In [7]:
```
from google.colab import drive
drive.mount('/content/drive')
```

```
Go to this URL in a browser: https://accounts.google.com/o/oauth2/auth?client_id=947
318989803-6bn6qk8qdgf4n4g3pfee6491hc0brc4i.apps.googleusercontent.com&redirect_uri=u
rn%3aietf%3awg%3aoauth%3a2.0%3aoob&response_type=code&scope=email%20https%3a%2f%2fww
w.googleapis.com%2fauth%2fdocs.test%20https%3a%2f%2fwww.googleapis.com%2fauth%2fdriv
e%20https%3a%2f%2fwww.googleapis.com%2fauth%2fdrive.photos.readonly%20https%3a%2f%2f
www.googleapis.com%2fauth%2fpeopleapi.readonly

Enter your authorization code:
 . . . . . .
Mounted at /content/drive
```

In [99]:
```
!pip install biopython
```

```
Collecting biopython
  Downloading https://files.pythonhosted.org/packages/96/01/7e5858a1e54bd0bd0d179cd7
4654740f07e86fb921a43dd20fb8beabe69d/biopython-1.75-cp36-cp36m-manylinux1_x86_64.whl
(2.3MB)
     |████████████████████████████████| 2.3MB 8.7MB/s
Requirement already satisfied: numpy in /usr/local/lib/python3.6/dist-packages (from
biopython) (1.17.4)
Installing collected packages: biopython
Successfully installed biopython-1.75
```

파이썬 기본 문법

- 파이썬의 변수는 값을 저장하는 주소를 가리키는 바인더

In [1]:
```
a = 10
print(a)
print(type(a))
```

```
10
<class 'int'>
```

- 논리연산자, True, False, and, or

In [2]:
```
print(True and False)
print(True or False)
print(not True and False)
```

```
False
True
False
```

- 조건문, if, elif, else

In [3]:
```
a = 10
if a < 0:
    print("Negative")
elif a >= 0 and a < 10:
    print("Less than 10")
else:
    print("Geater than 10")
    print("Or equal to 10")
```

```
Geater than 10
Or equal to 10
```

- 반복문 for, while

In [4]:
```
for i in [0, 1, 2, 3]:
        print("for1", i)
        print("for2", i)

a = 4
i = 0
while i < a:
    print("while", i)
    if i == 2:
        print("stop")
        break
    i = i+1
```

```
for1 0
for2 0
for1 1
for2 1
for1 2
for2 2
for1 3
for2 3
while 0
while 1
while 2
stop
```

파이썬 기본 자료 구조

List (리스트)

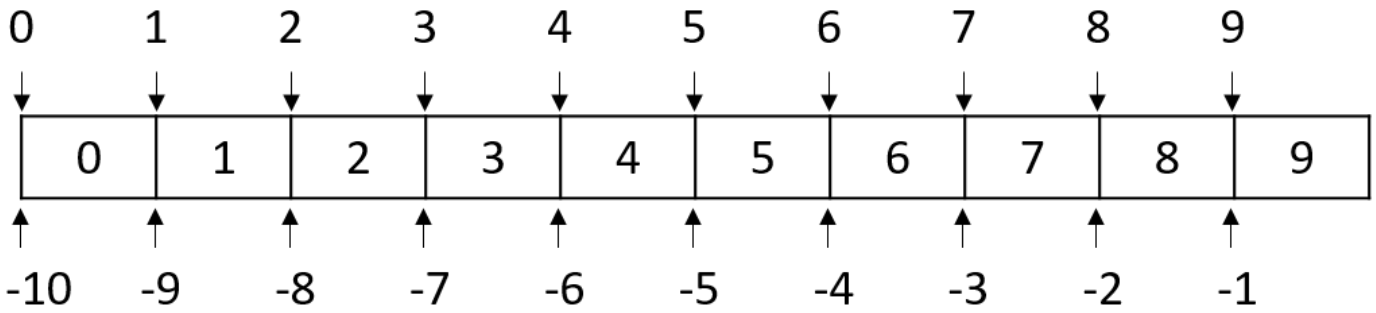
- 리스트는 여러 개의 데이터를 순서대로 저장하고 관리할 때 사용

In [ ]:
```
expression = ["geneA", 1]
expression = [1, 2, 3]
expression = []
```

- 인덱싱은 값 자체 (1은 두 번째값)
- 슬라이싱은 값 사이 경계선 (1은 첫 번째 값과 두 번째 값 사이)

In [6]:
```
!ls
```

```
sample_data
```



In [23]:
```
import os
os.getcwd()
```

Out[23]:
```
'/content'
```

In [26]:
```
geneids = [x for x in range(10)] # 리스트 컴프리헨션
print(geneids)
print(geneids[0])
print(geneids[-1])
print(geneids[2:-3])
print(geneids[:])
print(geneids[:-1])
print(geneids[1:])
print(geneids[:-10])
```

```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
0
9
[2, 3, 4, 5, 6]
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
[0, 1, 2, 3, 4, 5, 6, 7, 8]
[1, 2, 3, 4, 5, 6, 7, 8, 9]
[]
```

- 리스트 데이터 삽입 삭제

In [27]:
```
geneids = [1, 2, 3]
print(geneids)
geneids.append(4)
print(geneids)
print("length: %d" % len(geneids))
geneids[len(geneids):] = [5]
print(geneids)
print(geneids.pop())
print(geneids)
```

```
[1, 2, 3]
[1, 2, 3, 4]
length: 4
[1, 2, 3, 4, 5]
5
[1, 2, 3, 4]
```

Tuple (튜플)

- 리스트와 같은 기능이지만 '(', ')'를 사용하고 원소를 변경할 수 없음
- 리스트보다 빠른 속도, 리스트와 동일한 인덱싱 방법

In [29]:
```
geneids = (1, 2, 3)
print(geneids[0:2])
#geneids[0] = 4 ## error
```

```
(1, 2)
```

- 반복문에서 리스트 또는 튜플 활용

In [30]:
```
geneids = ['123', '456', '789']
for geneid in geneids:
    print("geneid: %s" %geneid)
```

```
geneid: 123
geneid: 456
geneid: 789
```

Dictionary (딕셔너리)

- 키(key)와 값(value)을 쌍으로 저장, '{'와 '}'를 사용

In [31]:
```
gene_expr = {}
gene_expr['A'] = 0.5
print(gene_expr)
gene_expr['B'] = 1.2
print(gene_expr)
print(len(gene_expr))
```

```
{'A': 0.5}
{'A': 0.5, 'B': 1.2}
2
```

- 인덱싱은 '[', ']' 사용, 키 값으로 인덱싱, 정수값 인덱싱 불가

In [32]:
```
print(gene_expr['A'])
## gene_expr[0] # error
```

```
0.5
```

- 데이터 추가는 key값 value값으로 수행, 삭제는 del 함수 이용

In [33]:
```
gene_expr['C'] = 0.3
print(gene_expr)
del gene_expr['C']
print(gene_expr)
```

```
{'A': 0.5, 'B': 1.2, 'C': 0.3}
{'A': 0.5, 'B': 1.2}
```

- key 값과 value 값 구하기

In [34]:
```
gene_expr_keys = list(gene_expr.keys())
print("keys:", gene_expr_keys)
gene_expr_values = list(gene_expr.values())
print("values:", gene_expr_values)
```

```
keys: ['A', 'B']
values: [0.5, 1.2]
```

- in 활용 키 값 탐색

In [35]:
```
print('D' in gene_expr_keys)
print('D' in gene_expr)
print('A' in gene_expr)
```

```
False
False
True
```

- 반복문에서 딕셔너리 활용 items()

In [36]:
```
gene_expr = {'A':0.5, 'B':1.2, 'C':0.3, 'D':3.2}
for geneid, expval in gene_expr.items():
    print("%s expression value is %s" %(geneid, expval))
```

```
A expression value is 0.5
B expression value is 1.2
C expression value is 0.3
D expression value is 3.2
```

파이썬 함수, 모듈, 클래스

함수

- 리스트 값 평균 리턴하는 함수

In [37]:
```
def average(input):
    if len(input) == 0:
        return None
    return sum(input) / len(input)

x = [1,2,3,4,5,6,7,8,9,10]
print(average(x))
```

```
5.5
```

모듈

- 위 average 함수를 mystat.py 라는 이름의 파일로 저장, 모듈로 활용

In [ ]:
```
#import mystat
#x = list(range(10))
#print(mystat.average(x))
```

- 모듈 직접 실행시 모듈 내 test 코드 실행 (**name** == **main**, True)

In [ ]:
```
#%run mystat
```

- 모듈 임포트

In [48]:
```
import os
os.getcwd()
```

Out[48]:
```
'/content'
```

In [ ]:
```
from os import getcwd
getcwd()
```

Out[ ]:
```
'/home/bioengml'
```

클래스

- Gene, Strain class 생성 연습
- Gene attribute: name, chromosomal location, length
- Strain attribute (변수): name, length of chromosome
- Strain method (함수): compute average length of the genes

In [ ]:
```
import statistics
class ORF:
    def __init__(self, location, length, seq):
        self.location = location
        self.length = length
        self.sequence = seq

class Strain:
    def __init__(self, name, chrlength):
        self.name = name
        self.chr_length = chrlength
        self.orfs = []
    def add_orf(self, location, length, seq):
        self.orfs.append(ORF(location, length, seq))
    def orf_length_average(self):
        return statistics.mean([s.length for s in self.orfs])
```

In [ ]:
```
ecoli = Strain("ecoli", 5000000)
ecoli.add_orf(1, 1000, "ATG")
ecoli.add_orf(1001, 2000, "CCT")
ecoli.add_orf(2001, 3000, "ATC")
```

In [54]:
```
print([g.location for g in ecoli.orfs])
print([g.sequence for g in ecoli.orfs])
ecoli.orf_length_average()
```

```
[1, 1001, 2001]
['ATG', 'CCT', 'ATC']
```

Out[54]:
```
2000
```

- 상속

In [ ]:
```
class Gene(ORF):
    def add_protein(self, prot_name, prot_seq):
        self.prot_name = prot_name
        self.prot_sequence = prot_seq
```

In [56]:
```
gene1 = Gene(1, 1000, "ATG")
print(gene1.location)
gene1.add_protein("myprotein", "M")
print(gene1.prot_name)
```

```
1
myprotein
```

파일 읽기 쓰기

In [ ]:
```
#f = open("README.md", 'rt')
#lines = f.readlines()
#for line in lines:
#    nline = line.split('Wn')[0]
#    print(nline)
```

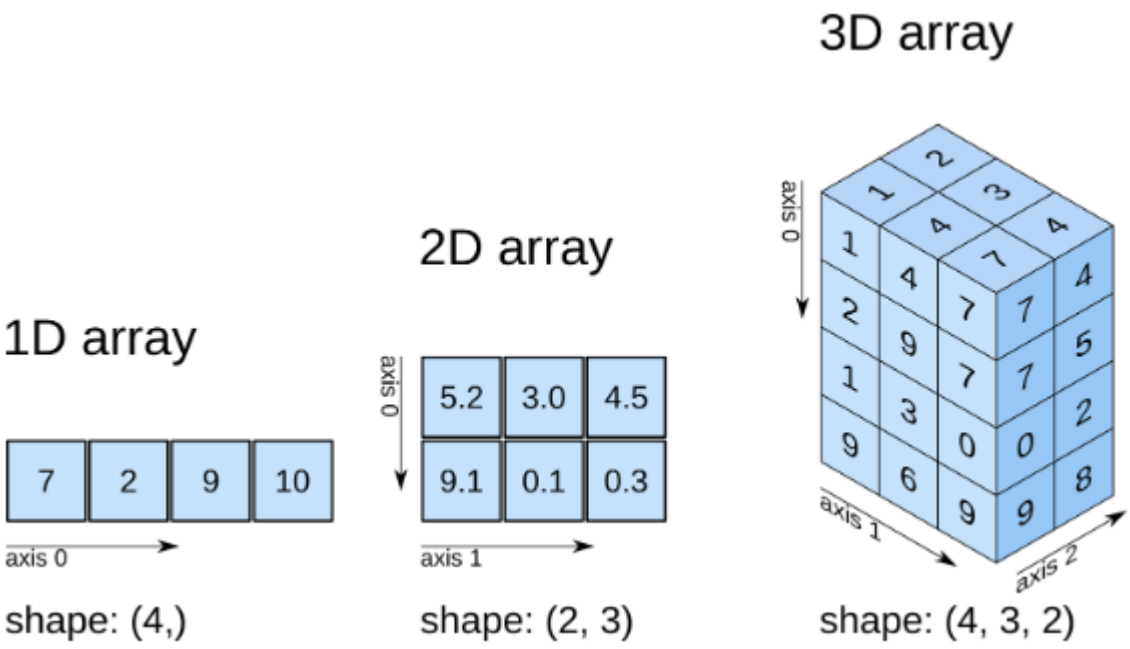
In [ ]:
```
f = open("write_test.txt", 'wt')
f.write('gene1;')
f.write('1;')
f.write('1000')
f.close()
```

In [62]:
```
f = open("write_test.txt", 'rt')
lines = f.readlines()
for line in lines:
    nline = line.split(';')
    print(nline)
```

```
['gene1', '1', '1000']
```

Numpy 자료구조 ndarray

- 행렬이나 다차원 배열 처리용 파이썬 라이브러리
- 같은 타입의 데이터만 허용
- 리스트에 비해 20배 이상 빠른 속도



In [ ]:
```
import numpy as np
```

In [64]:
```
arr = [1, 2, 3]
print(arr)
print(type(arr))

a = np.array([1,2,3])
print(a)
print(a.dtype)
print(a.shape)
print(type(a))
```

```
[1, 2, 3]
<class 'list'>
[1 2 3]
int64
(3,)
<class 'numpy.ndarray'>
```

- numpy 자료형
  - 부호가 있는 정수 int(8, 16, 32, 64)
  - 부호가 없는 정수 uint(8 ,16, 32, 54)
  - 실수 float(16, 32, 64, 128)
  - 복소수 complex(64, 128, 256)
  - 불리언 bool
  - 문자열 string_
  - 파이썬 오프젝트 object
  - 유니코드 unicode_

- np.zeros(), np.ones(), np.arange()
- 행렬 연산 지원

In [65]:
```
a = np.arange(1, 10).reshape(3,3) # [1, 10)
print(a)
a = np.ones((3,4), dtype=np.int16)
b = np.ones((3,4), dtype=np.int16)
print(a)
print(b)
print(a+b)
print(a-b)
```

```
[[1 2 3]
 [4 5 6]
 [7 8 9]]
[[1 1 1 1]
 [1 1 1 1]
 [1 1 1 1]]
[[1 1 1 1]
 [1 1 1 1]
 [1 1 1 1]]
[[2 2 2 2]
 [2 2 2 2]
 [2 2 2 2]]
[[0 0 0 0]
 [0 0 0 0]
 [0 0 0 0]]
```

- numpy 함수
  - np.sqrt()
  - np.log()
  - np.square()
  - np.log()
  - np.ceil()
  - np.floor()
  - np.isnan()
  - np.sum()
  - np.mean()
  - np.std()
  - np.min()

Pandas 자료구조 Series, DataFrame

- Pandas의 Series는 1차원, DataFrame은 2차원 데이터를 다루는 자료구조
- 리스트와 딕셔너리의 조합형
- 숫자형, 문자형, 범주형 등의 다양한 데이터 입력 가능

In [ ]:
```
from pandas import Series, DataFrame
```

In [68]:
```
genes = Series([0.1, 0.2, 1.4, 0.6, 1.1])
print(genes)
```

```
0    0.1
1    0.2
2    1.4
3    0.6
4    1.1
dtype: float64
```

In [69]:
```
genes = Series([0.1, 0.2, 1.4, 0.6, 1.1], index=['A', 'B', 'C', 'D', 'E'])
print(genes)
```

```
A    0.1
B    0.2
C    1.4
D    0.6
E    1.1
dtype: float64
```

- 인덱스 자동 정렬, 행렬 연산

In [70]:
```
genes1 = Series([0.1, 0.2, 1.4, 0.6, 1.1], index=['A', 'B', 'C', 'D', 'E'])
genes2 = Series([0.1, 0.2, 1.4, 0.6, 1.1], index=['B', 'C', 'D', 'E', 'A'])
genes1 + genes2
```

Out[70]:
```
A    1.2
B    0.3
C    1.6
D    2.0
E    1.7
dtype: float64
```

In [71]:
```
print(genes2.sort_values())
print(genes2.sort_index())
```

```
B    0.1
C    0.2
E    0.6
A    1.1
D    1.4
dtype: float64
A    1.1
B    0.1
C    0.2
D    1.4
E    0.6
dtype: float64
```

- DataFrame 생성은 '{', '}' 이용
- DataFrame은 Series의 집합

In [72]:
```
genes = {'A': [0.5, 0.1, 0.3],
         'B': [0.8, 0.9, 0.4]}
print(genes)
genes_df = DataFrame(genes)
print(genes_df)
print(genes_df['A'])
print(type(genes_df['A']))
```

```
{'A': [0.5, 0.1, 0.3], 'B': [0.8, 0.9, 0.4]}
     A    B
0  0.5  0.8
1  0.1  0.9
2  0.3  0.4
0    0.5
1    0.1
2    0.3
Name: A, dtype: float64
<class 'pandas.core.series.Series'>
```

In [73]:
```
genes = {'A': [0.5, 0.1, 0.3],
         'B': [0.8, 0.9, 0.4]}
genes_df = DataFrame(genes, columns=['B', 'A'], index=['day1', 'day2', 'day3'])
print(genes_df)
```

```
        B    A
day1  0.8  0.5
day2  0.9  0.1
day3  0.4  0.3
```

In [74]:
```
print(genes_df['A'])
print(genes_df.loc['day1'])
print(genes_df.index)
print(list(genes_df.columns))
```

```
day1    0.5
day2    0.1
day3    0.3
Name: A, dtype: float64
B    0.8
A    0.5
Name: day1, dtype: float64
Index(['day1', 'day2', 'day3'], dtype='object')
['B', 'A']
```

다차원 numpy 자료구조 텐서 (Tensor)

- 딥러닝 프레임워크 (라이브러리 모듈 묶어놓은 패키지)
  - tensorflow - 구글 개발, 가장 높은 인기
  - theano - python 기반 최초 딥러닝 라이브러리
  - PyTorch - 페이스북 개발, 낮은 진입 장벽
  - CNTK (Cognitive Toolkit) - Microsoft 개발, 높은 성능
  - 참고로 Keras는 tensorflow, theano, CNTK를 백엔드엔진으로 사용해서 동작하는 고수준 라이브러리

- 텐서는 수치형 (float32, uint8, float64) 데이터를 주로 다룸
- 임의의 차원 개수를 가지는 행렬의 일반화된 모습
- 0D 텐서는 스칼라, 1D 텐서는 벡터, 2D 텐서는 행렬, ...
- 랭크(ndim), 크기(shape), 타입(dtype) 속성이 있음

In [75]:
```
import numpy as np
x = np.array(12)
print(x)
print(x.ndim)
```

```
12
0
```

In [76]:
```
x = np.array([1, 2, 3, 4, 5])
print(x.ndim)
```

```
1
```

In [77]:
```
x = np.array([[1,2,3,4,5],
              [6,7,8,9,10],
              [11,12,13,14,15]])
print(x.ndim)
```

```
2
```

In [ ]:
```
x = np.array([[[1,2,3],
               [2,3,4]],
              [[5,6,7],
               [8,9,10]],
              [[11,12,13],
               [14,15,16]]])
```

In [79]:
```
x.shape
```

Out[79]: (3, 2, 3)

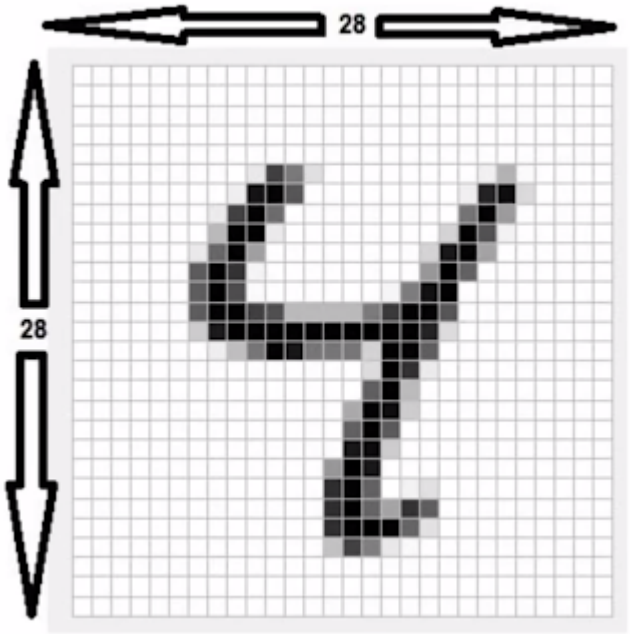
Neural Network 예제

- 유명 예제 중 하나인 MNIST 예제
- 흑백 손글씨 숫자 이미지 (28x28픽셀)을 10개 범주에서 (0 부터 9까지)로 분류하는 문제
- 미국 국립표준기술연구소 (NIST)에서 수집한 60000개 훈련 이미지와 1만개 테스트 이미지 구성

In [ ]:
```
from keras.datasets import mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()
```

In [101]:
```
print(train_images.shape)
print(train_labels.shape)
print(test_images.shape)
print(test_labels.shape)
```

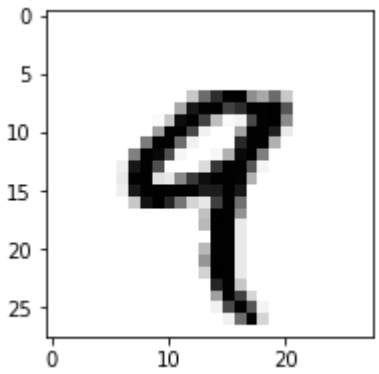
```
(60000, 28, 28)
(60000,)
(10000, 28, 28)
(10000,)
```



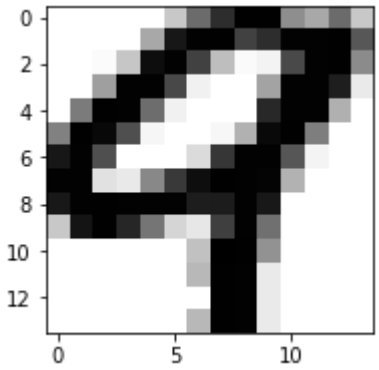
In [102]:
```
digit = train_images[4]
print(digit.shape)

import matplotlib.pyplot as plt
plt.imshow(digit, cmap=plt.cm.binary)
plt.show()
```

```
(28, 28)
```



In [103]:
```
my_slice = train_images[4,7:-7,7:-7]
plt.imshow(my_slice, cmap=plt.cm.binary)
plt.show()
```



- 배치 (batch) - 훈련 데이터를 나누어 입력
- 에폭 (epoch) - 전체 훈련 데이터에 수행되는 각 반복

In [ ]:
```
batch1 = train_images[:128]
batch2 = train_images[129:256]
#...
```

- 배열 변환

In [ ]:
```
train_images = train_images.reshape((60000, 28*28))
train_images = train_images.astype('float32')/255
test_images = test_images.reshape((10000, 28*28))
test_images = test_images.astype('float32')/255
```

In [106]:
```
print(train_images.shape)
print(train_labels.shape)
print(test_images.shape)
print(test_labels.shape)
```

```
(60000, 784)
(60000,)
(10000, 784)
(10000,)
```

In [107]:
```
print(test_labels[:10])
```

```
[7 2 1 0 4 1 4 9 5 9]
```

- 신경망

In [ ]:
```
from keras import models
from keras import layers
from keras.utils import to_categorical

network = models.Sequential()
network.add(layers.Dense(512, activation='relu', input_shape=(28*28,)))
network.add(layers.Dense(10, activation='softmax'))

network.compile(optimizer='rmsprop', loss='categorical_crossentropy', metrics=['acc
uracy'])
train_labels = to_categorical(train_labels)
test_labels = to_categorical(test_labels)
```

In [109]:
```
print("train_images shape:", train_images.shape)
print("test_images shape:", test_images.shape)
print("train_labels shape:", train_labels.shape)
print("test_labels shape:", test_labels.shape)
print(test_labels[:2,])
```

```
train_images shape: (60000, 784)
test_images shape: (10000, 784)
train_labels shape: (60000, 10)
test_labels shape: (10000, 10)
[[0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]]
```

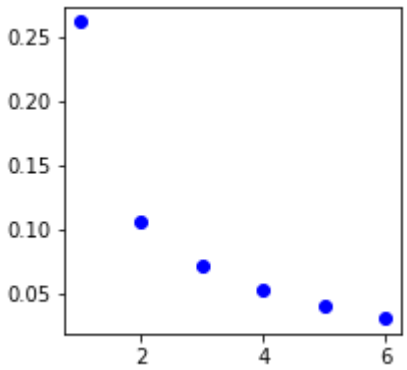
In [110]:
```
history = network.fit(train_images, train_labels, epochs=6, batch_size=128)
```

```
Epoch 1/6
60000/60000 [==============================] - 5s 78us/step - loss: 0.2570 - acc: 0.
9253
Epoch 2/6
60000/60000 [==============================] - 4s 74us/step - loss: 0.1058 - acc: 0.
9684
Epoch 3/6
60000/60000 [==============================] - 4s 71us/step - loss: 0.0693 - acc: 0.
9787
Epoch 4/6
60000/60000 [==============================] - 4s 74us/step - loss: 0.0516 - acc: 0.
9842
Epoch 5/6
60000/60000 [==============================] - 4s 71us/step - loss: 0.0392 - acc: 0.
9883
Epoch 6/6
60000/60000 [==============================] - 4s 71us/step - loss: 0.0306 - acc: 0.
9907
```

In [93]:
```
import matplotlib.pyplot as plt

history_dict = history.history
print(history_dict.keys())
loss =history_dict['loss']
acc = history_dict['acc']
epochs = range(1, len(loss)+1)
plt.rcParams["figure.figsize"] = (3,3)
plt.plot(epochs, loss, 'bo')
plt.show()
```

```
dict_keys(['loss', 'acc'])
```



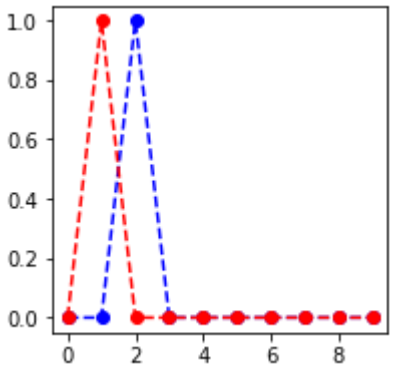
- 테스트 세트에서 모델 작동 확인

In [94]:
```
results = network.predict(test_images)
print(results.shape)
```

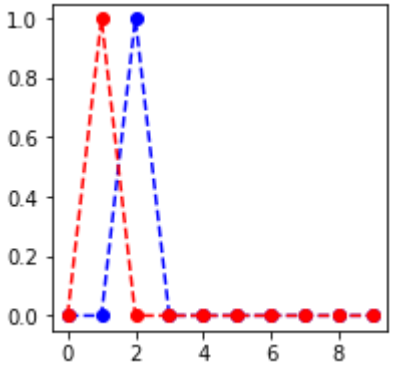
```
(10000, 10)
```

In [95]:
```
import matplotlib.pyplot as plt
plt.rcParams["figure.figsize"] = (3,3)
print([round(x) for x in list(results[1,])])
plt.plot(results[1,], "bo--")
plt.plot(results[2,], "ro--")
plt.show()
```

```
[0.0, 0.0, 1.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0]
```



In [96]:
```
plt.plot(test_labels[1,], "bo--")
plt.plot(test_labels[2,], "ro--")
plt.show()
print(test_labels[1,])
```




```
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
```

In [97]:
```
results = network.evaluate(test_images, test_labels)
print(results)
```

```
10000/10000 [==============================] - 1s 55us/step
[0.06716508627363364, 0.9798]
```

Biopython - Sequence objects

In [111]:
```
from Bio.Seq import Seq
from Bio.Alphabet import IUPAC
my_seq = Seq("AGTACACTGGT", IUPAC.unambiguous_dna)
my_seq
```

Out[111]:
```
Seq('AGTACACTGGT', IUPACUnambiguousDNA())
```

In [112]:
```
for index, letter in enumerate(my_seq):
    print("%i %s " % (index, letter))
```

```
0 A
1 G
2 T
3 A
4 C
5 A
6 C
7 T
8 G
9 G
10 T
```

In [113]:
```
x = [1, 4, 5, 7, 8]
for i in enumerate(x):
    print(i)
```

```
(0, 1)
(1, 4)
(2, 5)
(3, 7)
(4, 8)
```

In [114]:
```
print(my_seq)
print(my_seq[0:3])
print(my_seq[0::2])
print(str(my_seq))
print(my_seq + "ATG")
print(my_seq=="ATG")
print("AGT" in my_seq)
```

```
AGTACACTGGT
AGT
ATCCGT
AGTACACTGGT
AGTACACTGGTATG
False
True
```

In [115]:
```
my_seq_low = my_seq.lower()
print(my_seq_low)
print(my_seq_low.upper())
print(my_seq.complement())
print(my_seq.reverse_complement())
```

```
agtacactggt
AGTACACTGGT
TCATGTGACCA
ACCAGTGTACT
```

- 전사, 번역

In [116]:
```
mrna = my_seq.transcribe()
print(mrna)
prot = mrna.translate() ## truncated
print(prot)
print(my_seq.translate())
```

```
AGUACACUGGU
STL
STL

/usr/local/lib/python3.6/dist-packages/Bio/Seq.py:2748: BiopythonWarning: Partial co
don, len(sequence) not a multiple of three. Explicitly trim the sequence or add trai
ling N before translation. This may become an error in future.
  BiopythonWarning)
```

In [117]:
```
from Bio.Data import CodonTable
standard_table = CodonTable.unambiguous_dna_by_id[1]
print(standard_table)
print(standard_table.start_codons)
print(standard_table.stop_codons)
print(type(standard_table))
```

```
Table 1 Standard, SGC0

  |  T      |  C      |  A      |  G      |
--+---------+---------+---------+---------+--
T | TTT F   | TCT S   | TAT Y   | TGT C   | T
T | TTC F   | TCC S   | TAC Y   | TGC C   | C
T | TTA L   | TCA S   | TAA Stop| TGA Stop| A
T | TTG L(s)| TCG S   | TAG Stop| TGG W   | G
--+---------+---------+---------+---------+--
C | CTT L   | CCT P   | CAT H   | CGT R   | T
C | CTC L   | CCC P   | CAC H   | CGC R   | C
C | CTA L   | CCA P   | CAA Q   | CGA R   | A
C | CTG L(s)| CCG P   | CAG Q   | CGG R   | G
--+---------+---------+---------+---------+--
A | ATT I   | ACT T   | AAT N   | AGT S   | T
A | ATC I   | ACC T   | AAC N   | AGC S   | C
A | ATA I   | ACA T   | AAA K   | AGA R   | A
A | ATG M(s)| ACG T   | AAG K   | AGG R   | G
--+---------+---------+---------+---------+--
G | GTT V   | GCT A   | GAT D   | GGT G   | T
G | GTC V   | GCC A   | GAC D   | GGC G   | C
G | GTA V   | GCA A   | GAA E   | GGA G   | A
G | GTG V   | GCG A   | GAG E   | GGG G   | G
--+---------+---------+---------+---------+--
['TTG', 'CTG', 'ATG']
['TAA', 'TAG', 'TGA']
<class 'Bio.Data.CodonTable.NCBICodonTableDNA'>
```

biopython - SeqRecord, SeqIO

- Sequence annotation objects
- 특정 서열의 identifier나 feature 정보 포함

In [ ]:
```
from Bio.Seq import Seq
from Bio.SeqRecord import SeqRecord

simple_seq = Seq("GATC")
simple_seq_r = SeqRecord(simple_seq)
```

In [119]:
```
simple_seq_r.id = "AC12345"
simple_seq_r.description = "Made up sequence I wish I could write a paper about"
print(simple_seq_r.description)
print(simple_seq_r.seq)
```

```
Made up sequence I wish I could write a paper about
GATC
```

In [120]:
```
#help(SeqRecord)
#SeqRecord.__dict__.keys()
SeqRecord.__init__.__code__.co_varnames
```

Out[120]:
```
('self',
 'seq',
 'id',
 'name',
 'description',
 'dbxrefs',
 'features',
 'annotations',
 'letter_annotations')
```

- Read fasta file
- *Yersinia pestis biovar Microtus* str. 91001 plasmid (페스트균)

In [ ]:
```
from Bio import SeqIO
record = SeqIO.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/NC_005816.fna", "fasta")
```

In [125]:
```
record
```

Out[125]:
```
SeqRecord(seq=Seq('TGTAACGAACGGTGCAATAGTGATCCACACCCAACGCCTGAAATCAGATCCAGG...CTG', SingleLetterAlphabet()), id='gi|45478711|ref|NC_005816.1|', name='gi|45478711|ref|NC_005816.1|', description='gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence', dbxrefs=[])
```

In [126]:
```
print(record.id)
print(record.name)
print(record.description)
```

```
gi|45478711|ref|NC_005816.1|
gi|45478711|ref|NC_005816.1|
gi|45478711|ref|NC_005816.1| Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence
```

- Read GenBank file

In [ ]:
```
from Bio import SeqIO
record = SeqIO.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/NC_005816.gb", "genbank")
```

In [130]:
```
print(record.id)
print(record.name)
print(record.description)
print(len(record.features))
print(record.features[0])
print(record.features[2])
print(record.features[3])
```

```
NC_005816.1
NC_005816
Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequence
41
type: source
location: [0:9609](+)
qualifiers:
    Key: biovar, Value: ['Microtus']
    Key: db_xref, Value: ['taxon:229193']
    Key: mol_type, Value: ['genomic DNA']
    Key: organism, Value: ['Yersinia pestis biovar Microtus str. 91001']
    Key: plasmid, Value: ['pPCP1']
    Key: strain, Value: ['91001']

type: gene
location: [86:1109](+)
qualifiers:
    Key: db_xref, Value: ['GeneID:2767718']
    Key: locus_tag, Value: ['YP_pPCP01']

type: CDS
location: [86:1109](+)
qualifiers:
    Key: codon_start, Value: ['1']
    Key: db_xref, Value: ['GI:45478712', 'GeneID:2767718']
    Key: locus_tag, Value: ['YP_pPCP01']
    Key: note, Value: ['similar to corresponding CDS from previously sequenced pPCP
plasmid of Yersinia pestis KIM (AF053945) and C092 (AL109969), also many transposase
entries for insertion sequence IS100 of Yersinia pestis. Contains IS21-like element
transposase, HTH domain (Interpro|IPR007101)']
    Key: product, Value: ['putative transposase']
    Key: protein_id, Value: ['NP_995567.1']
    Key: transl_table, Value: ['11']
    Key: translation, Value: ['MVTFETVMEIKILHKQGMSSRAIARELGISRNTVKRYLQAKSEPPKYTPRPAV
ASLLDEYRDYIRQRIADAHPYKIPATVIAREIRDQGYRGGMTILRAFIRSLSVPQEQEPAVRFETEPGRQMQVDWGTMRNGRSP
LHVFVAVLGYSRMLYIEFTDNMRYDTLETCHRNAFRFFGGVPREVLYDNMKTVVLQRDAYQTGQHRFHPSLWQFGKEMGFSPRL
CRPFRAQTKGKVERMVQYTRNSFYIPLMTRLRPMGITVDVETANRHGLRWLHDVANQRKHETIQARPCDRWLEEQQSMLALPPE
KKEYDVHLDENLVNFDKHPLHHPLSIYDSFCRGVA']
```

- 위치 탐색 in 활용

In [131]:
```
for feature in record.features:
    if 4350 in feature:
        print(feature)
        print("%s %s" % (feature.type, feature.qualifiers.get("db_xref")))
```

```
type: source
location: [0:9609](+)
qualifiers:
    Key: biovar, Value: ['Microtus']
    Key: db_xref, Value: ['taxon:229193']
    Key: mol_type, Value: ['genomic DNA']
    Key: organism, Value: ['Yersinia pestis biovar Microtus str. 91001']
    Key: plasmid, Value: ['pPCP1']
    Key: strain, Value: ['91001']

source ['taxon:229193']
type: gene
location: [4342:4780](+)
qualifiers:
    Key: db_xref, Value: ['GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']

gene ['GeneID:2767712']
type: CDS
location: [4342:4780](+)
qualifiers:
    Key: codon_start, Value: ['1']
    Key: db_xref, Value: ['GI:45478716', 'GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']
    Key: note, Value: ['similar to many previously sequenced pesticin immunity prote
in entries of Yersinia pestis plasmid pPCP, e.g. gi| 16082683|,ref|NP_395230.1| (NC_
003132) , gi|1200166|emb|CAA90861.1| (Z54145 ) , gi|1488655| emb|CAA63439.1| (X9285
6) , gi|2996219|gb|AAC62543.1| (AF053945) , and gi|5763814|emb|CAB531 67.1| (AL10996
9)']
    Key: product, Value: ['pesticin immunity protein']
    Key: protein_id, Value: ['NP_995571.1']
    Key: transl_table, Value: ['11']
    Key: translation, Value: ['MGGGMISKLFCLALIFLSSSGLAEKNTYTAKDILQNLELNTFGNSLSHGIYGK
QTTFKQTEFTNIKSNTKKHIALINKDNSWMISLKILGIKRDEYTVCFEDFSLIRPPTYVAIHPLLIKKVKSGNFIVVKEIKKSI
PGCTVYYH']

CDS ['GI:45478716', 'GeneID:2767712']
```

- format 함수

In [ ]:
```
#record.format("fasta") ##"fasta", "genbank"
```

- Slicing

In [133]:
```
print(len(record))
print(len(record.features))
```

```
9609
41
```

In [134]:
```
print(record.features[20])
print(record.features[21])
```

```
type: gene
location: [4342:4780](+)
qualifiers:
    Key: db_xref, Value: ['GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']

type: CDS
location: [4342:4780](+)
qualifiers:
    Key: codon_start, Value: ['1']
    Key: db_xref, Value: ['GI:45478716', 'GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']
    Key: note, Value: ['similar to many previously sequenced pesticin immunity prote
in entries of Yersinia pestis plasmid pPCP, e.g. gi| 16082683|,ref|NP_395230.1| (NC_
003132) , gi|1200166|emb|CAA90861.1| (Z54145 ) , gi|1488655| emb|CAA63439.1| (X9285
6) , gi|2996219|gb|AAC62543.1| (AF053945) , and gi|5763814|emb|CAB531 67.1| (AL10996
9)']
    Key: product, Value: ['pesticin immunity protein']
    Key: protein_id, Value: ['NP_995571.1']
    Key: transl_table, Value: ['11']
    Key: translation, Value: ['MGGGMISKLFCLALIFLSSSGLAEKNTYTAKDILQNLELNTFGNSLSHGIYGK
QTTFKQTEFTNIKSNTKKHIALINKDNSWMISLKILGIKRDEYTVCFEDFSLIRPPTYVAIHPLLIKKVKSGNFIVVKEIKKSI
PGCTVYYH']
```

- 서열 위치로 직접 슬라이싱

In [135]:
```
sub_record = record[4300:4800]
print(sub_record)
print(len(sub_record))
print(len(sub_record.features))
print(sub_record.features[0])
print(sub_record.features[1])
```

```
ID: NC_005816.1
Name: NC_005816
Description: Yersinia pestis biovar Microtus str. 91001 plasmid pPCP1, complete sequ
ence
Number of features: 2
Seq('ATAAATAGATTATTCCAAATAATTTATTTATGTAAGAACAGGATGGGAGGGGGA...TTA', IUPACAmbiguousDN
A())
500
2
type: gene
location: [42:480](+)
qualifiers:
    Key: db_xref, Value: ['GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']

type: CDS
location: [42:480](+)
qualifiers:
    Key: codon_start, Value: ['1']
    Key: db_xref, Value: ['GI:45478716', 'GeneID:2767712']
    Key: gene, Value: ['pim']
    Key: locus_tag, Value: ['YP_pPCP05']
    Key: note, Value: ['similar to many previously sequenced pesticin immunity prote
in entries of Yersinia pestis plasmid pPCP, e.g. gi| 16082683|,ref|NP_395230.1| (NC_
003132) , gi|1200166|emb|CAA90861.1| (Z54145 ) , gi|1488655| emb|CAA63439.1| (X9285
6) , gi|2996219|gb|AAC62543.1| (AF053945) , and gi|5763814|emb|CAB531 67.1| (AL10996
9)']
    Key: product, Value: ['pesticin immunity protein']
    Key: protein_id, Value: ['NP_995571.1']
    Key: transl_table, Value: ['11']
    Key: translation, Value: ['MGGGMISKLFCLALIFLSSSGLAEKNTYTAKDILQNLELNTFGNSLSHGIYGK
QTTFKQTEFTNIKSNTKKHIALINKDNSWMISLKILGIKRDEYTVCFEDFSLIRPPTYVAIHPLLIKKVKSGNFIVVKEIKKSI
PGCTVYYH']
```

Biopython - Entrez

- 파일 읽기/쓰기 with 문 사용

In [137]:
```
from Bio import Entrez
from Bio import SeqIO
Entrez.email = "*****@gmail.com"
entid = "6273291"
with Entrez.efetch(db="nucleotide", rettype="gb", retmode="text", id=entid) as han
dle:
    seq_record = SeqIO.read(handle, "gb")
print("%s with %i features" % (seq_record.id, len(seq_record.features)))
print(type(seq_record))
SeqIO.write(seq_record, "/content/drive/My Drive/Colab Notebooks/bioengml/dataset
s/"+seq_record.id+".fa", "fasta")
print(seq_record)
```

```
AF191665.1 with 3 features
<class 'Bio.SeqRecord.SeqRecord'>
ID: AF191665.1
Name: AF191665
Description: Opuntia marenae rpl16 gene; chloroplast gene for chloroplast product, p
artial intron sequence
Number of features: 3
/molecule_type=DNA
/topology=linear
/data_file_division=PLN
/date=07-NOV-1999
/accessions=['AF191665']
/sequence_version=1
/keywords=['']
/source=chloroplast Grusonia marenae
/organism=Grusonia marenae
/taxonomy=['Eukaryota', 'Viridiplantae', 'Streptophyta', 'Embryophyta', 'Tracheophyt
a', 'Spermatophyta', 'Magnoliophyta', 'eudicotyledons', 'Gunneridae', 'Pentapetala
e', 'Caryophyllales', 'Cactineae', 'Cactaceae', 'Opuntioideae', 'Grusonia']
/references=[Reference(title='Phylogeny of the subfamily Opuntioideae (Cactaceae)',
...), Reference(title='Direct Submission', ...)]
Seq('TATACATTAAAGGAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAAAAAA...AGA', IUPACAmbiguousDN
A())
```

- 여러개 record에 대해서는 parse 함수를 사용

In [139]:
```
entids = "6273290,6273289"
with Entrez.efetch(db="nucleotide", rettype="gb", retmode="text", id=entids) as ha
ndle:
    for seq_record in SeqIO.parse(handle, "gb"):
        print("%s %s..." % (seq_record.id, seq_record.description[:50]))
        print("Sequence length %i, %i features, from: %s"
              % (len(seq_record), len(seq_record.features), seq_record.annotations[
"source"]))
        SeqIO.write(seq_record, "/content/drive/My Drive/Colab Notebooks/bioengml/d
atasets/"+seq_record.id+".gb", "gb")
```

```
AF191664.1 Opuntia clavata rpl16 gene; chloroplast gene for c...
Sequence length 899, 3 features, from: chloroplast Grusonia clavata
AF191663.1 Opuntia bradtiana rpl16 gene; chloroplast gene for...
Sequence length 899, 3 features, from: chloroplast Grusonia bradtiana
```

Biopython - multiple sequence alignment objects

- http://biopython.org/DIST/docs/tutorial/Tutorial.html#htoc70 (http://biopython.org/DIST/docs/tutorial/Tutorial.html#htoc70)
- Bio.AlignIO.read() returns a single MultipleSeqAlignment object
- Bio.AlignIO.parse() returns MultipleSeqAlignment objects

- Alignment tools

In [140]:
```
import Bio.Align.Applications as alnapps
dir(alnapps)
```

Out[140]:
```
['ClustalOmegaCommandline',
 'ClustalwCommandline',
 'DialignCommandline',
 'MSAProbsCommandline',
 'MafftCommandline',
 'MuscleCommandline',
 'PrankCommandline',
 'ProbconsCommandline',
 'TCoffeeCommandline',
 '_ClustalOmega',
 '_Clustalw',
 '_Dialign',
 '_MSAProbs',
 '_Mafft',
 '_Muscle',
 '_Prank',
 '_Probcons',
 '_TCoffee',
 '__all__',
 '__builtins__',
 '__cached__',
 '__doc__',
 '__file__',
 '__loader__',
 '__name__',
 '__package__',
 '__path__',
 '__spec__']
```

- Clustalw를 이용한 서열 정렬 (cactus family Opuntia(선인장))

In [143]:
```
from Bio.Align.Applications import ClustalwCommandline as clw
#help(clw)
cline = clw("clustalw2", infile="/content/drive/My Drive/Colab Notebooks/bioengml/datasets/opuntia.fasta")
#stdout, stderr = cline()
print(cline)
#print(stdout)
```

```
clustalw2 -infile="/content/drive/My Drive/Colab Notebooks/bioengml/datasets/opuntia.fasta"
```

In [144]:
```
#print(stdout)
from Bio import AlignIO
align = AlignIO.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/opuntia.aln", "clustal")
print(align)
```

```
SingleLetterAlphabet() alignment with 7 rows and 906 columns
TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273285|gb|AF191659.1|AF191
TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273284|gb|AF191658.1|AF191
TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273287|gb|AF191661.1|AF191
TATACATAAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273286|gb|AF191660.1|AF191
TATACATTAAAGGAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273290|gb|AF191664.1|AF191
TATACATTAAAGGAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273289|gb|AF191663.1|AF191
TATACATTAAAGGAGGGGGATGCGGATAAATGGAAAGGCGAAAG...AGA gi|6273291|gb|AF191665.1|AF191
```

In [147]:
```
from Bio import Phylo
tree = Phylo.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/opuntia.dnd", "newick")
Phylo.draw_ascii(tree)
```

```
                                 ________________ gi|6273291|gb|AF191665.1|AF191665
  ______________________________|
 |                              |    ______ gi|6273290|gb|AF191664.1|AF191664
 |                              |___|
 |                                  |_____ gi|6273289|gb|AF191663.1|AF191663
 |
_|__________________ gi|6273287|gb|AF191661.1|AF191661
 |
 |___________ gi|6273286|gb|AF191660.1|AF191660
 |
 |     __ gi|6273285|gb|AF191659.1|AF191659
 |____|
      | gi|6273284|gb|AF191658.1|AF191658
```

Biopython - Position specific scoring matrix (PSSM) matrix

In [148]:
```
from Bio.Seq import Seq
test_seq=Seq("TAAGCGTGCACGCGCAACACGTGCATTA")
test_seq
print(test_seq)
```

```
TAAGCGTGCACGCGCAACACGTGCATTA
```

In [ ]:
```
from Bio import AlignIO
from Bio.Align import AlignInfo
```

- Pfam은 단백질 페밀리 database, 각 서열 그룹을 align 한 파일이 제공됨
- Family: Sigma54_activ_2 (PF14532) https://pfam.xfam.org/family/PF14532#tabview=tab3 (https://pfam.xfam.org/family/PF14532#tabview=tab3)

In [151]:
```
align = AlignIO.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/PF14532_full.txt", "stockholm")
#print(align)
print(len(align))
print(align[0])
print("############################################################")
print(align[0].seq)
```

```
1240
ID: A0A1F7TK17_9BACT/134-279
Name: A0A1F7TK17_9BACT
Description: A0A1F7TK17_9BACT/134-279
Number of features: 0
/accession=A0A1F7TK17.1
/start=134
/end=279
Seq('-------------------------------------------------------...---', SingleLetterAlphabet())
############################################################
------------------------------------------------------------------------------------------GNDP
K-V-D-A-L-C-S-A---L---E---E---A---A--------G---D----L-------R--------P-----L---V-L-L
--GER-GT-GK----R----H-L-A----H-----V--------L-------H--------N--------R--------G----
----I--------T-------R--------E--------G-------P--------F----A----P----L--HCR-------
--S--------------LAspkrks-------------------------------------dIqasIRR-L---LPK--------
---------------------E-------------------------GS-G---T--V-YL-DG--W--EQAP--A-EE-------R
AG-I----L-D---A--LAA-----------------------------------WT----K---D----G-----H---R--L---
----L-V-A--I---D---E---D-G----G---E-----------------A---V---S-L--W-D-Q-A-A-E-RL-R-A--
R-KLHLPPL-----------------------------------------------------------------------------
--------
```

- slicing alignment

In [152]:
```
# print(align[3:8].format("clustal"))
print(align[3:8,100:200].format("clustal"))
print(align[3:8,197])
```

```
CLUSTAL X (1.81) multiple sequence alignment


V7EPJ0_9RHOB/141-283            --V---A---R---V---M--------N---T----D-------L---
--
B1ZTM1_OPITP/145-296            --V---K---K---L---A--------A---V----R-------T---
--
W3ANH6_9FIRM/219-355            --A---E---K---L---S--------R---T----D-------C---
--
Q6LNI3_PHOPR/144-289            --I---A---N---I---A--------L---T----N-------K---
--
A0A1G8U4Y5_9RHOB/145-284        --V---R---L---V---A--------R---A----G-------A---
--

V7EPJ0_9RHOB/141-283            ---A-----V---L-V-T--GES-GT-GK----S----L-I-A----K
--
B1ZTM1_OPITP/145-296            ---P-----V---L-L-I--GEN-GS-GK----S----A-V-A----E
--
W3ANH6_9FIRM/219-355            ---P-----K---L-I-V--EPV-GN-LH----R----A-F-I----N
--
Q6LNI3_PHOPR/144-289            ---D-----V---L-I-D--GES-GT-GR----R----T-V-S----K
--
A0A1G8U4Y5_9RHOB/145-284        ---E-----V---L-V-T--GPT-GS-GT----A----K-V-A----E
--



KENKE
```

- Turn the alignment object into an array of letters

In [154]:
```
import numpy as np
from Bio import AlignIO
align = AlignIO.read("/content/drive/My Drive/Colab Notebooks/bioengml/datasets/opuntia.aln", "clustal")
align_array = np.array([list(rec) for rec in align], np.character)
print("Align shape %i by %i" % align_array.shape)
print(align_array)
```

```
Align shape 7 by 906
[[b'T' b'A' b'T' ... b'A' b'G' b'A']
 [b'T' b'A' b'T' ... b'A' b'G' b'A']
 [b'T' b'A' b'T' ... b'A' b'G' b'A']
 ...
 [b'T' b'A' b'T' ... b'A' b'G' b'A']
 [b'T' b'A' b'T' ... b'A' b'G' b'A']
 [b'T' b'A' b'T' ... b'A' b'G' b'A']]
```

Note that this leaves the original Biopython alignment object and the NumPy array in memory as separate objects - editing one will not update the other!

In [155]:
```
align_array.shape
```

Out[155]:
```
(7, 906)
```

- SummaryInfo 클래스
  - consensus sequence, position specific score matrix 계산
  - information content와 substitution 정보 계산 가능

In [156]:
```
summary_align = AlignInfo.SummaryInfo(align)
consensus = summary_align.dumb_consensus()
print(consensus)
my_pssm = summary_align.pos_specific_score_matrix(consensus, chars_to_ignore = ['N'
, '-'])
#print(my_pssm)
# your_pssm[sequence_number][residue_count_name]
my_pssm[1]['A']
[s for s in my_pssm][:10]
```

```
TATACATTAAAGXAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAAAAAAATGAATCTAAATGATATAXGATTCCACTAT
GTAAGGTCTTTGAATCATATCATAAAAGACAATGTAATAAAGCATGAATACAGATTCACACATAATTATCTGATATGAATCTAT
TCATAGAAAAAAGAAAAAAGTAAGAGCCTCCGGCCAATAAAGACTAAGAGGGTTGGCTCAAGAACAAAGTTCATTAAGAGCTCC
ATTGTAGAATTCAGACCTAATCATTAATCAAGAAGCGATGGGAACGATGTAATCCATGAATACAGAAGATTCAATTGAAAAAGA
TCCTAATXXXTCATTGGGAAGGATGGCGGAACGAACCAGAGACCAATTCATCTATTCTGAAAAGTGATAAACTAATCCTATAAA
ACTAAAATAGATATTGAAAGAGTAAATATTCGCCCGCGAAAATTCCTTTTTTATTTAAATTGCTCATATTTTXTTTTAGCAATG
CAATCTAATAAAATATATCTATACAAAAAAAXATAGACAAACTATATATATATATATATATAATATATTTCAAATTXCCTTATA
TATCCAAATATAAAAATATCTAATAAATTAGATGAATATCAAAGAATCTATTGATTTAGTGTATTATTAAATGTATATXTTAAT
TCAATATTATTATTCTATTCATTTTTATTCATTTTCAAATTTATAATATATTAATCTATATATTAATTTAXAATTCTATTCTAA
TTCGAATTCAATTTTTAAATATTCATATTCAATTAAAATTGAAATTTTTTCATTCGCGAGGAGCCGGATGAGAAGAAACTCTCA
TGTCCGGTTCTGTAGTAGAGATGGAATTAAGAAAAAACCATCAACTATAACCCCAAXAGAACCAGA
```

Out[156]:
```
[{'A': 0, 'C': 0, 'G': 0, 'T': 7.0},
 {'A': 7.0, 'C': 0, 'G': 0, 'T': 0},
 {'A': 0, 'C': 0, 'G': 0, 'T': 7.0},
 {'A': 7.0, 'C': 0, 'G': 0, 'T': 0},
 {'A': 0, 'C': 7.0, 'G': 0, 'T': 0},
 {'A': 7.0, 'C': 0, 'G': 0, 'T': 0},
 {'A': 0, 'C': 0, 'G': 0, 'T': 7.0},
 {'A': 1.0, 'C': 0, 'G': 0, 'T': 6.0},
 {'A': 7.0, 'C': 0, 'G': 0, 'T': 0},
 {'A': 7.0, 'C': 0, 'G': 0, 'T': 0}]
```

In [157]:
```
instances = [al.seq for al in align[:10]]
print(instances)
```

```
[Seq('TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAAAAAA...AGA', SingleLetterAlp
habet()), Seq('TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAAAAAA...AGA', Single
LetterAlphabet()), Seq('TATACATTAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAAAAAA...AG
A', SingleLetterAlphabet()), Seq('TATACATAAAAGAAGGGGGATGCGGATAAATGGAAAGGCGAAAGAAAGAA
AAAA...AGA', SingleLetterAlphabet()), Seq('TATACATTAAAGGAGGGGGATGCGGATAAATGGAAAGGCGA
AAGAAAGAAAAAA...AGA', SingleLetterAlphabet()), Seq('TATACATTAAAGGAGGGGGATGCGGATAAATG
GAAAGGCGAAAGAAAGAAAAAA...AGA', SingleLetterAlphabet()), Seq('TATACATTAAAGGAGGGGGATGC
GGATAAATGGAAAGGCGAAAGAAAGAAAAAA...AGA', SingleLetterAlphabet())]
```

Biopython - Motif

- Bio.motifs package included in Biopython 1.61

In [ ]:
```
from Bio import motifs
from Bio.Seq import Seq
```

In [ ]:
```
instances = [Seq("TACAA"),
             Seq("TACGA"),
             Seq("TACAA"),
             Seq("TAGAA"),
             Seq("TACAA"),
             Seq("AACGA"),
            ]
```

In [160]:
```
m = motifs.create(instances)
print(m)
```

```
TACAA
TACGA
TACAA
TAGAA
TACAA
AACGA
```

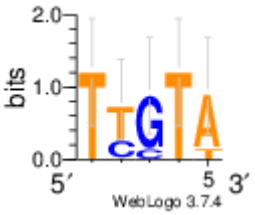
In [161]:
```
m.counts
```

Out[161]:
```
{'A': [1, 6, 0, 4, 6],
 'C': [0, 0, 5, 0, 0],
 'G': [0, 0, 1, 2, 0],
 'T': [5, 0, 0, 0, 0]}
```

In [162]:
```
m.counts["A", 1]
r = m.reverse_complement()
print(r.consensus)
#r.weblogo("mymotif.png")
```

```
TTGTA
```

In [165]:
```
from IPython.display import Image, display
display(Image(filename="/content/drive/My Drive/Colab Notebooks/bioengml/mymotif.png"))
```



- Position-weight matrices 계산
- .counts 특성 사용

In [166]:
```
pwm = m.counts.normalize(pseudocounts=0.5)
print(pwm)
```

```
        0     1     2     3     4
A:   0.19  0.81  0.06  0.56  0.81
C:   0.06  0.06  0.69  0.06  0.06
G:   0.06  0.06  0.19  0.31  0.06
T:   0.69  0.06  0.06  0.06  0.06
```

In [167]:
```
pssm = pwm.log_odds()
print(pssm)
```

```
        0     1     2     3     4
A:  -0.42  1.70 -2.00  1.17  1.70
C:  -2.00 -2.00  1.46 -2.00 -2.00
G:  -2.00 -2.00 -0.42  0.32 -2.00
T:   1.46 -2.00 -2.00 -2.00 -2.00
```

In [168]:
```
background = {"A":0.3,"C":0.2,"G":0.2,"T":0.3}
pssm = pwm.log_odds(background)
print(pssm)
```

```
        0     1     2     3     4
A:  -0.68  1.44 -2.26  0.91  1.44
C:  -1.68 -1.68  1.78 -1.68 -1.68
G:  -1.68 -1.68 -0.09  0.64 -1.68
T:   1.20 -2.26 -2.26 -2.26 -2.26
```

- 서열 내 모티프 존재 유무 탐색

In [169]:
```
test_seq=Seq("TACACTGCATTACAACCCAAGCATTA")
for pos, seq in m.instances.search(test_seq):
    print("%i %s " % (pos, seq))
print(m)
```

```
10 TACAA
TACAA
TACGA
TACAA
TAGAA
TACAA
AACGA
```

In [170]:
```
for pos, seq in r.instances.search(test_seq):
    print("%i %s " % (pos, seq))
print(r)
```

```
TTGTA
TCGTA
TTGTA
TTCTA
TTGTA
TCGTT
```

- Using the PSSM score

In [171]:
```
for pos, score in pssm.search(test_seq, threshold=3.0):
    print("%d, %f " % (pos, score))
print(pssm.calculate(test_seq))
```

```
0, 3.643981
10, 6.759458
[  3.643981    -8.560285    -2.4004133   -5.6533937   -4.2748823
  -0.05645879 -10.145247    -3.3293302   -5.9753222   -3.5703382
   6.759458    -5.3903594   -5.8598447   -0.81545067  -0.81545067
   0.7695118   -6.3903594   -3.5379167    0.4255574   -1.9309279
 -10.145247    -3.3293302 ]
```

In [172]:
```
m.pseudocounts = 0.1
print(m.counts)
print(m.pwm)
print(m.pssm)
```

```
        0      1      2      3      4
A:   1.00   6.00   0.00   4.00   6.00
C:   0.00   0.00   5.00   0.00   0.00
G:   0.00   0.00   1.00   2.00   0.00
T:   5.00   0.00   0.00   0.00   0.00

        0      1      2      3      4
A:   0.17   0.95   0.02   0.64   0.95
C:   0.02   0.02   0.80   0.02   0.02
G:   0.02   0.02   0.17   0.33   0.02
T:   0.80   0.02   0.02   0.02   0.02

        0      1      2      3      4
A:  -0.54   1.93  -4.00   1.36   1.93
C:  -4.00  -4.00   1.67  -4.00  -4.00
G:  -4.00  -4.00  -0.54   0.39  -4.00
T:   1.67  -4.00  -4.00  -4.00  -4.00
```

기계학습 K-Nearest Neighbor (KNN)

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

from sklearn.datasets import load_breast_cancer
from sklearn.metrics import confusion_matrix
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import train_test_split
import seaborn as sns
sns.set()
```

In [ ]:
```
breast_cancer = load_breast_cancer()
```

In [176]:
```
print(breast_cancer.data.shape)
X = pd.DataFrame(breast_cancer.data, columns=breast_cancer.feature_names)
```

```
(569, 30)
```

In [177]:
```
print(X.loc[0:3,])
```

```
   mean radius  mean texture  ...  worst symmetry  worst fractal dimension
0        17.99         10.38  ...          0.4601                  0.11890
1        20.57         17.77  ...          0.2750                  0.08902
2        19.69         21.25  ...          0.3613                  0.08758
3        11.42         20.38  ...          0.6638                  0.17300

[4 rows x 30 columns]
```

In [178]:
```
X[['mean area', 'mean compactness']]
```

Out[178]:

	mean area	mean compactness
0	1001.0	0.27760
1	1326.0	0.07864
2	1203.0	0.15990
3	386.1	0.28390
4	1297.0	0.13280
...	...	...
564	1479.0	0.11590
565	1261.0	0.10340
566	858.1	0.10230
567	1265.0	0.27700
568	181.0	0.04362

569 rows × 2 columns

In [179]:
```
y = pd.Categorical.from_codes(breast_cancer.target, breast_cancer.target_names)
y = pd.get_dummies(y, drop_first=True)
y
```

Out[179]:

	benign
0	0
1	0
2	0
3	0
4	0
...	...
564	0
565	0
566	0
567	0
568	1

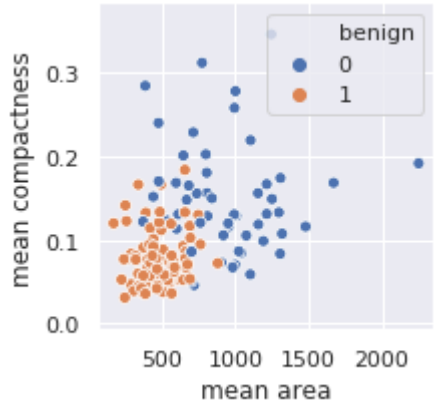
569 rows × 1 columns

In [ ]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)
```

In [181]:
```
knn = KNeighborsClassifier(n_neighbors=5, metric='euclidean')
knn.fit(X_train, y_train)
y_pred = knn.predict(X_test)
sns.scatterplot(
    x='mean area',
    y='mean compactness',
    hue='benign',
    data=X_test.join(y_test, how='outer')
)
```

```
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:2: DataConversionWarnin
g: A column-vector y was passed when a 1d array was expected. Please change the shap
e of y to (n_samples, ), for example using ravel().
```

Out[181]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7fcbeaedacf8>
```



In [182]:
```
results = pd.DataFrame([y_test["benign"].values, y_pred], index=("test", "predict"
)).T
print(results)
```

```
     test  predict
0       1        0
1       0        0
2       1        1
3       0        0
4       0        0
..    ...      ...
138     1        1
139     1        1
140     0        0
141     0        0
142     1        1

[143 rows x 2 columns]
```

In [183]:
```
results[results["test"]+results["predict"] == 1]
```

Out[183]:

	test	predict
0	1	0
33	0	1
38	0	1
63	1	0
76	0	1
77	0	1
110	0	1
127	1	0
137	1	0

In [184]:
```
from sklearn import metrics
print("Accuracy:",metrics.accuracy_score(y_test, y_pred))
```

```
Accuracy: 0.9370629370629371
```

Labeling problem of Bio-data

- Genotype - Phenotype
  - Sequence (SNP) - Disease : 의약 (임상 데이터) 1M samples
  - Sequence - ? : 생물공학 Low throughput

Sequence에서 filter와 pooling 의미

- 아래 예는 N=569개 샘플, P=30개 feature

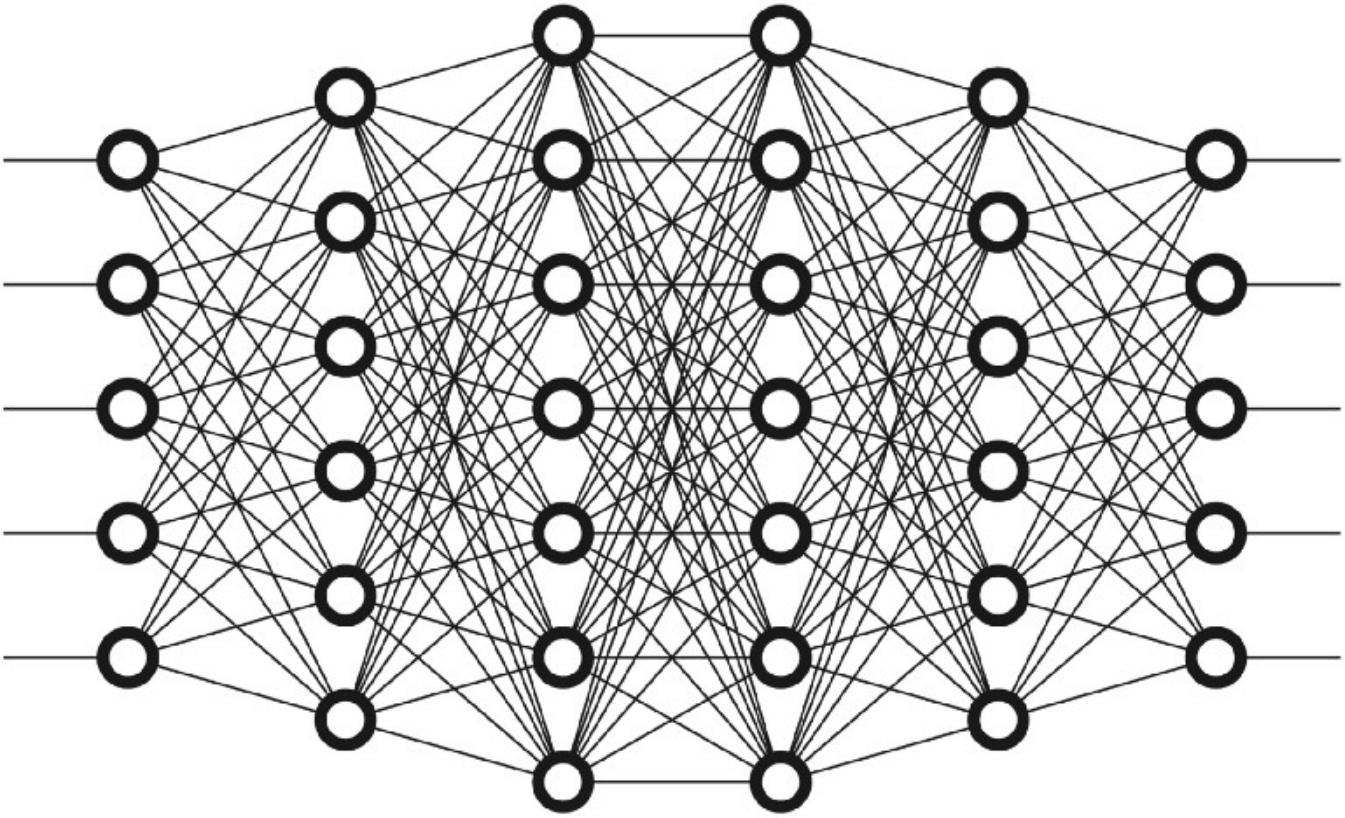
```
[176] print(breast_cancer.data.shape)
      X = pd.DataFrame(breast_cancer.data, columns=breast_cancer.feature_names)
```

```
(569, 30)
```

```
[177] print(X.loc[0:3,])
```

```
   mean radius  mean texture  ...  worst symmetry  worst fractal dimension
0        17.99         10.38  ...          0.4601                  0.11890
1        20.57         17.77  ...          0.2750                  0.08902
2        19.69         21.25  ...          0.3613                  0.08758
3        11.42         20.38  ...          0.6638                  0.17300

[4 rows x 30 columns]
```



filter: 서열에서 motif (e.g. conserved sequences)

filter 1 = first motif
...
filter P = Pth motif
N Sample x P filters

Pooling: 특정 서열에 모티프가 있다 (높은 score를 갖는 부분이 있다)

이미지의 10x10 픽셀은 1x100 으로 변환 수행, 즉, 이미지 1장 서열 1개 와 같음

CNN이 생물공학에서 가장 쉽게 접근 가능한 딥러닝 알고리즘

In [ ]: