BME1063 HW1 Visualization and Analyzation

package information

- python version 3.7.6
- numpy version 1.18.1
- pandas version 1.0.3
- matplotlib version 3.1.3

```
import os
import numpy as np
import pandas as pd
import matplotlib as mpl
import matplotlib.pyplot as plt
```

```
figure_path='../FinalReport/images'
```

Runtime vidualization

- Runtime information path: `FinalReport/time_summary`

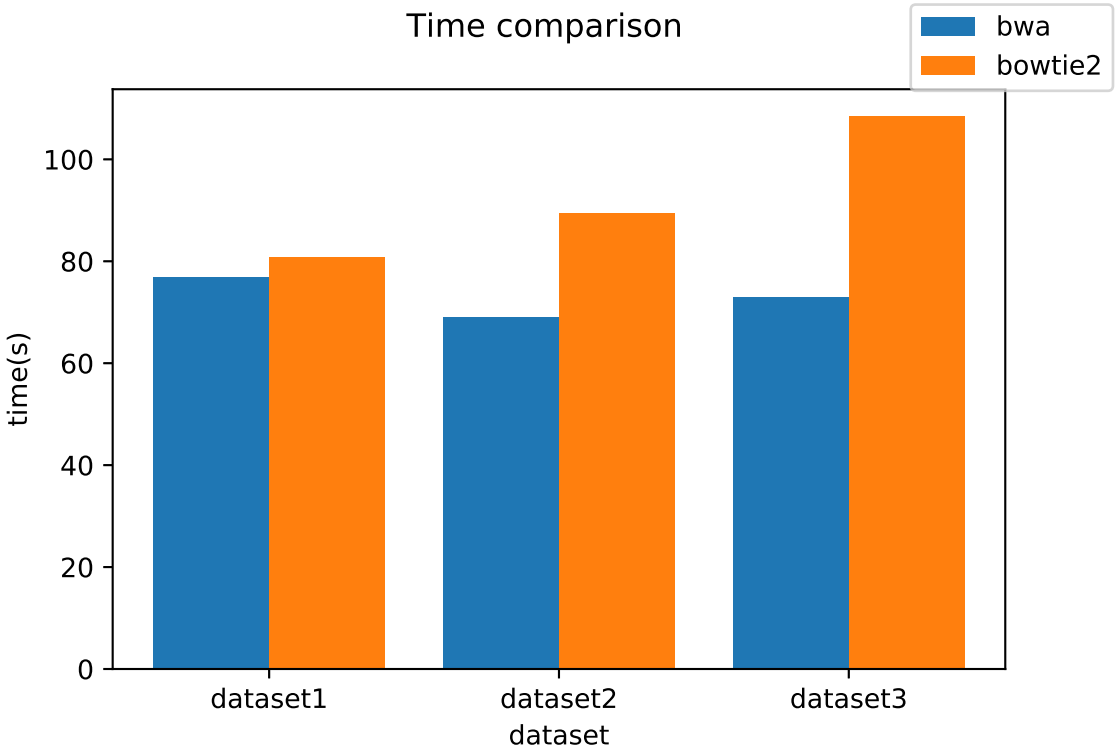
```
info_path = '../FinalReport/time_summary'

# read data from time summary
bwa_time = []
bowtie_time = []

with open(os.path.join(info_path, 'bwa_time_summary.txt'), 'r') as f:
    line = f.readline()
    # loop over the file and find 3 line start with 'user'
    while line != '':
        if line.split()[0] == 'user':
            time = line.split()[1]
            bwa_time.append(float(time.split('m')[1][:-1]) +
float(time.split('m')[0])*60)
        line = f.readline()

with open(os.path.join(info_path, 'bowtie2_time_summary.txt'), 'r') as f:
    line = f.readline()
    # loop over the file and find 3 line start with 'user'
    while line != '':
        if line.split()[0] == 'user':
            time = line.split()[1]
            bowtie_time.append(float(time.split('m')[1][:-1]) +
float(time.split('m')[0])*60)
        line = f.readline()
```

```
fig = plt.figure()
ax = fig.add_subplot(111)
ax.bar(range(3), bwa_time, width=0.4, label='bwa')
ax.bar([i + 0.4 for i in range(3)], bowtie_time, width=0.4, label='bowtie2')
# set ticks, tick labels and labels
ax.set(
    xticks=[i+0.2 for i in range(3)],
    xticklabels=['dataset1', 'dataset2', 'dataset3'],
    xlabel='dataset',
    ylabel='time(s)',
)
fig.legend()
fig.suptitle('Time comparison')
fig.savefig(os.path.join(figure_path, 'time_comparison.svg'))
```



mapping quality analyzation and visualization

```
quality_path = '../FinalReport/mapping_summary'
bwa_quality = os.path.join(quality_path, 'bwa_mapping')
bowtie2_quality = os.path.join(quality_path, 'bowtie2_mapping')
dwgsim_eval_cols = [ # data types given by dwgsim_eval
    'thr',
    'mc',
    'mi',
    'mu',
    'um',
    'uu',
    'mc+mi+mu+um+uu',
    "mc'",
    "mi'",
    "mu'",
    "um'",
    "uu'",
```

```
    "mc'+mi'+mu'+um'+uu'",
    "mc/(mc'+mi'+mu')",
    "mc/(mc'+mi')",
    "um/(um'+uu')",
    "mc'/(mc'+mi'_mu')",
    "mc'/(mc'+mi')",
    "um'/(um'+uu')"
]
```

```
# read data for mapping quality
bwa_dfs = [pd.read_csv(os.path.join(bwa_quality, name), delimiter=r"\s+",
header=None) for name in os.listdir(bwa_quality)]
# the code is indeed ugly but it is the simplest way to do the job
for df in bwa_dfs:
    df.columns=dwgsim_eval_cols

bowtie2_dfs = [pd.read_csv(os.path.join(bowtie2_quality, name),
delimiter=r"\s+", header=None) for name in os.listdir(bowtie2_quality)]
for df in bowtie2_dfs:
    df.columns=dwgsim_eval_cols
```

TP, TN, FP, FN

The definition for TP, TN, FP, FN is as follows:

- TP: true positive, number of sequences correctly mapped
- TN: true negative, number of sequences correctly unmapped
- FN: false negative, unmapped sequences should be mapped
- FP: false positive, mapped sequences should not be mapped, including wrongly mapped ones

```
# calculate TP, TN, FN, FP
for df in bwa_dfs:
    df['TP'] = df['mc']
    df['TN'] = df['uu']
    df['FP'] = df['mi'] + df['um']
    df['FN'] = df['mu']

for df in bowtie2_dfs:
    df['TP'] = df['mc']
    df['TN'] = df['uu']
    df['FP'] = df['mi'] + df['um']
    df['FN'] = df['mu']

# for i in range(3):
#     bwa_dfs[i] = bwa_dfs[i][['thr', 'TP', 'TN', 'FP', 'FN']]
#     bowtie2_dfs[i] = bowtie2_dfs[i][['thr', 'TP', 'TN', 'FP', 'FN']]
```

Precision and Recall

calculate Precision and Recall as follows:

$Precision = \frac{TP}{TP+FP}$
$Recall = \frac{TP}{TP+FN}$

$$Fscore = \frac{2*Precision*Recall}{Precision+Recall}$$

```
mapping_compare = pd.DataFrame(
    columns = ['software', 'dataset', 'precision', 'recall']
)
for i in range(3):
    df =bwa_dfs[i]
    mapping_compare = mapping_compare.append(
        {
            'software': 'bwa',
            'dataset': 'dataset' + str(i+1),
            'precision': df['TP'].sum() / (df['TP'].sum() + df['FP'].sum()),
            'recall': df['TP'].sum() / (df['TP'].sum() + df['FN'].sum())
        },
        ignore_index=True,
    )
    df =bowtie2_dfs[i]
    mapping_compare = mapping_compare.append(
        {
            'software': 'bowtie2',
            'dataset': 'dataset' + str(i + 1),
            'precision': df['TP'].sum() / (df['TP'].sum() + df['FP'].sum()),
            'recall': df['TP'].sum() / (df['TP'].sum() + df['FN'].sum())
        },
        ignore_index=True,
    )

mapping_compare['Fscore'] =
2*mapping_compare['precision']*mapping_compare['recall']/(mapping_compare['preci
sion'] + mapping_compare['recall'])

mapping_compare.to_csv(os.path.join(quality_path, 'precision_recall.csv'))
mapping_compare
```

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

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

	software	dataset	precision	recall	Fscore
0	bwa	dataset1	0.930225	1.000000	0.963852
1	bowtie2	dataset1	0.909904	0.999397	0.952553
2	bwa	dataset2	0.915926	1.000000	0.956119
3	bowtie2	dataset2	0.883572	0.998894	0.937701
4	bwa	dataset3	0.923573	1.000000	0.960268
5	bowtie2	dataset3	0.900112	0.999278	0.947106

Cumulative precision

Since a mapping quality score is made in each alignment, we can further validate the performance by computing `Cumulative precision`, defined as follows:

$$\text{Cumulative precision} = \frac{\text{TP considering cases with score higher than threshold}}{\text{TP + FP considering cases with score higher than threshold}}$$

$$\text{Cumulative recall} = \frac{\text{TP considering cases with score higher than threshold}}{\text{TP + FN considering cases with score higher than threshold}}$$

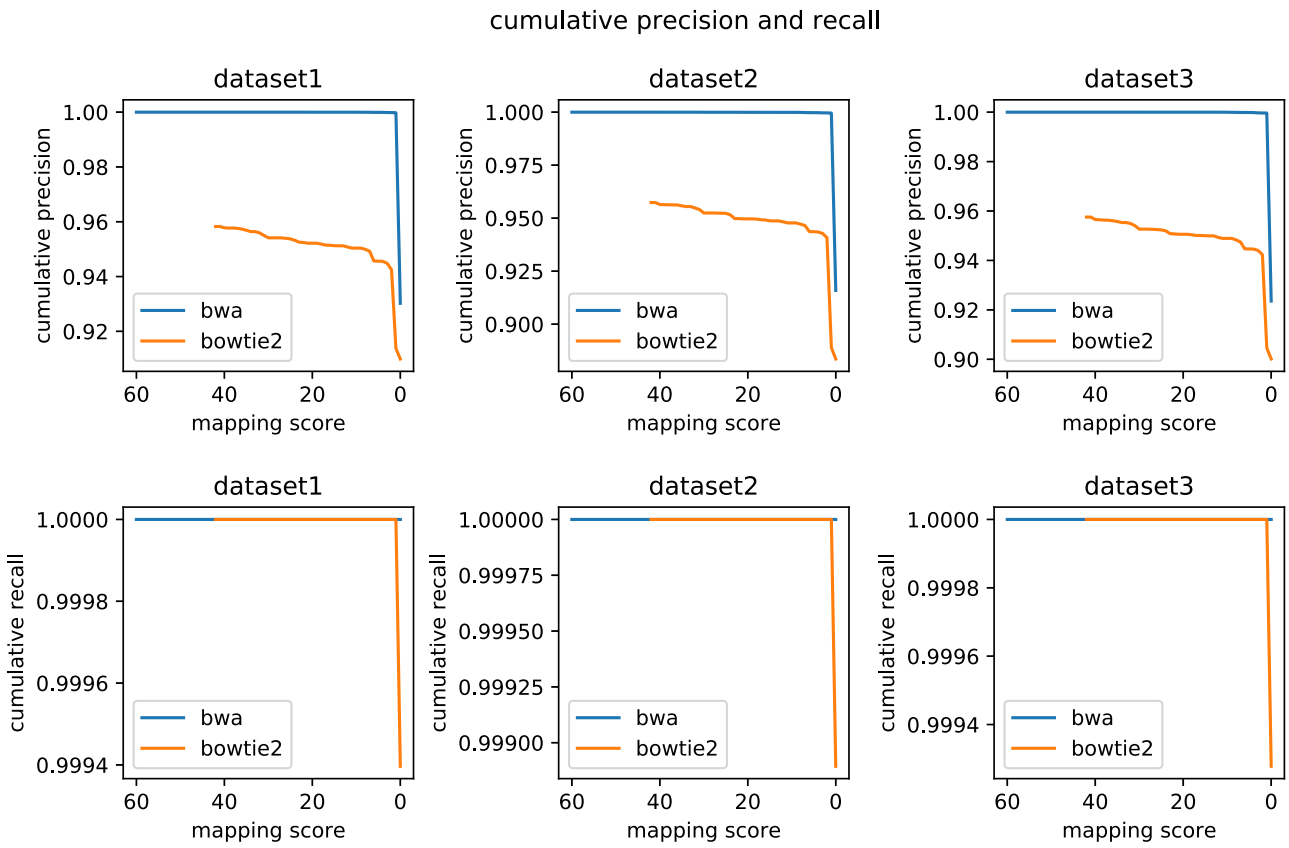
```
def calculate_cumulative_precision_recall(df):
    for i in range(df.shape[0]):
        # select first i+1 rows
        temp=df.loc[range(i+1)]
        df.loc[i, 'cumulative_precision'] = temp['TP'].sum() / (temp['TP'].sum() +
temp['FP'].sum())
        df.loc[i, 'cumulative_recall'] = temp['TP'].sum() / (temp['TP'].sum() +
temp['FN'].sum())
```

```
for i in range(3):
    calculate_cumulative_precision_recall(bwa_dfs[i])
    calculate_cumulative_precision_recall(bowtie2_dfs[i])
```

```
fig, axes = plt.subplots(2,3, figsize=(10,6), )
for i in range(3):
    axes[0, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['cumulative_precision'], label='bwa')
    axes[0, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['cumulative_precision'],
label='bowtie2')
    axes[0, i].set(xticks=[-60,-40,-20,0], xticklabels=[60,40,20,0], xlabel='mapping
score', ylabel='cumulative precision')
    axes[0, i].legend()
    axes[0, i].set_title('dataset{}'.format(str(i+1)))

    axes[1, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['cumulative_recall'], label='bwa')
    axes[1, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['cumulative_recall'],
label='bowtie2')
    axes[1, i].set(xticks=[-60,-40,-20,0], xticklabels=[60,40,20,0], xlabel='mapping
score', ylabel='cumulative recall')
    axes[1, i].legend()
    axes[1, i].set_title('dataset{}'.format(str(i+1)))
```

```
fig.subplots_adjust(wspace=0.5, hspace=0.5)
fig.suptitle('cumulative precision and recall')
fig.savefig(os.path.join(figure_path, 'cumulative_precision_recall.svg'), dpi=72)
```

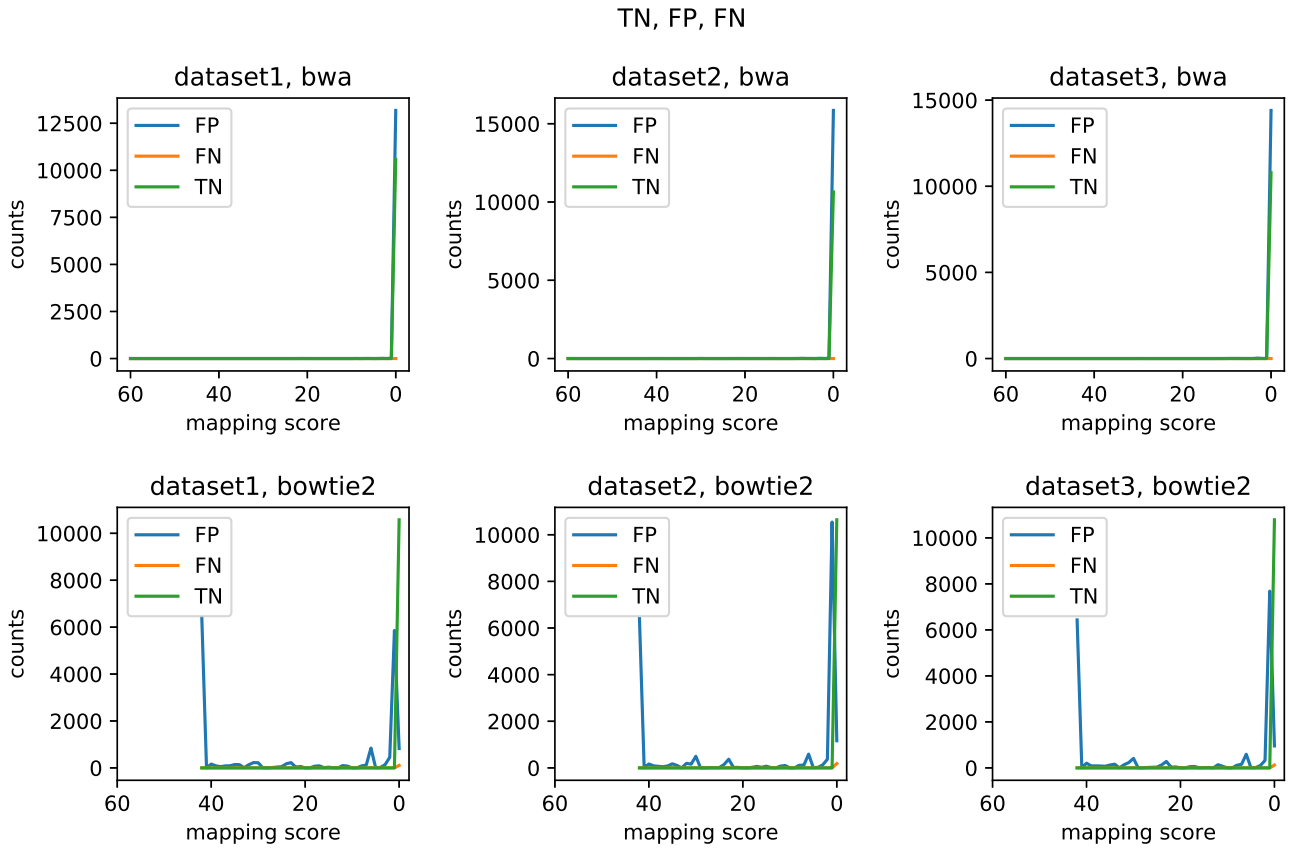


TP, TN, FP, FN distribution

if we plot TP, TN, FP, FN against the mapping quality

```
fig, axes = plt.subplots(2,3, figsize=(10,6), )
for i in range(3):
    axes[0, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['FP'], label='FP')
    axes[0, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['FN'], label='FN')
    # axes[0, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['TP'], label='TP')
    axes[0, i].plot(-bwa_dfs[i]['thr'], bwa_dfs[i]['TN'], label='TN')
    axes[0, i].set(xticks=[-60,-40,-20,0], xticklabels=[60,40,20,0], xlabel='mapping
score', ylabel='counts')
    axes[0, i].legend()
    axes[0, i].set_title('dataset{}, bwa'.format(str(i+1)))

    axes[1, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['FP'], label='FP')
    axes[1, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['FN'], label='FN')
    # axes[1, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['TP'], label='TP')
    axes[1, i].plot(-bowtie2_dfs[i]['thr'], bowtie2_dfs[i]['TN'], label='TN')
    axes[1, i].set(xticks=[-60,-40,-20,0], xticklabels=[60,40,20,0], xlabel='mapping
score', ylabel='counts')
    axes[1, i].legend()
    axes[1, i].set_title('dataset{}, bowtie2'.format(str(i+1)))
fig.subplots_adjust(wspace=0.5, hspace=0.5)
fig.suptitle('TN, FP, FN')
fig.savefig(os.path.join(figure_path, 'TN_FP_FN.svg'), dpi=72)
```



See if there are random sequences mapped.

```
for i in range(3):
    print(bwa_dfs[i]['um'].sum(), bowtie2_dfs[i]['um'].sum())
```

```
0 0
0 0
0 0
```