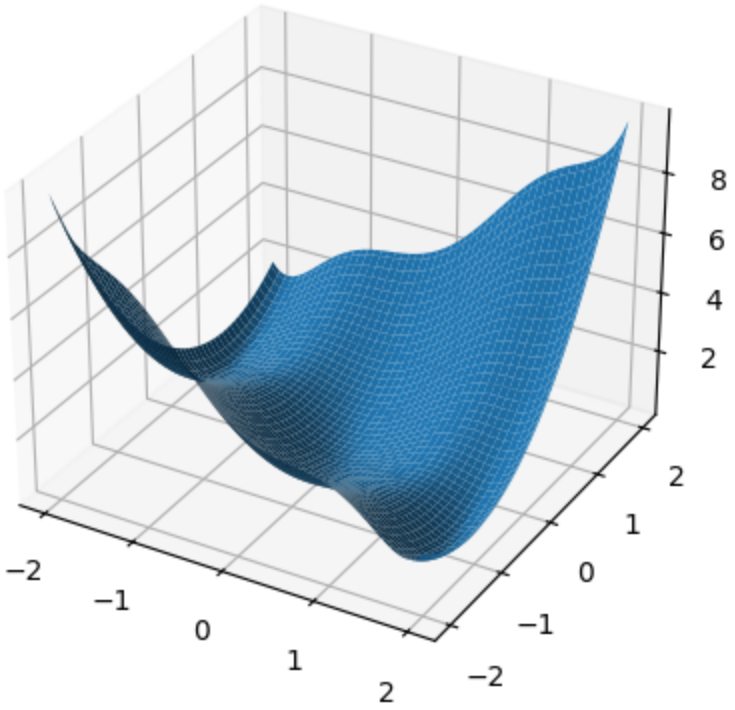
4. Simulated Annealing (for HW#2)

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

def Camel(point):
    x, y = point
    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)
```



No description has been provided for this image

- Random Displacement:

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

- Metropolis Rule:

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

TODO: Finish SA code

In [ ]:
```
def SA(solution, func, schedule, delta, boundary, n_iter, report_interval=Nc
    """
    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_interavl: int
        Number of temperature steps to report result

    Returns
    -------
    res: dict
        Minimized point and its evaulation 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
            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(len(trial)) - 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.randc
                    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}
```

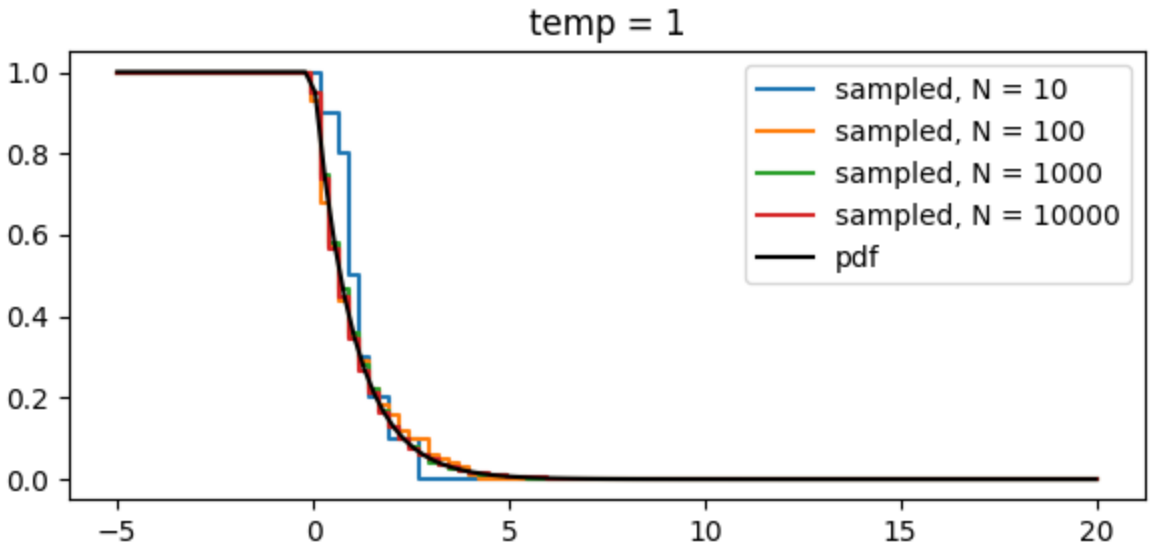
Metropolis algo for sampling

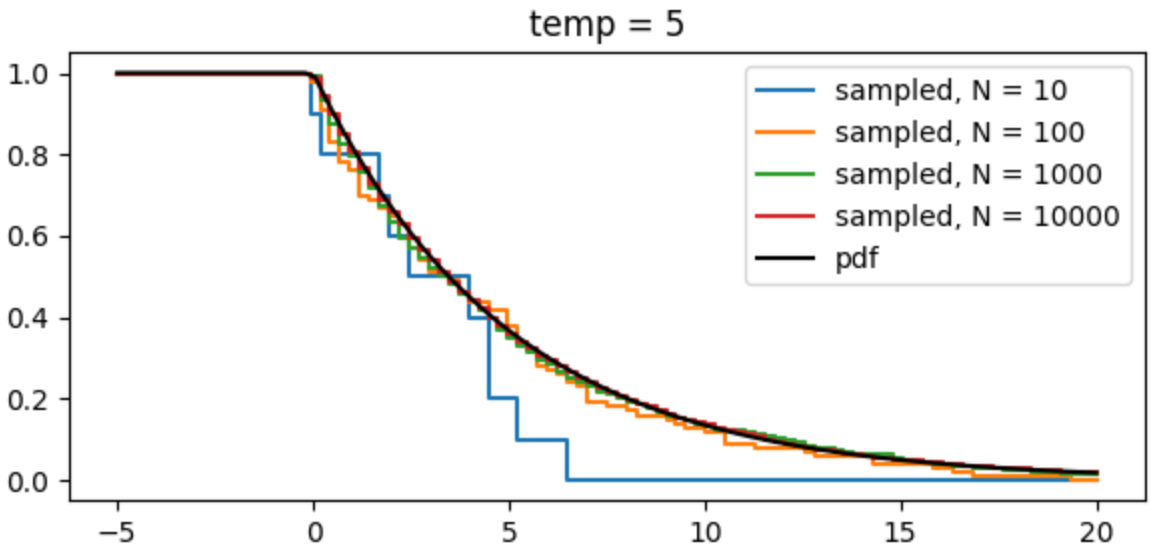
In [ ]:
```
def pdf(x,args):
    return np.where(x>0,np.exp(-x/args[0]),1)

temp = 5
for temp in [1,5]:
    x = np.linspace(-5,20,100)
    plt.figure(figsize=(6,3))

    for N in [10,100,1000,10000]:
        samples = (pdf(x,[temp])[:,None]>np.random.random(N)[None,:]).sum(1)
        plt.step(x,samples/N,where='mid',label=f'sampled, N = {N}',)

    plt.plot(x,pdf(x,[temp]),'k',label='pdf')
    plt.title(f'temp = {temp}')
    plt.legend()
    plt.tight_layout()
```



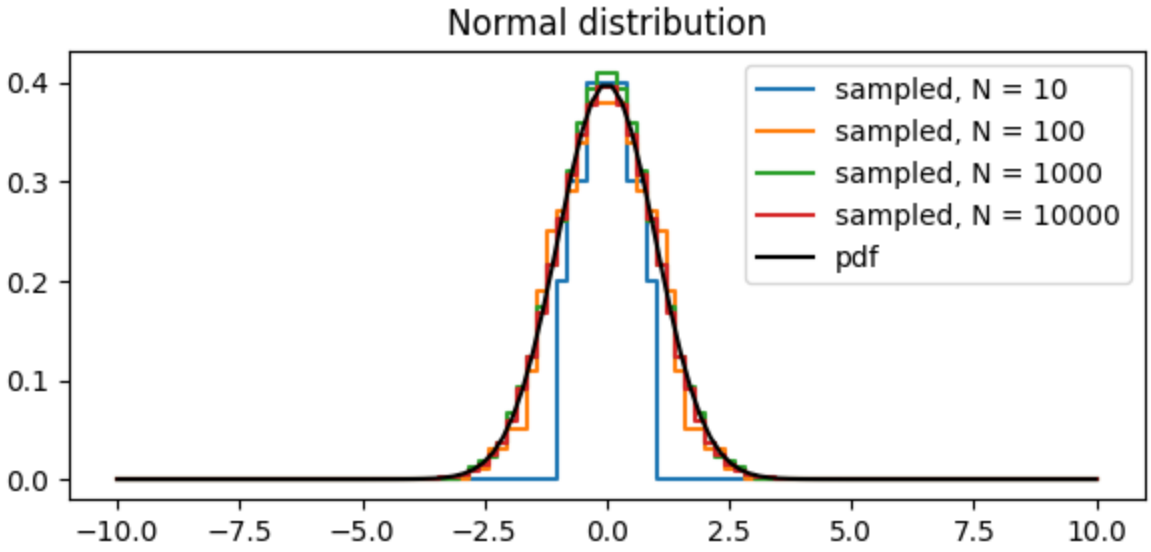


In [ ]:
```
def pdf(x,args):
    return np.exp(-x**2 / 2) / np.sqrt(2 * np.pi)


x = np.linspace(-10,10,100)
plt.figure(figsize=(6,3))

for N in [10,100,1000,10000]:
    samples = (pdf(x,[])[:,None]>np.random.random(N)[None,:]).sum(1)
    plt.step(x,samples/N,where='mid',label=f'sampled, N = {N}',)

plt.plot(x,pdf(x,[]),'k',label='pdf')
plt.title(f'Normal distribution')
plt.legend()
plt.tight_layout()
```



Local minimization method fails

In [ ]:
```
from scipy.optimize import minimize

starting_point = np.array([-1.7, 0.7])
minimize(Camel, starting_point, method="BFGS")
```

Out[ ]:
```
  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
```

SA with linear cooling

In [ ]:
```
# Start from a point which is close to local minimum
linear_cooling = np.linspace(3000, 50, 1000)
SA(starting_point, Camel, linear_cooling, 0.1, (-2, 2), 5, 100)
```

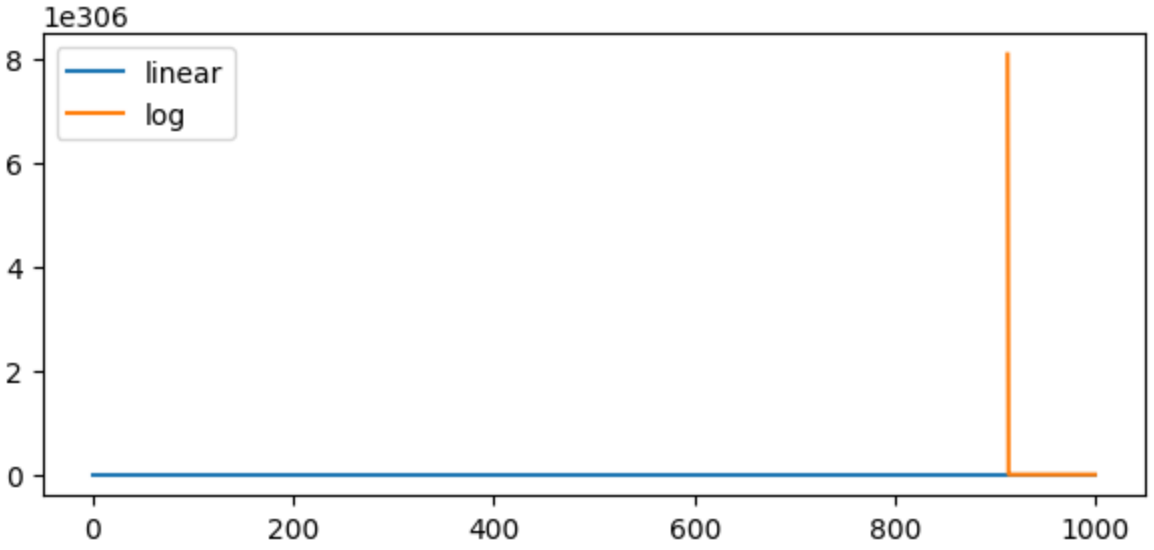
```
1/1000, Temp: 3000.00, Best solution: [-1.7  0.7], Value: 0.3332232
100/1000, Temp: 2707.66, Best solution: [-1.73741446  0.92389844], Value: 0.
3022725
200/1000, Temp: 2412.36, Best solution: [-1.73741446  0.92389844], Value: 0.
3022725
300/1000, Temp: 2117.07, Best solution: [-1.73486069  0.8456993 ], Value: 0.
3000280
400/1000, Temp: 1821.77, Best solution: [-0.1816215   0.43222392], Value: 0.
1731526
500/1000, Temp: 1526.48, Best solution: [-0.1816215   0.43222392], Value: 0.
1731526
600/1000, Temp: 1231.18, Best solution: [-0.12066591  0.27221605], Value: 0.
0701528
700/1000, Temp: 935.89, Best solution: [-0.12066591  0.27221605], Value: 0.0
701528
800/1000, Temp: 640.59, Best solution: [-0.12066591  0.27221605], Value: 0.0
701528
900/1000, Temp: 345.30, Best solution: [-0.12066591  0.27221605], Value: 0.0
701528
1000/1000, Temp: 50.00, Best solution: [-0.12066591  0.27221605], Value: 0.0
701528
```

Out[ ]:
```
{'solution': array([-0.12066591,  0.27221605]),
 'evaluation': 0.07015281989297005}
```

TODO: Try SA with logarithmic cooling

In [ ]:
```
log_cooling = np.logspace(3000, 50, 1000)

plt.figure(figsize=(6,3))
plt.plot(linear_cooling,label='linear')
plt.plot(log_cooling,label='log')
plt.legend()
plt.tight_layout()
```



In [ ]:
```
SA(starting_point, Camel, log_cooling, 0.1, (-2, 2), 5, 100)
```

```
1/1000, Temp: inf, Best solution: [-1.7  0.7], Value: 0.3332232
100/1000, Temp: inf, Best solution: [-1.68538129  0.72718695], Value: 0.3320
861
200/1000, Temp: inf, Best solution: [-1.73735266  0.87310791], Value: 0.2992
532
300/1000, Temp: inf, Best solution: [-1.73735266  0.87310791], Value: 0.2992
532
400/1000, Temp: inf, Best solution: [-0.18476388  0.42695259], Value: 0.1704
615
500/1000, Temp: inf, Best solution: [ 0.00779412 -0.0297886 ], Value: 0.0007
767
600/1000, Temp: inf, Best solution: [ 0.00779412 -0.0297886 ], Value: 0.0007
767
700/1000, Temp: inf, Best solution: [ 0.00779412 -0.0297886 ], Value: 0.0007
767
800/1000, Temp: inf, Best solution: [ 0.00779412 -0.0297886 ], Value: 0.0007
767
900/1000, Temp: inf, Best solution: [ 0.00779412 -0.0297886 ], Value: 0.0007
767
1000/1000, Temp: 1000000000000000076297698410918870032949649709465 60.00, Bes
t solution: [ 0.00779412 -0.0297886 ], Value: 0.0007767
```

Out[ ]:
```
{'solution': array([ 0.00779412, -0.0297886 ]),
 'evaluation': 0.0007766772987190596}
```