NetRAX Experiment Evaluation

February 9, 2021

[1]:
```
%matplotlib inline
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
sns.set(style="darkgrid")
```

[2]:
```
def bic_stats(df):
    print("Inferred BIC better or equal: " + str(len(df[df['bic_inferred'] <=␣
 ↪df['bic_true']])))
    print("Inferred BIC worse: " + str(len(df[df['bic_inferred'] >␣
 ↪df['bic_true']])))

def reticulation_stats(df):
    print("Inferred n_reticulations less: " +␣
 ↪str(len(df[df['n_reticulations_inferred'] < df['n_reticulations']])))
    print("Inferred n_reticulations equal: " +␣
 ↪str(len(df[df['n_reticulations_inferred'] == df['n_reticulations']])))
    print("Inferred n_reticulations more: " +␣
 ↪str(len(df[df['n_reticulations_inferred'] > df['n_reticulations']])))

def weirdness_stats(df):
    df['true_network_weirdness'].plot.hist(bins=10, alpha=0.5, range=(0,1),␣
 ↪title='True network weirdness')

def zero_branches_stats(df):
    df['near_zero_branches_raxml'].plot.hist(bins=10, alpha=0.5,␣
 ↪title='Near-zero branches raxml')

def distances(df):
    fig, axes = plt.subplots(3, 2, constrained_layout=True)
    df['hardwired_cluster_distance'].plot.hist(bins=10, alpha=0.5,␣
 ↪title='Hardwired cluster distance', ax=axes[0,0])
    df['softwired_cluster_distance'].plot.hist(bins=10, alpha=0.5,␣
 ↪title='Softwired cluster distance', ax=axes[0,1])
    df['displayed_trees_distance'].plot.hist(bins=10, alpha=0.5,␣
 ↪title='Displayed trees distance', ax=axes[1,0])
```

```
    df['tripartition_distance'].plot.hist(bins=10, alpha=0.5,␣
 ↪title='Tripartition distance', ax=axes[1,1])
    df['nested_labels_distance'].plot.hist(bins=10, alpha=0.5, title='Nested␣
 ↪labels distance', ax=axes[2,0])
    df['path_multiplicity_distance'].plot.hist(bins=10, alpha=0.5, title='Path␣
 ↪multiplicity distance', ax=axes[2,1])

def build_stats(df):
    plt.figure(0)
    bic_stats(df)
    print("")
    plt.figure(1)
    reticulation_stats(df)
    print("")
    plt.figure(2)
    weirdness_stats(df)
    print("")
    plt.figure(3)
    zero_branches_stats(df)
    print("")
    plt.figure(4)
    distances(df)
```

Load the result CSV:

[3]:
```
#df = pd.read_csv('small_network_results.csv')
#df = pd.read_csv('medium_network_norandom_results.csv')
#df = pd.read_csv('small_network_uniform_results.csv')
df = pd.read_csv('medium_network_norandom_uniform_results.csv')
```

[4]:
```
pd.set_option('display.max_columns', None)
df.head()
```

[4]:

	name	n_taxa	n_trees	n_reticulations	msa_size	sampling_type	simulation_type
0	datasets_medium_network_norandom_uniform_0_0/0…	26	4	2	200	PERFECT_SAMPLING	CELINE
1	datasets_medium_network_norandom_uniform_0_0/0…	26	4	2	200	PERFECT_SAMPLING	CELINE
2	datasets_medium_network_norandom_uniform_0_0/0…	26	4	2	400	PERFECT_SAMPLING	CELINE
3	datasets_medium_network_norandom_uniform_0_0/0…	26	4	2	400	PERFECT_SAMPLING	CELINE
4	datasets_medium_network_norandom_uniform_0_1/0…	22	2	1	100	PERFECT_SAMPLING	CELINE

```
                                    celine_params  \
0  {'to': 0.14860997437546947| 'lambda': 21.63797…
1  {'to': 0.14860997437546947| 'lambda': 21.63797…
2  {'to': 0.14860997437546947| 'lambda': 21.63797…
3  {'to': 0.14860997437546947| 'lambda': 21.63797…
4  {'to': 0.12766349262110696| 'lambda': 24.51074…

                  seqgen_params  near_zero_branches_raxml  \
0  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                         0
1  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                         0
2  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                         0
3  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                         0
4  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                         0

   n_equal_tree_pairs  true_network_weirdness  \
0                   0                       0
1                   0                       0
2                   0                       0
3                   0                       0
4                   0                       0

                                 true_network_path  \
0  datasets_medium_network_norandom_uniform_0_0/0…
1  datasets_medium_network_norandom_uniform_0_0/0…
2  datasets_medium_network_norandom_uniform_0_0/0…
3  datasets_medium_network_norandom_uniform_0_0/0…
4  datasets_medium_network_norandom_uniform_0_1/0…

                            inferred_network_path likelihood_type  \
0  datasets_medium_network_norandom_uniform_0_0/0…         AVERAGE
1  datasets_medium_network_norandom_uniform_0_0/0…            BEST
2  datasets_medium_network_norandom_uniform_0_0/0…         AVERAGE
3  datasets_medium_network_norandom_uniform_0_0/0…            BEST
4  datasets_medium_network_norandom_uniform_0_1/0…         AVERAGE

  brlen_linkage_type  start_type  timeout  n_random_start_networks  \
0             LINKED  FROM_RAXML        0                        0
1             LINKED  FROM_RAXML        0                        0
2             LINKED  FROM_RAXML        0                        0
3             LINKED  FROM_RAXML        0                        0
4             LINKED  FROM_RAXML        0                        0

   n_parsimony_start_networks  runtime_inference  n_reticulations_inferred  \
0                           0          18670.640                       1.0
1                           0           1029.402                       0.0
2                           0           1217.179                       0.0
3                           0            709.402                       0.0
```

```
4                          0           2056.276                        0.0

      bic_true    logl_true  bic_inferred  logl_inferred    bic_raxml  \
0  3913.384732 -1554.540913   3963.151211   -1596.536980  3984.670570
1  3913.384533 -1554.540813   3984.670570   -1624.409487  3984.670570
2  7306.336325 -3218.438792   7490.636097   -3347.586922  7490.636097
3  7306.336325 -3218.438792   7490.636097   -3347.586922  7490.636097
4  1611.070345  -559.256368   1592.876235    -565.551738  1592.875978

    logl_raxml  rf_absolute_raxml  rf_relative_raxml  rf_absolute_inferred  \
0 -1624.409487                 -1                 -1                    -1
1 -1624.409487                 -1                 -1                    -1
2 -3347.586922                 -1                 -1                    -1
3 -3347.586922                 -1                 -1                    -1
4  -565.551610                 -1                 -1                    -1

   rf_relative_inferred  hardwired_cluster_distance  \
0                    -1                        12.0
1                    -1                         9.0
2                    -1                        10.0
3                    -1                        10.0
4                    -1                         7.0

   softwired_cluster_distance  displayed_trees_distance  \
0                        14.5                       2.5
1                        11.5                       2.5
2                         9.5                       2.5
3                         9.5                       2.5
4                         7.5                       1.5

   tripartition_distance  nested_labels_distance  path_multiplicity_distance
0                   14.5                    17.0                        10.5
1                   14.0                    16.0                        11.0
2                   13.0                    15.0                        12.0
3                   13.0                    15.0                        12.0
4                    8.5                    12.0                         9.0
```

[5]:
```
df.columns
```

[5]:
```
Index(['name', 'n_taxa', 'n_trees', 'n_reticulations', 'msa_size',
       'sampling_type', 'simulation_type', 'celine_params', 'seqgen_params',
       'near_zero_branches_raxml', 'n_equal_tree_pairs',
       'true_network_weirdness', 'true_network_path', 'inferred_network_path',
       'likelihood_type', 'brlen_linkage_type', 'start_type', 'timeout',
       'n_random_start_networks', 'n_parsimony_start_networks',
       'runtime_inference', 'n_reticulations_inferred', 'bic_true',
       'logl_true', 'bic_inferred', 'logl_inferred', 'bic_raxml', 'logl_raxml',
```

```
       'rf_absolute_raxml', 'rf_relative_raxml', 'rf_absolute_inferred',
       'rf_relative_inferred', 'hardwired_cluster_distance',
       'softwired_cluster_distance', 'displayed_trees_distance',
       'tripartition_distance', 'nested_labels_distance',
       'path_multiplicity_distance'],
      dtype='object')
```

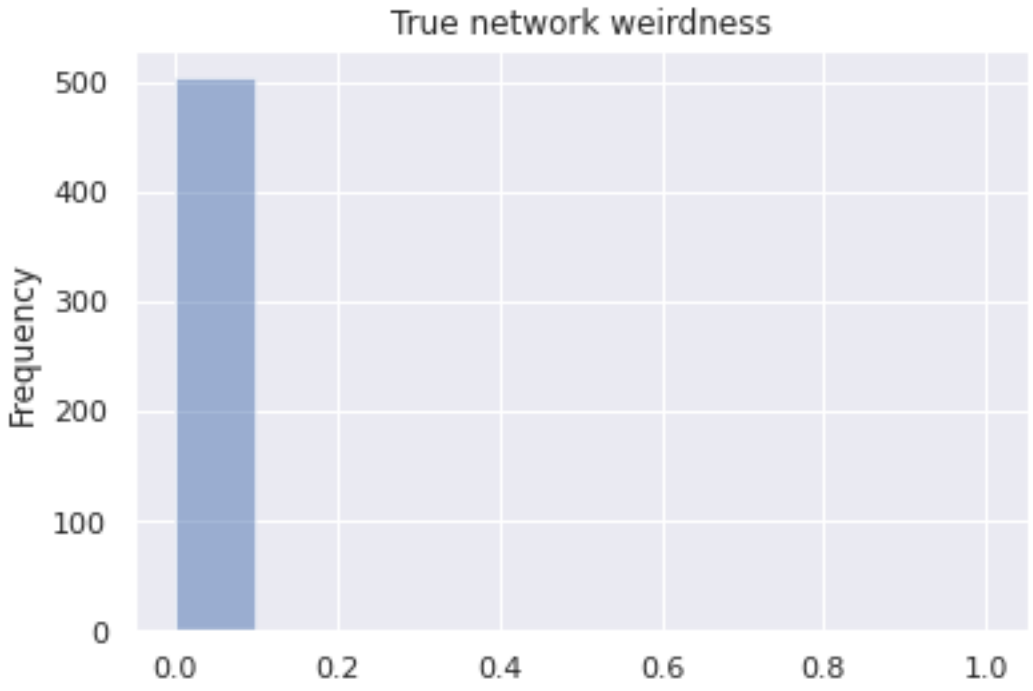
[6]:
```
build_stats(df)
```

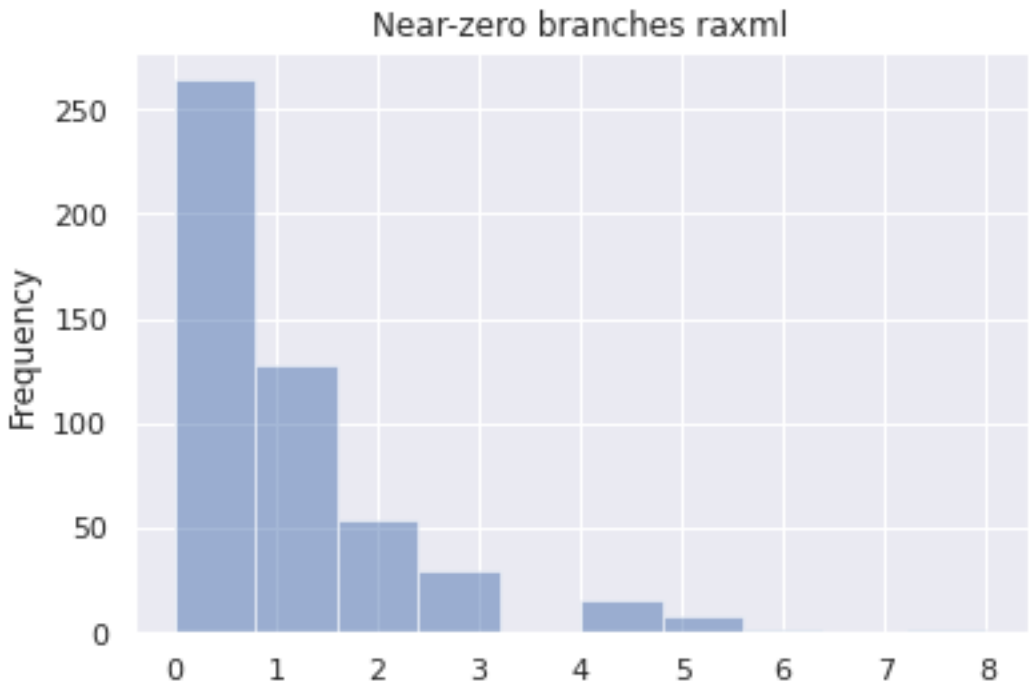
```
Inferred BIC better or equal: 382
Inferred BIC worse: 122

Inferred n_reticulations less: 415
Inferred n_reticulations equal: 89
Inferred n_reticulations more: 0
```

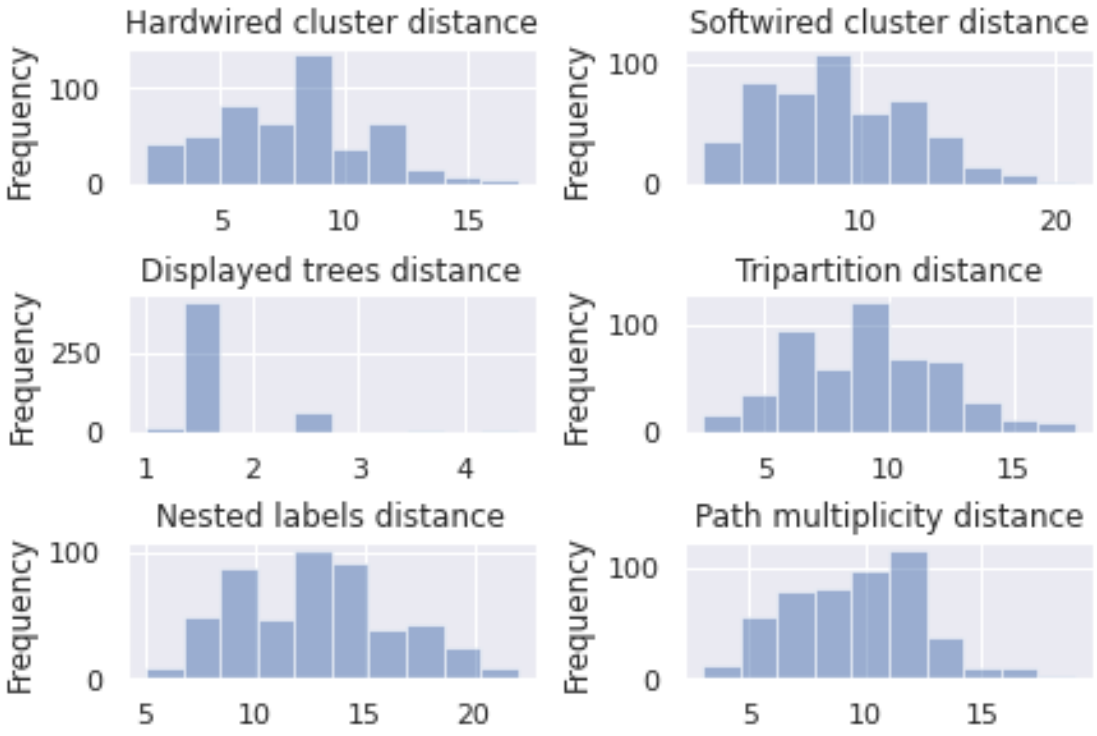
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



1 Plots for starting with raxml-ng best tree only

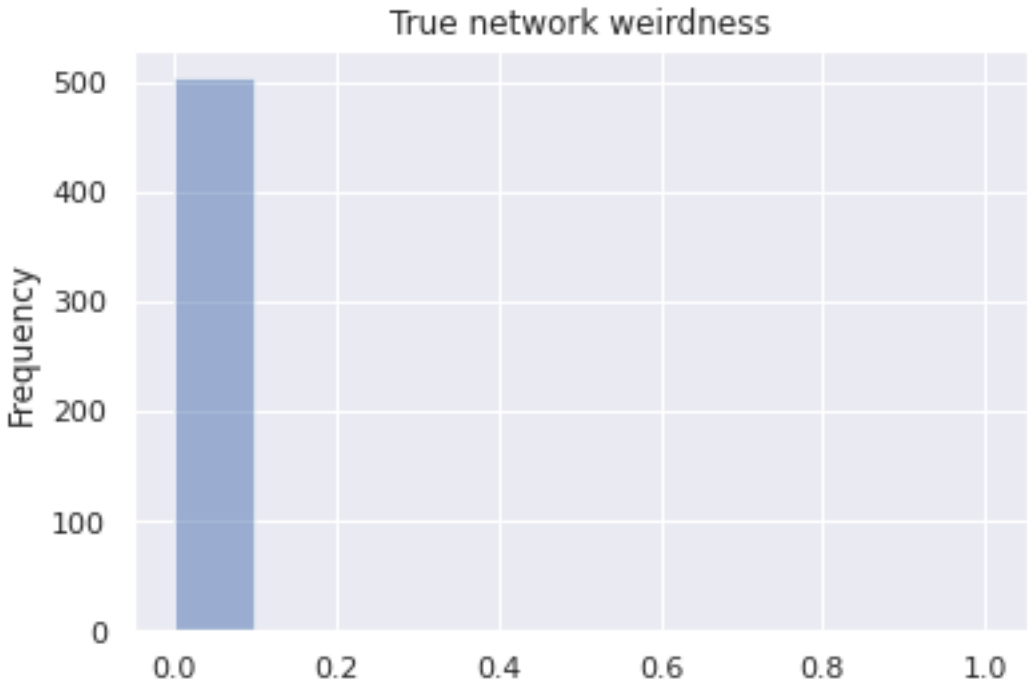
[7]:
```
df_raxml_only = df.query('start_type == "FROM_RAXML"')
build_stats(df_raxml_only)
```

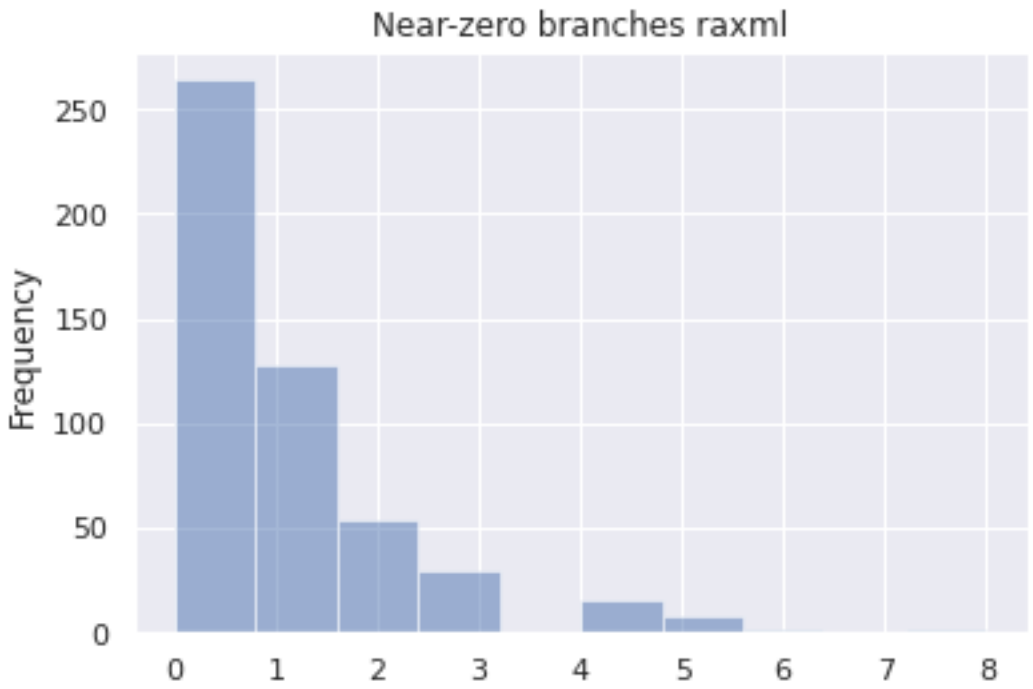
```
Inferred BIC better or equal: 382
Inferred BIC worse: 122

Inferred n_reticulations less: 415
Inferred n_reticulations equal: 89
Inferred n_reticulations more: 0
```

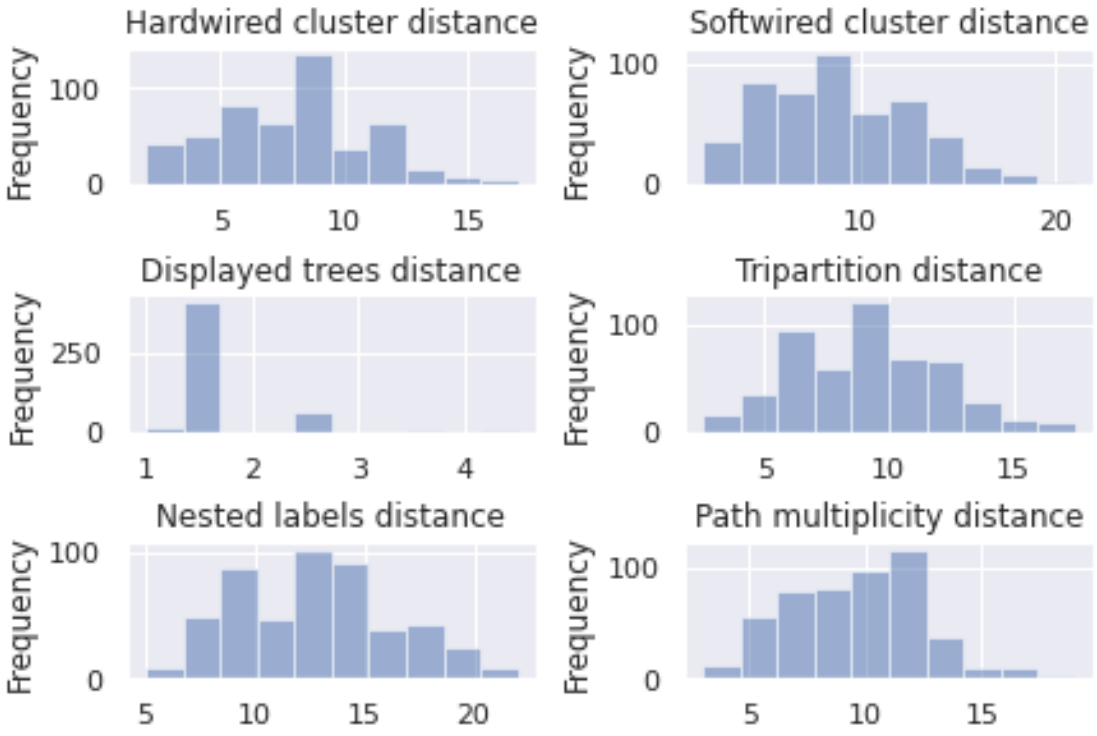
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



1.1 Plots for MSA_size ~ 100*n_trees

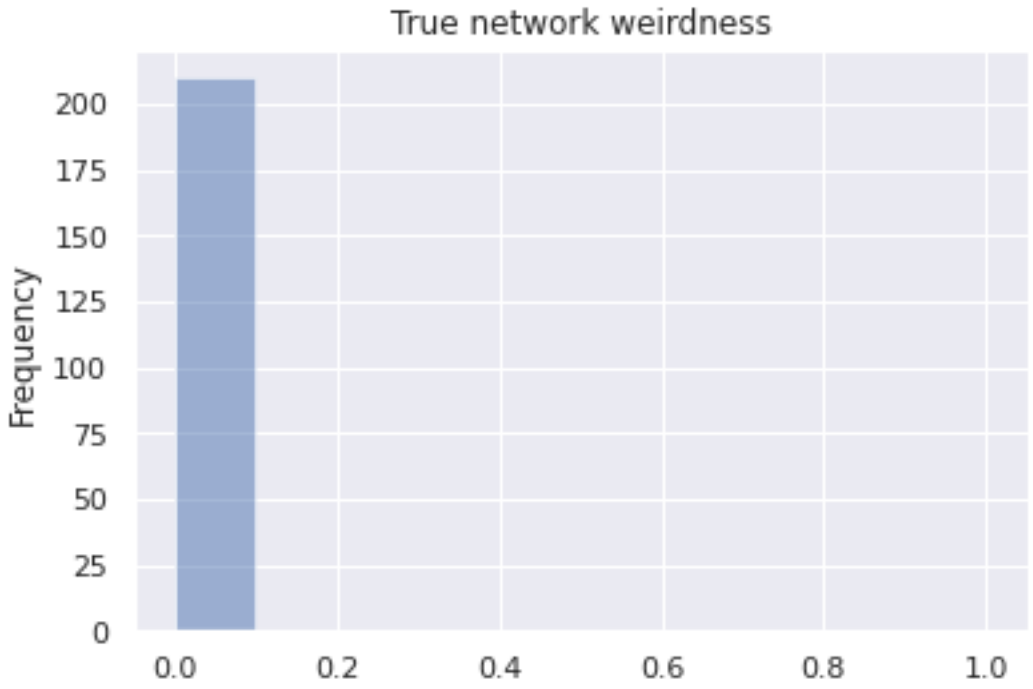
[8]:
```
df_raxml_only_msasize_100 = df_raxml_only.query('msa_size == 100')
build_stats(df_raxml_only_msasize_100)
```

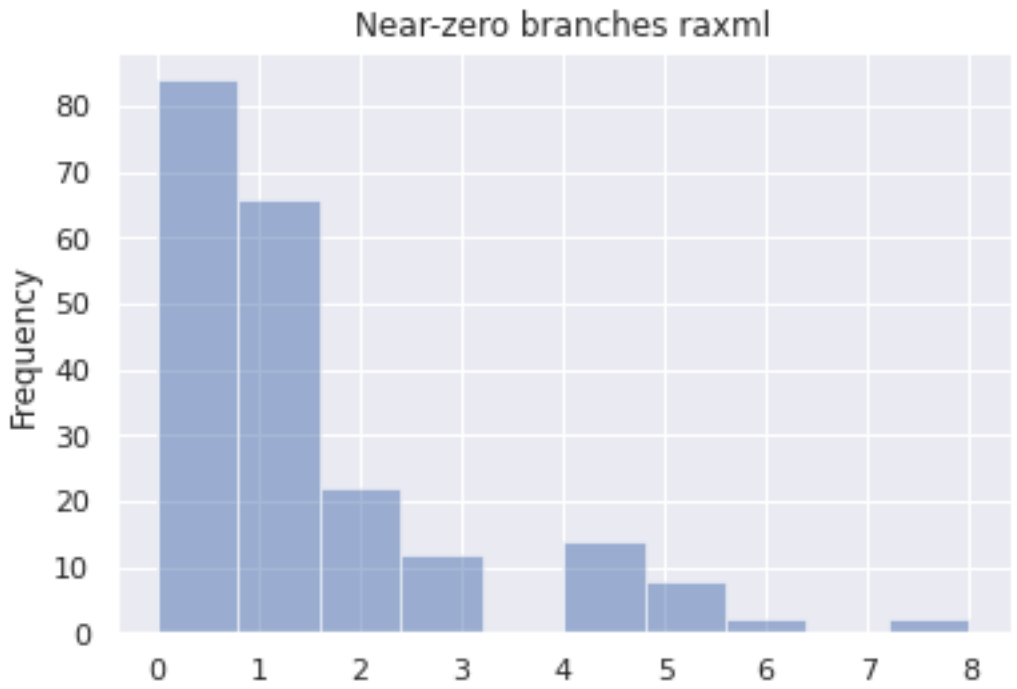
```
Inferred BIC better or equal: 190
Inferred BIC worse: 20

Inferred n_reticulations less: 179
Inferred n_reticulations equal: 31
Inferred n_reticulations more: 0
```

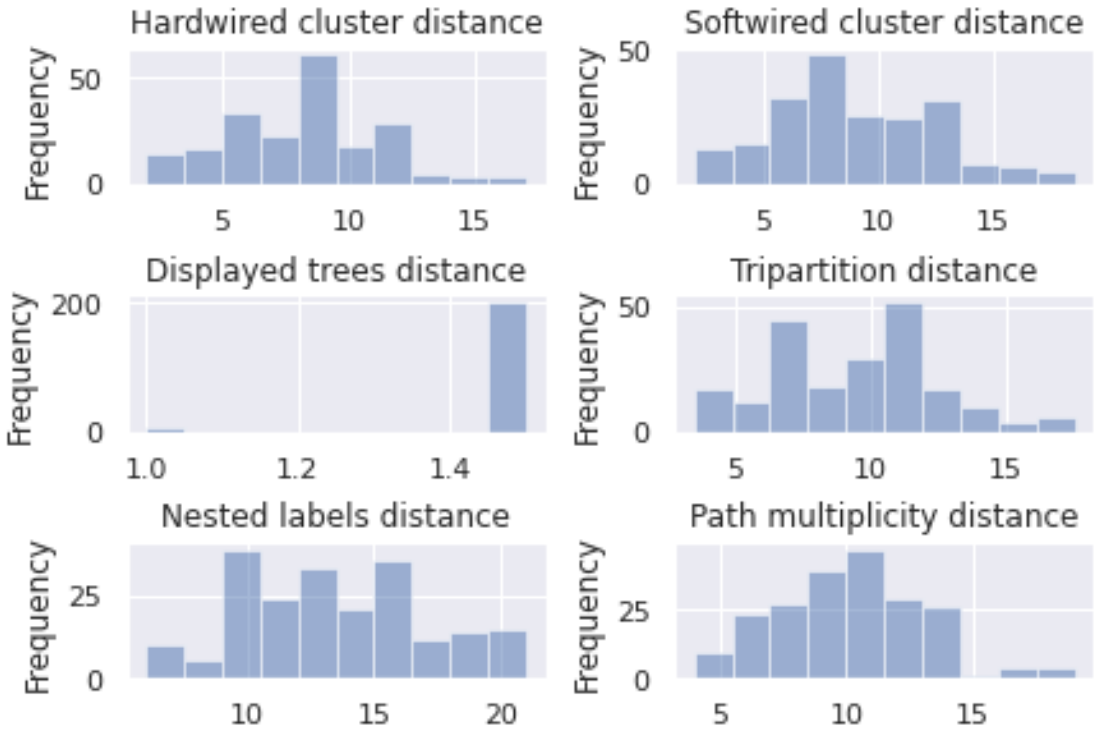
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



1.1.1 Plots for LikelihodType.AVERAGE

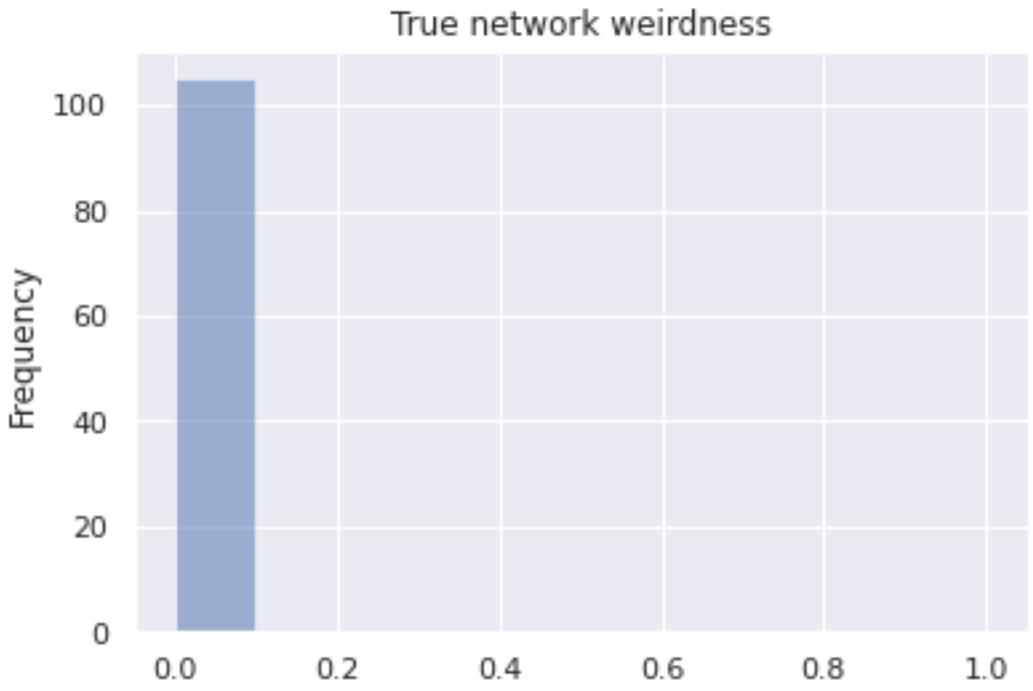
[9]:
```
df_raxml_only_msasize_100_average = df_raxml_only_msasize_100.
 ↪query('likelihood_type == "AVERAGE"')
build_stats(df_raxml_only_msasize_100_average)
```

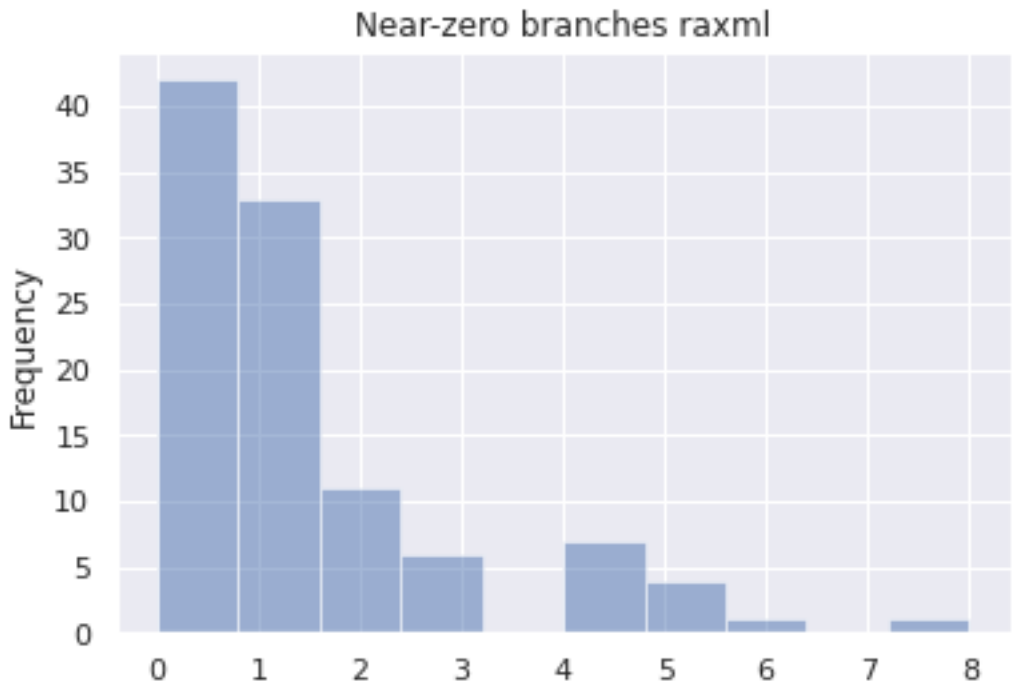
```
Inferred BIC better or equal: 98
Inferred BIC worse: 7

Inferred n_reticulations less: 87
Inferred n_reticulations equal: 18
Inferred n_reticulations more: 0
```

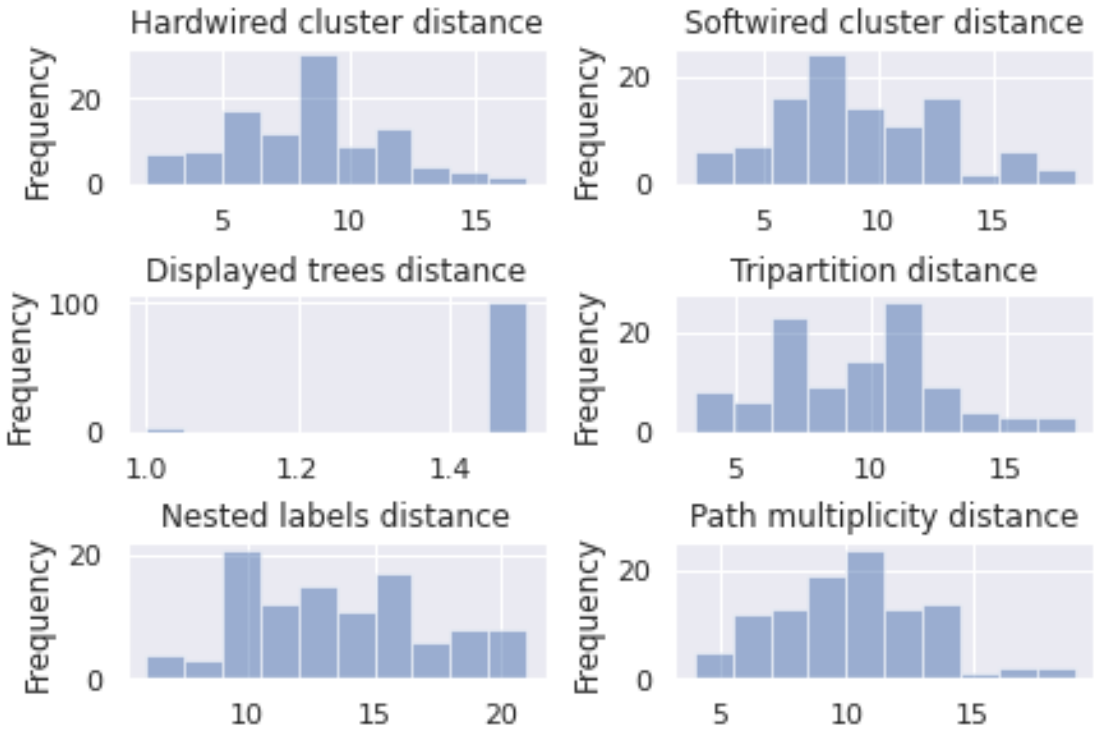
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```






```
<Figure size 432x288 with 0 Axes>
```



1.1.2 Plots for LikelihoodType.BEST

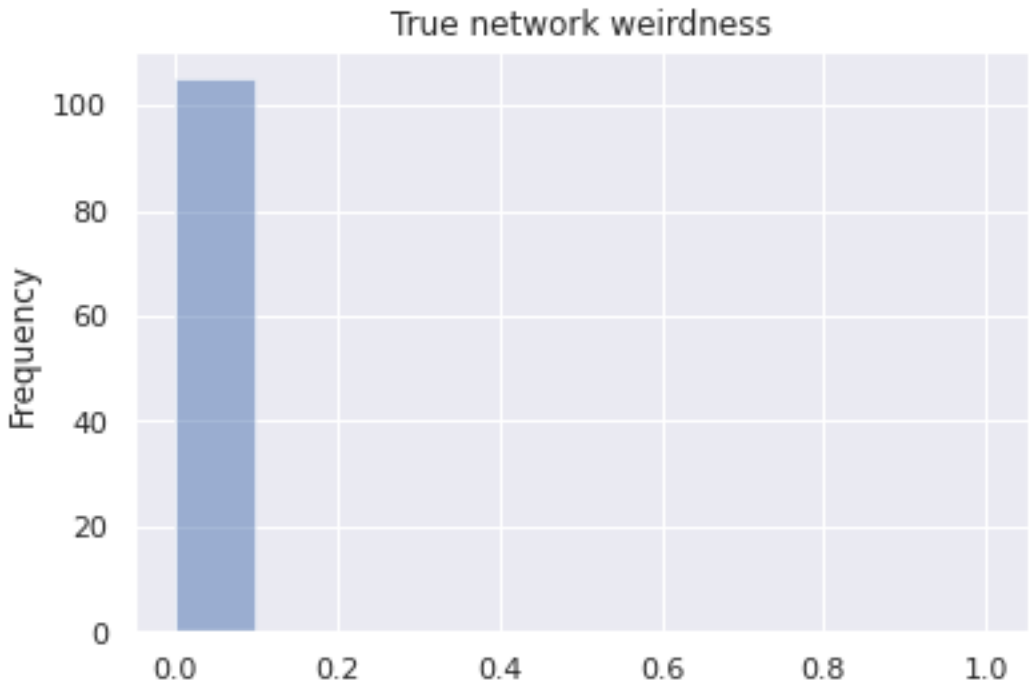
[10]:
```
df_raxml_only_msasize_100_best = df_raxml_only_msasize_100.
 ↪query('likelihood_type == "BEST"')
build_stats(df_raxml_only_msasize_100_best)
```

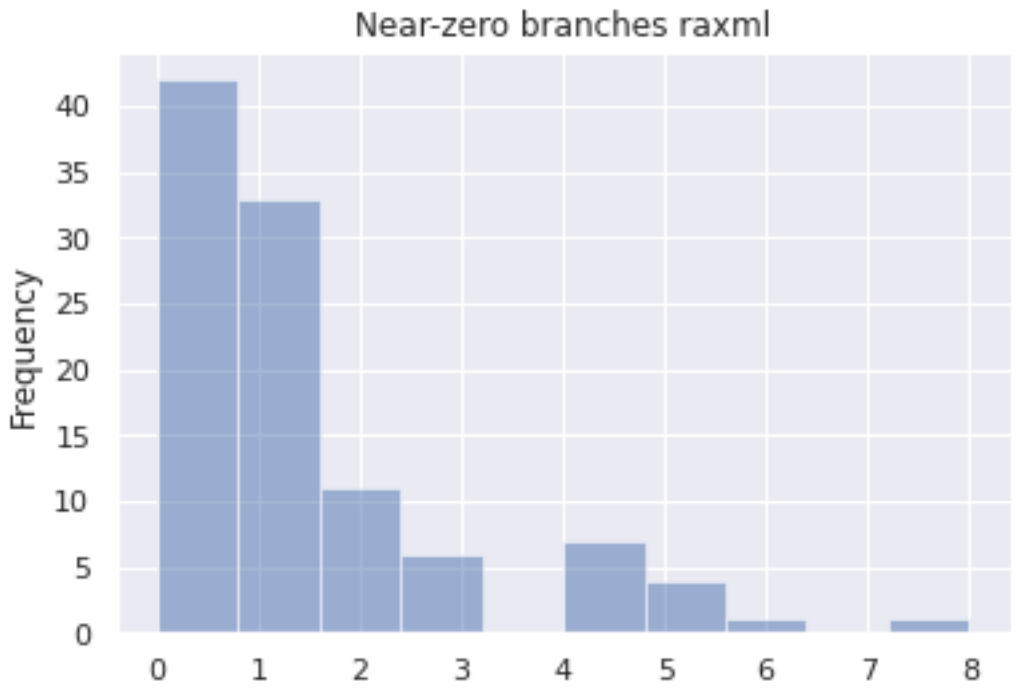
```
Inferred BIC better or equal: 92
Inferred BIC worse: 13

Inferred n_reticulations less: 92
Inferred n_reticulations equal: 13
Inferred n_reticulations more: 0
```

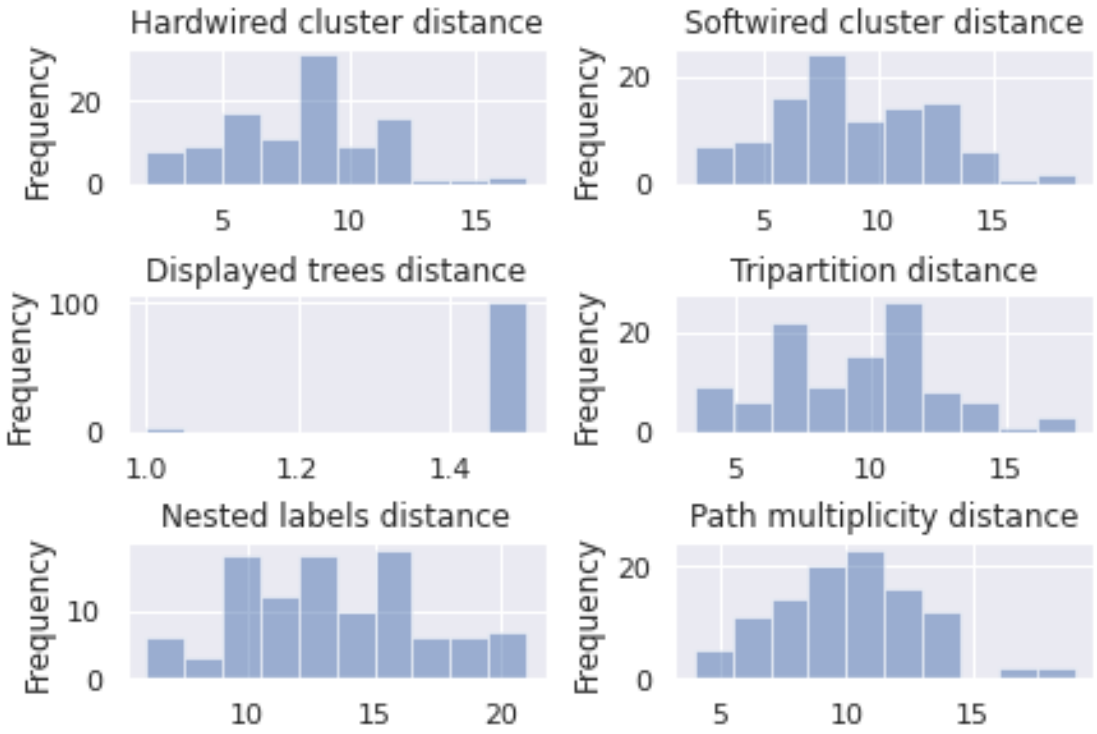
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```






```
<Figure size 432x288 with 0 Axes>
```



1.2 Plots for MSA_size ~ 200*n_trees

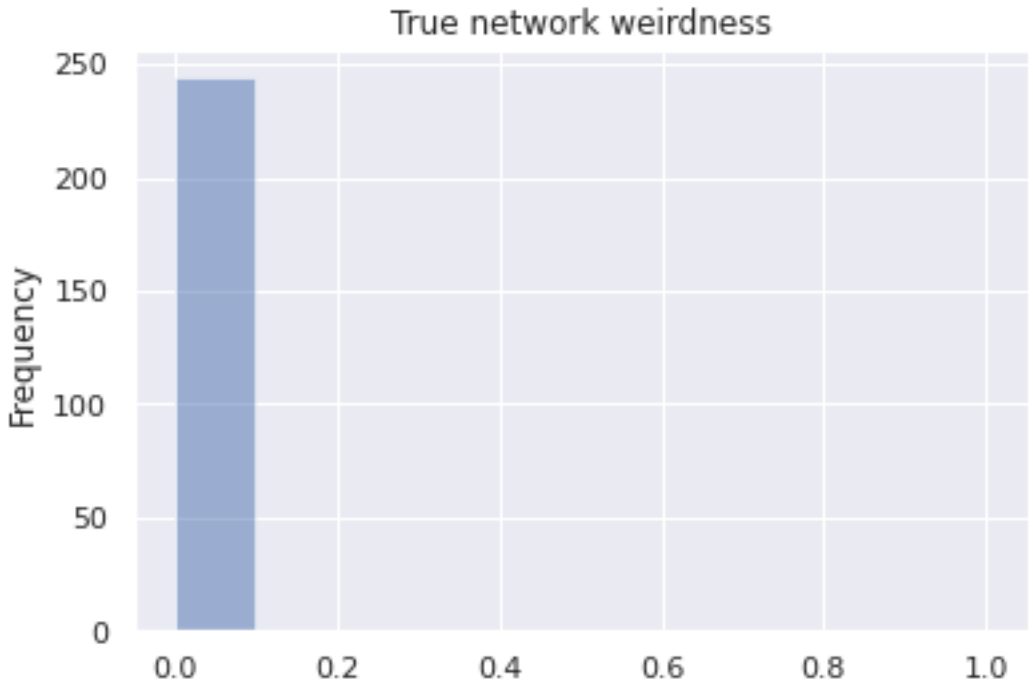
[11]:
```
df_raxml_only_msasize_200 = df_raxml_only.query('msa_size == 200')
build_stats(df_raxml_only_msasize_200)
```

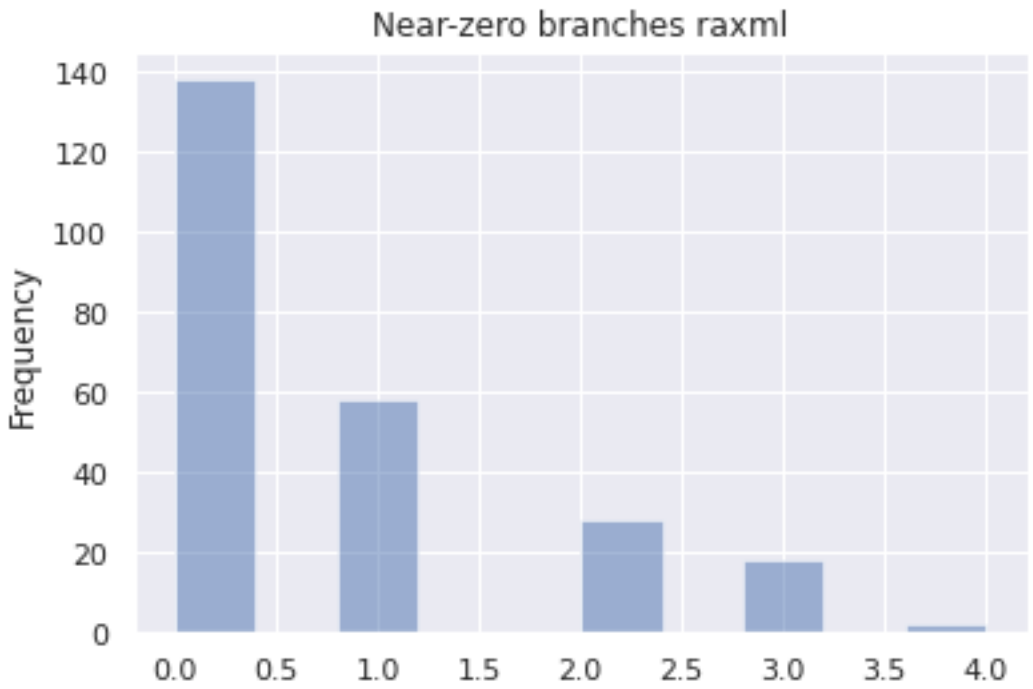
```
Inferred BIC better or equal: 170
Inferred BIC worse: 74

Inferred n_reticulations less: 187
Inferred n_reticulations equal: 57
Inferred n_reticulations more: 0
```

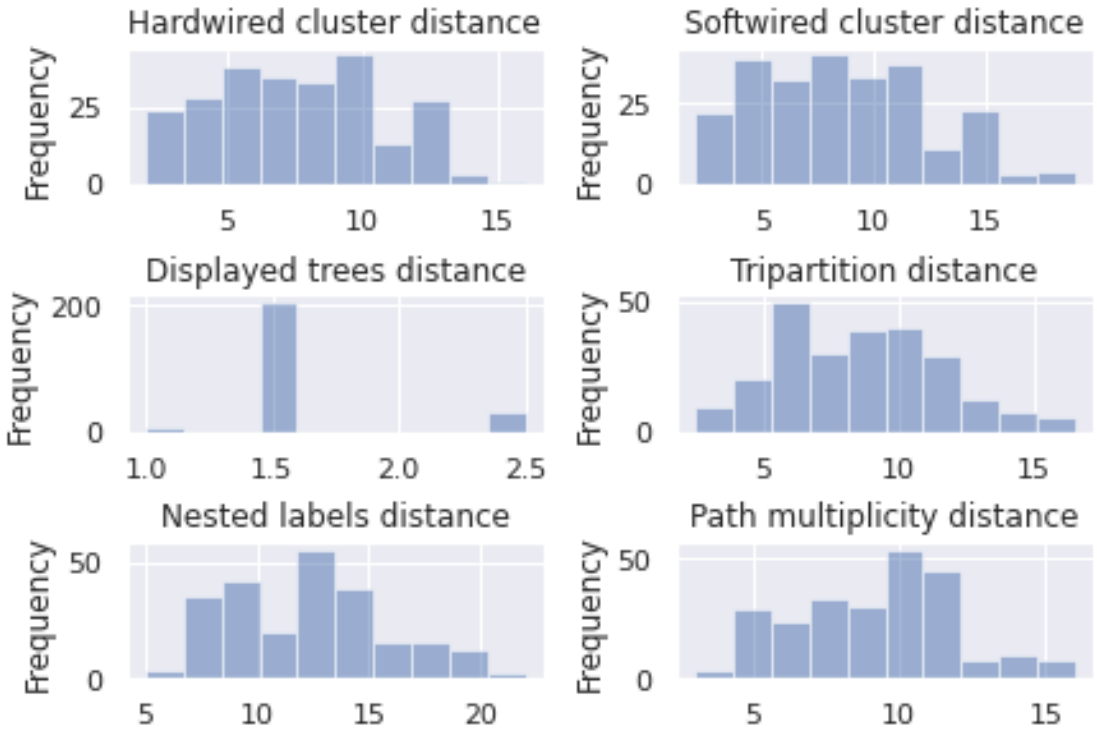
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



1.2.1 Plots for LikelihodType.AVERAGE

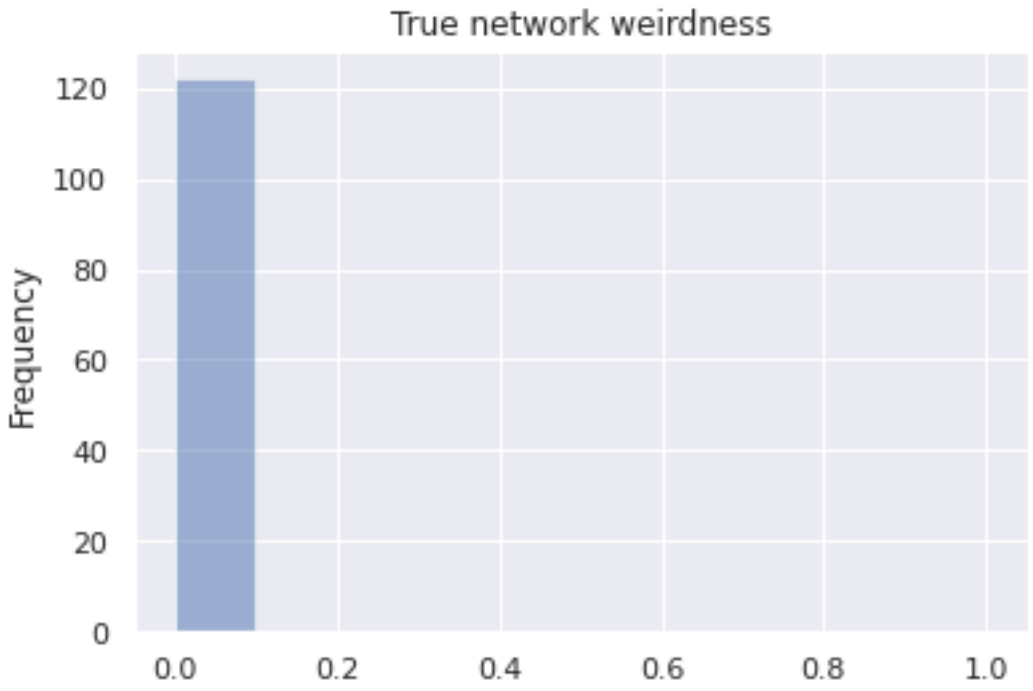
[12]:
```
df_raxml_only_msasize_200_average = df_raxml_only_msasize_200.
 ↪query('likelihood_type == "AVERAGE"')
build_stats(df_raxml_only_msasize_200_average)
```

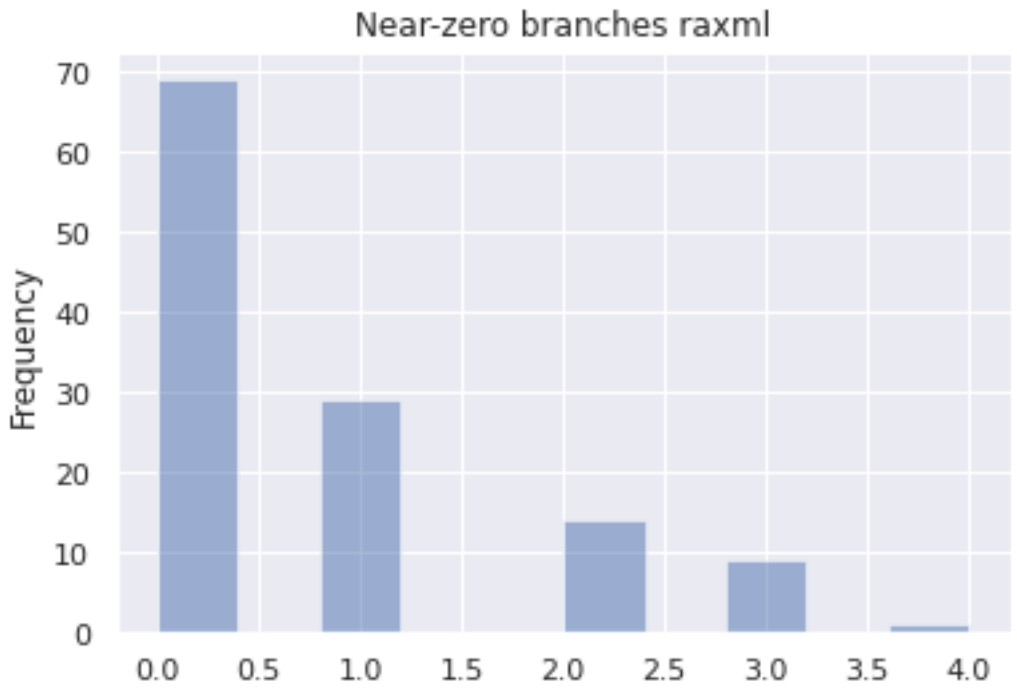
```
Inferred BIC better or equal: 85
Inferred BIC worse: 37

Inferred n_reticulations less: 93
Inferred n_reticulations equal: 29
Inferred n_reticulations more: 0
```

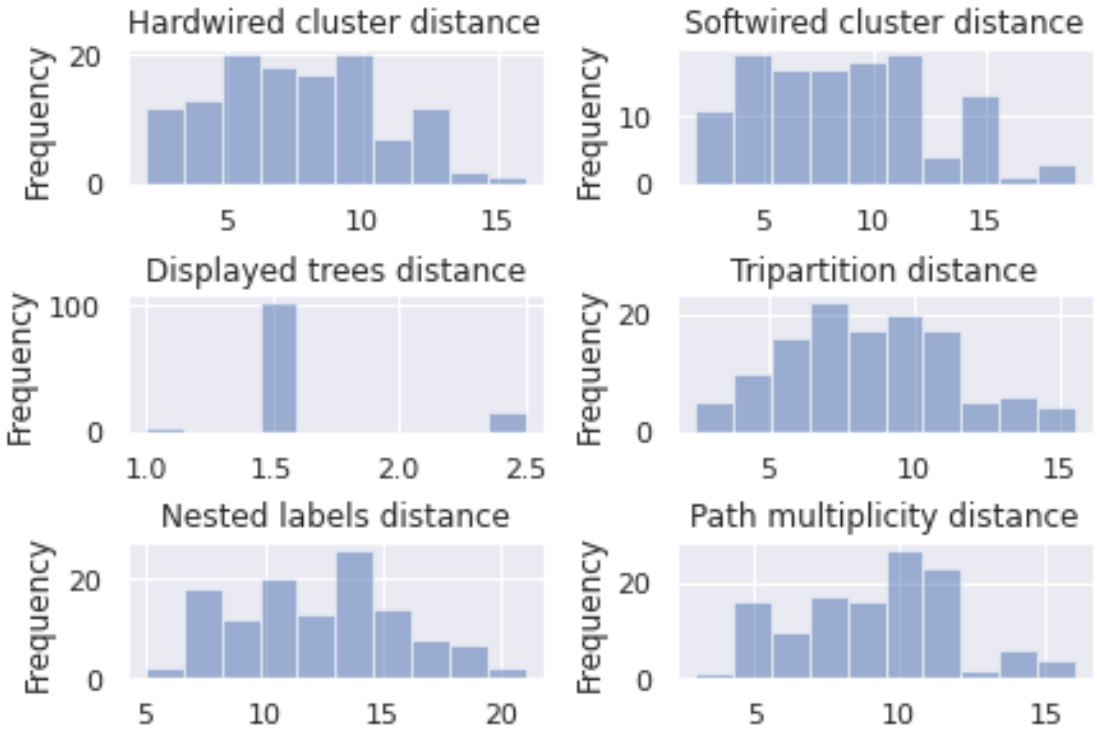
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



1.2.2 Plots for LikelihoodType.BEST

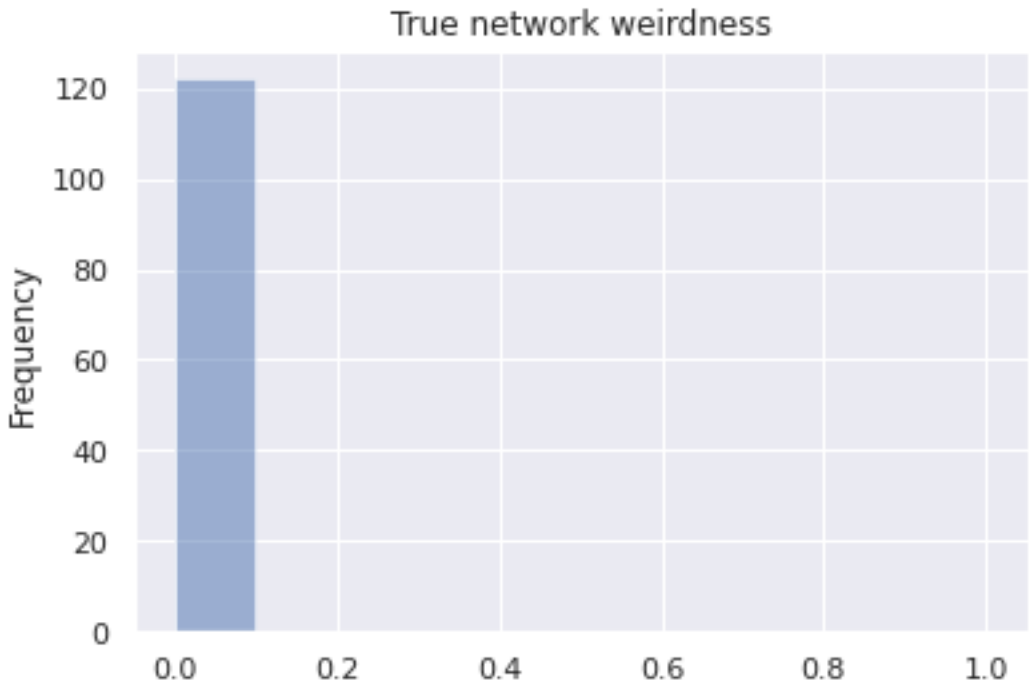
[13]:
```
df_raxml_only_msasize_200_best = df_raxml_only_msasize_200.
 ↪query('likelihood_type == "BEST"')
build_stats(df_raxml_only_msasize_200_best)
```

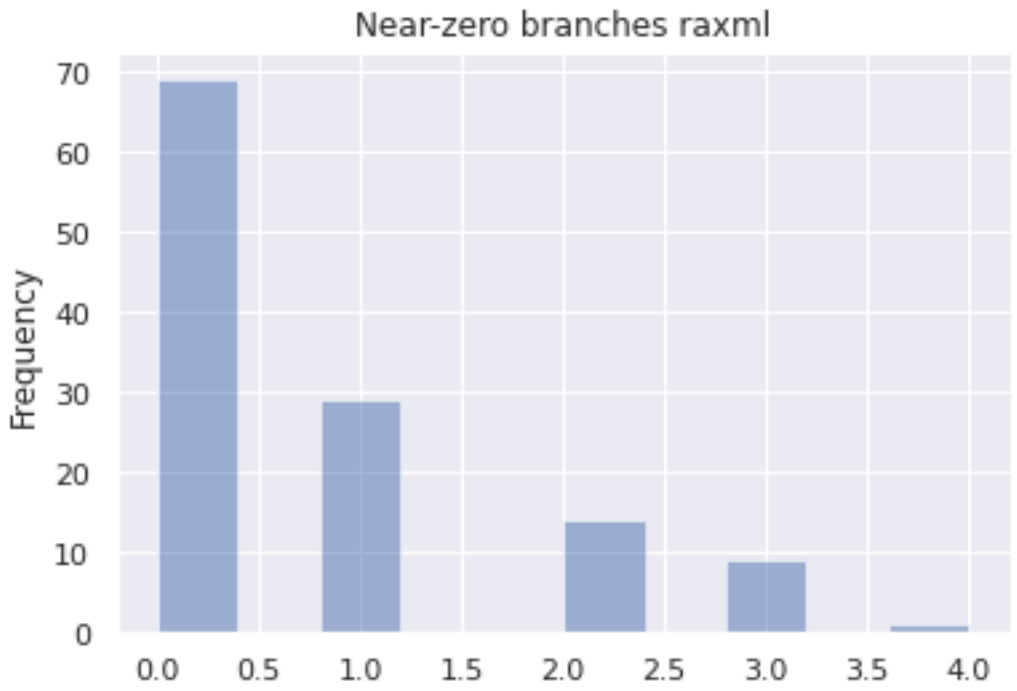
```
Inferred BIC better or equal: 85
Inferred BIC worse: 37

Inferred n_reticulations less: 94
Inferred n_reticulations equal: 28
Inferred n_reticulations more: 0
```

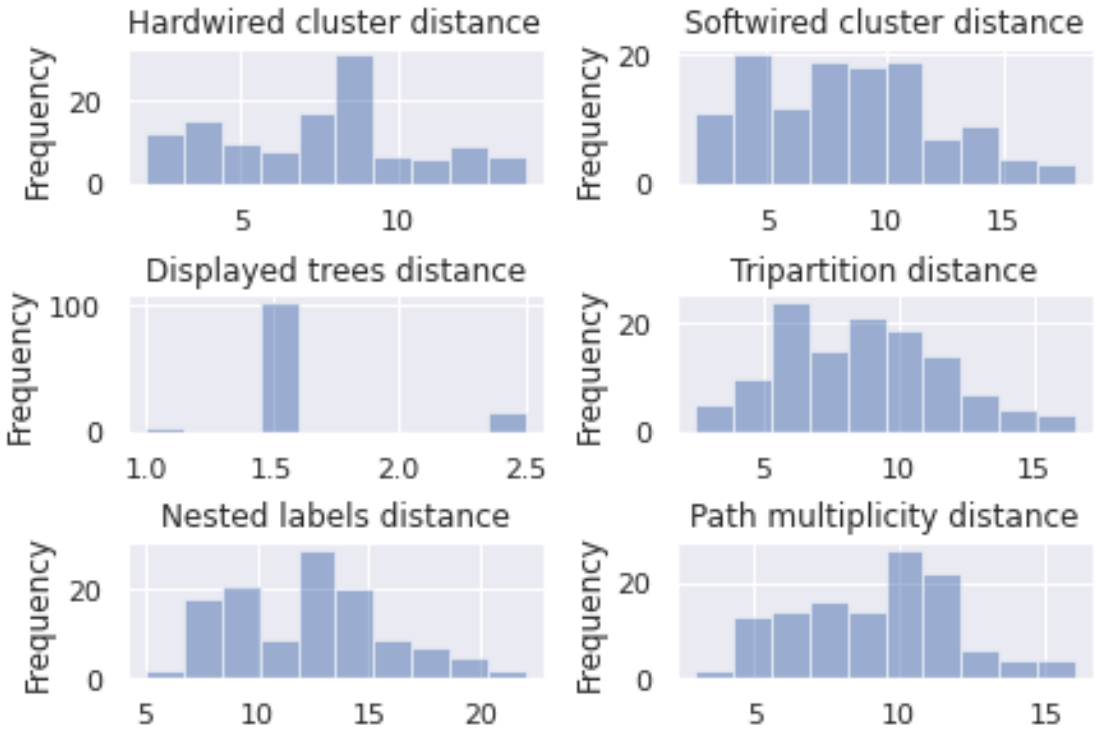
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2 Plots for starting with 5 random, 5 parsimony trees

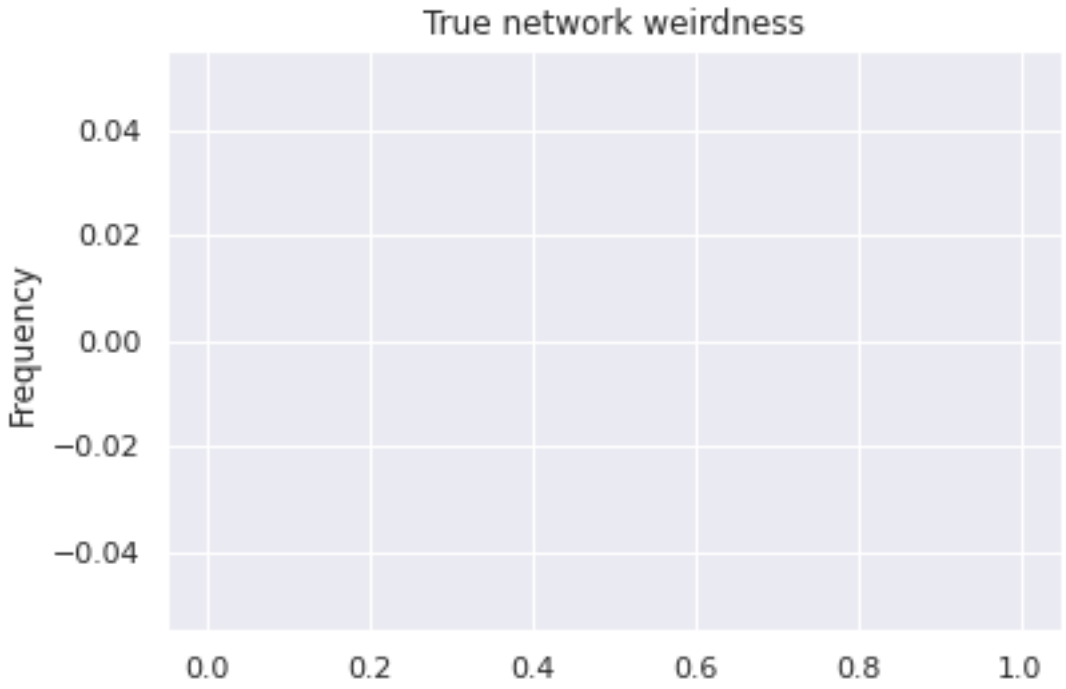
[14]:
```
df_random = df.query('start_type == "RANDOM"')
build_stats(df_random)
```

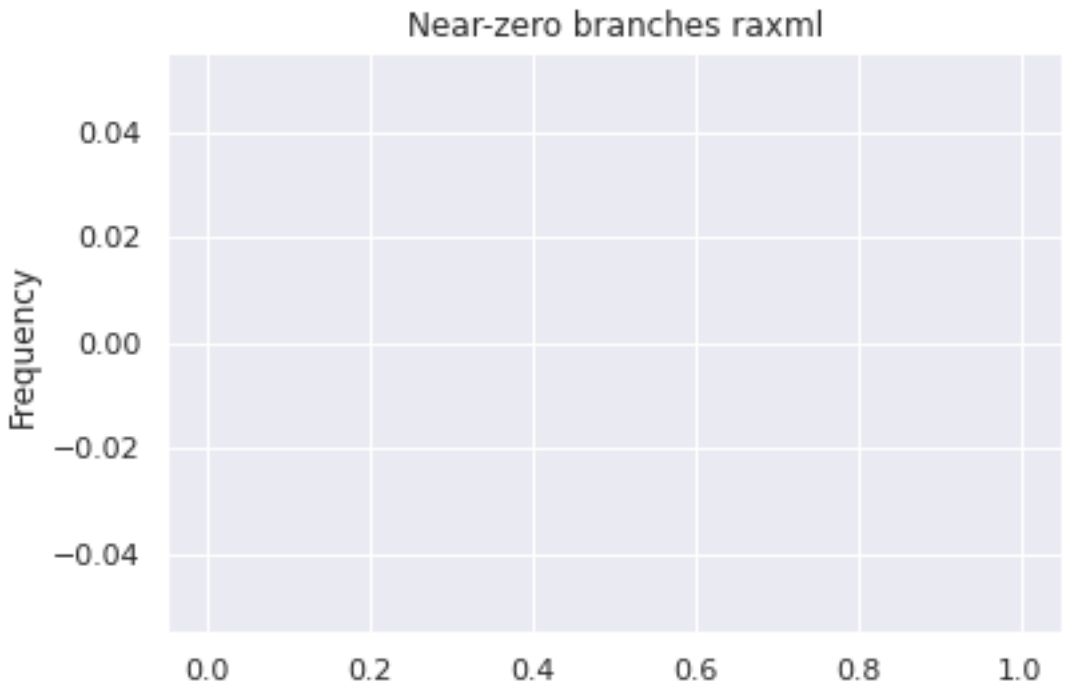
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

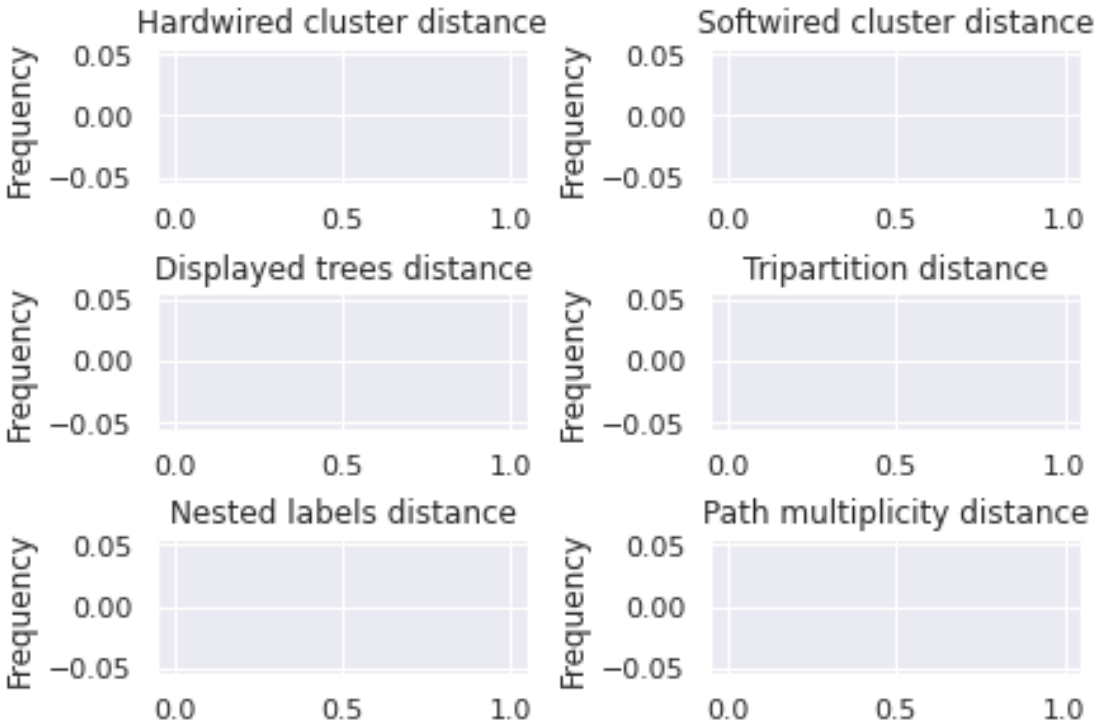
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.1 Plots for MSA_size ~ 100*n_trees

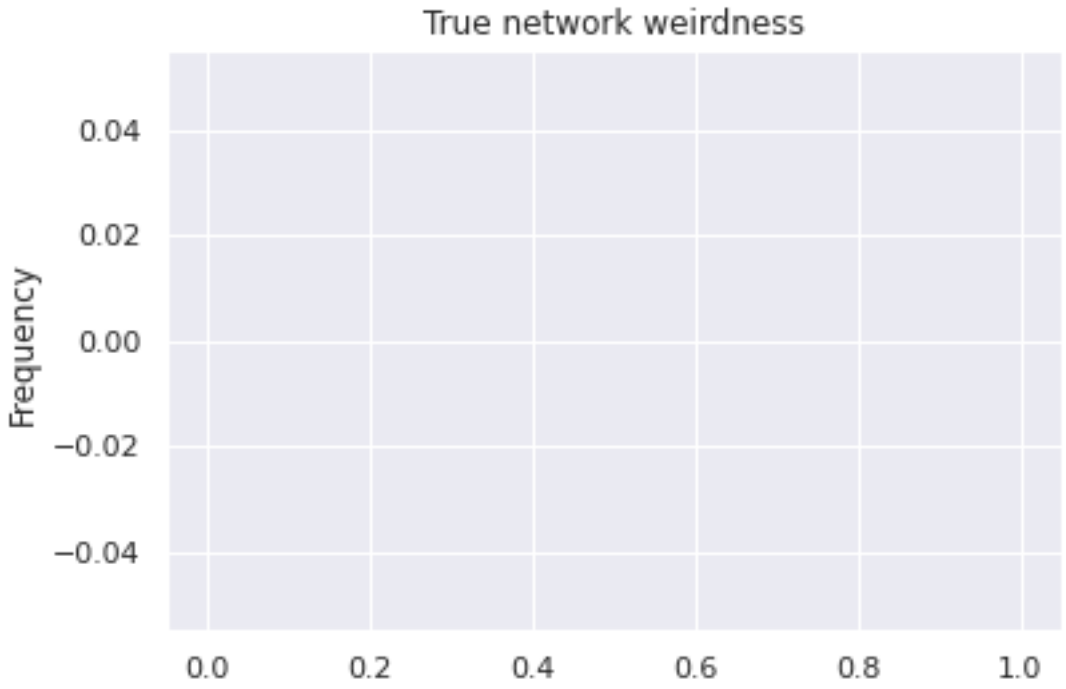
[15]:
```
df_random_msasize_100 = df_random.query('msa_size == 100')
build_stats(df_random_msasize_100)
```

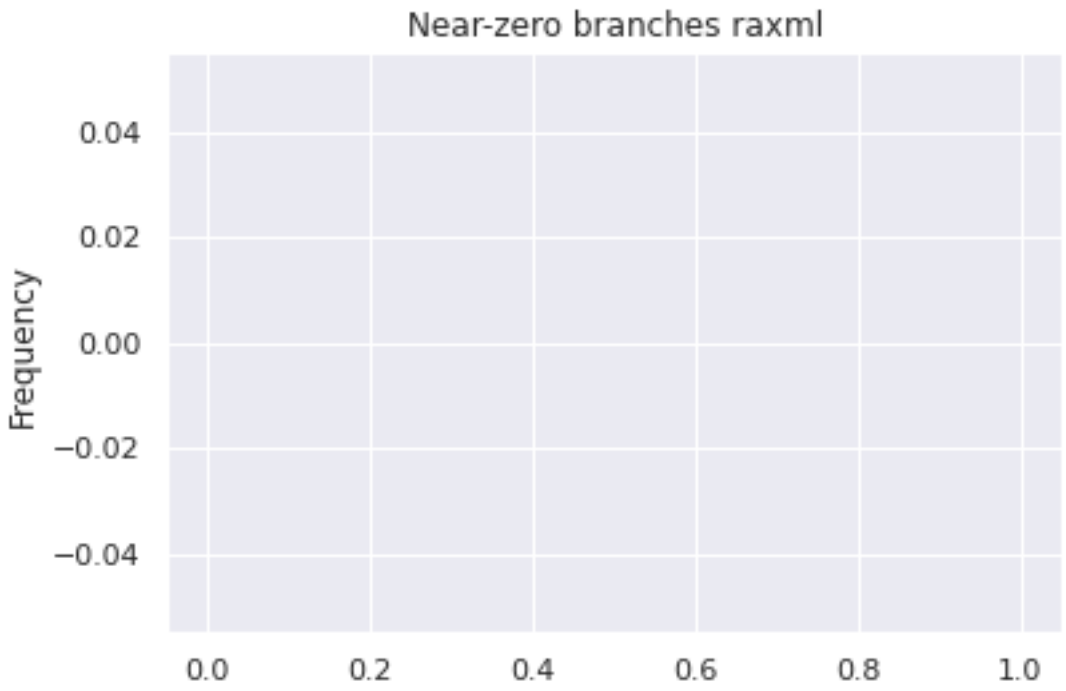
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

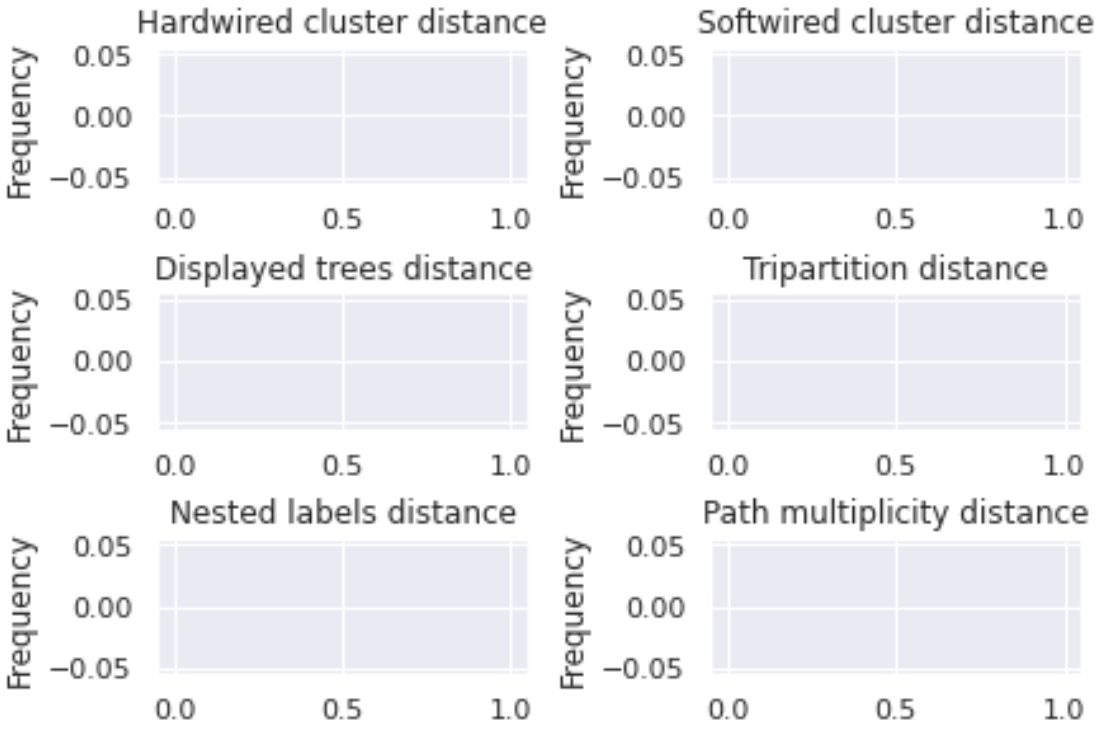
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.1.1 Plots for LikelihodType.AVERAGE

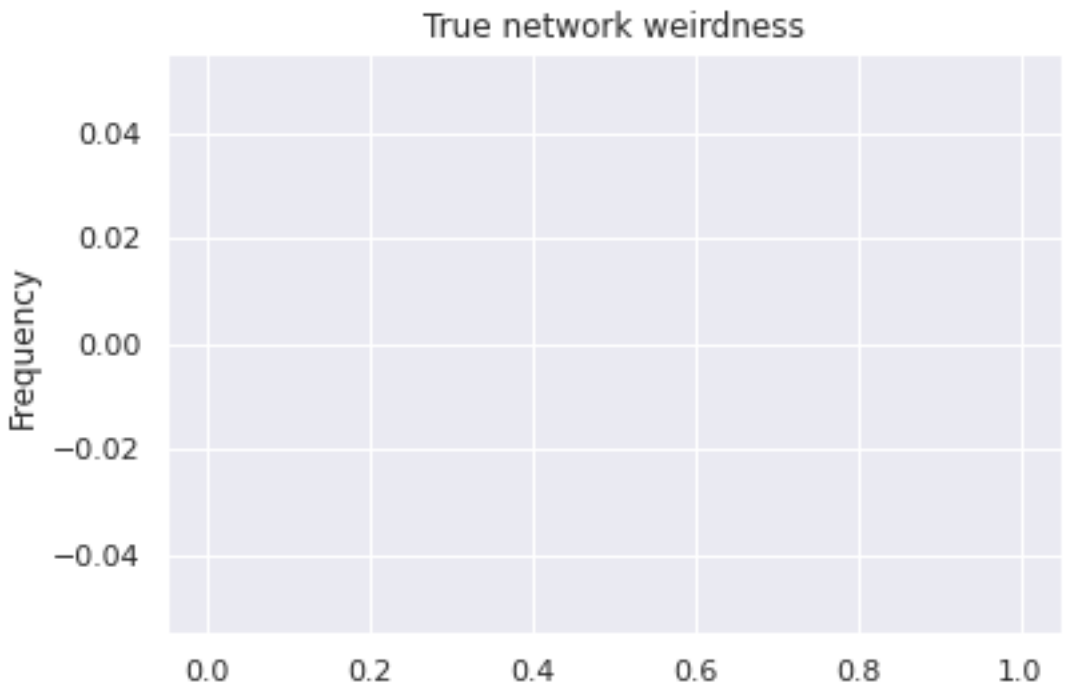
[16]:
```
df_random_msasize_100_average = df_random_msasize_100.query('likelihood_type ==␣
↪"AVERAGE"')
build_stats(df_random_msasize_100_average)
```

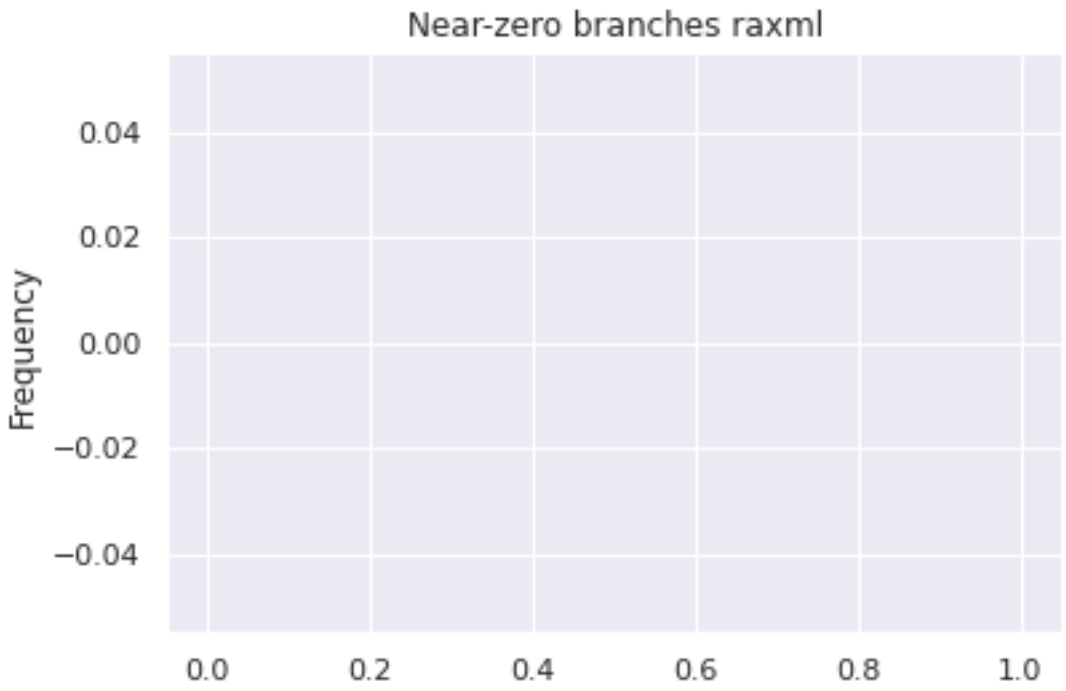
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

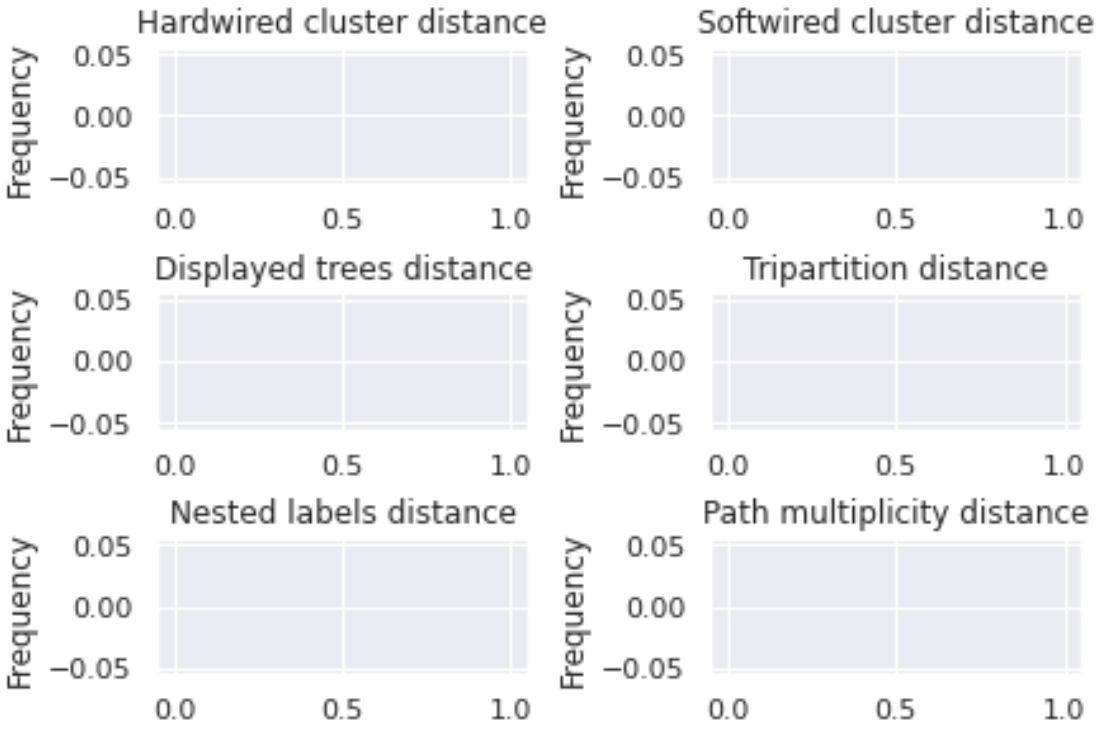
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.1.2 Plots for LikelihoodType.BEST

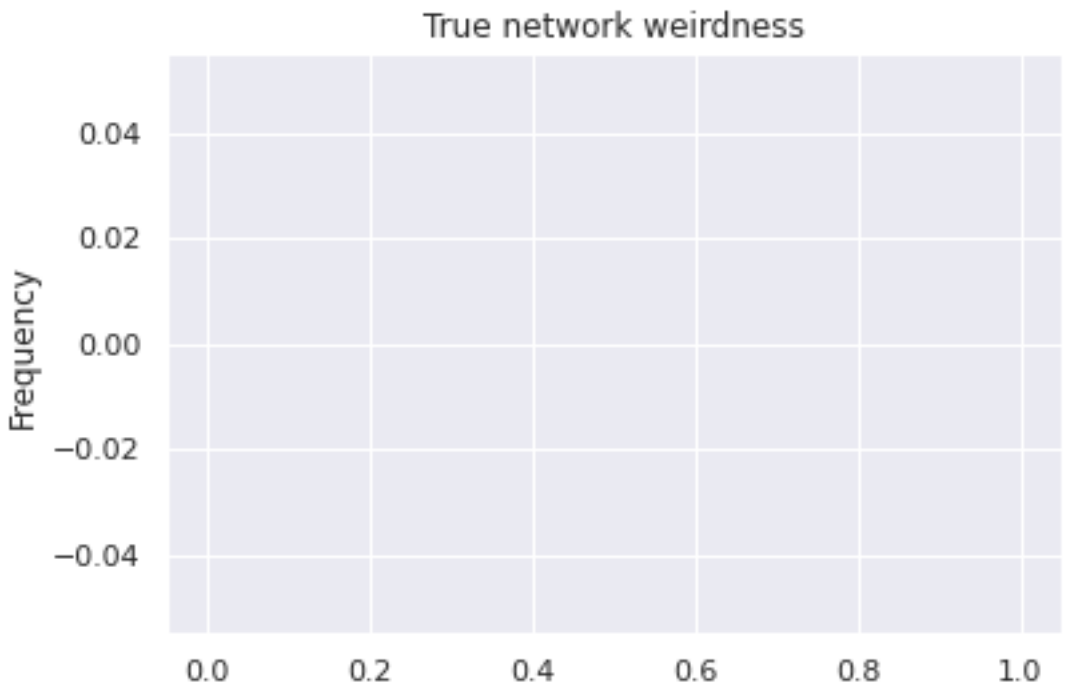
[17]:
```
df_random_msasize_100_best = df_random_msasize_100.query('likelihood_type ==␣
↪"BEST"')
build_stats(df_random_msasize_100_best)
```

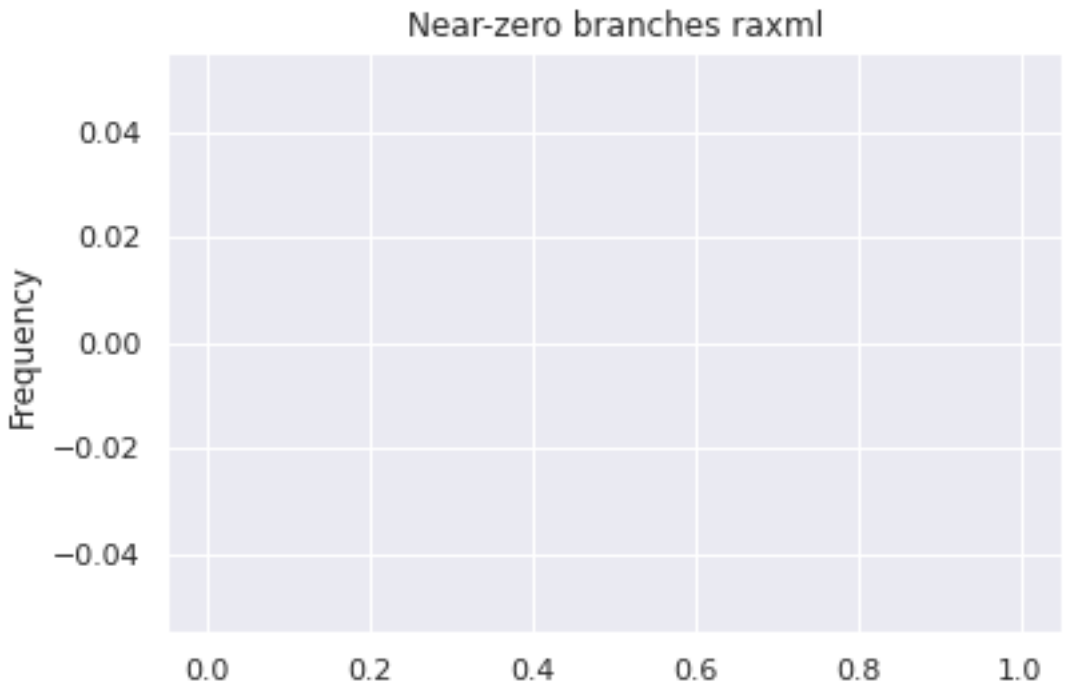
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

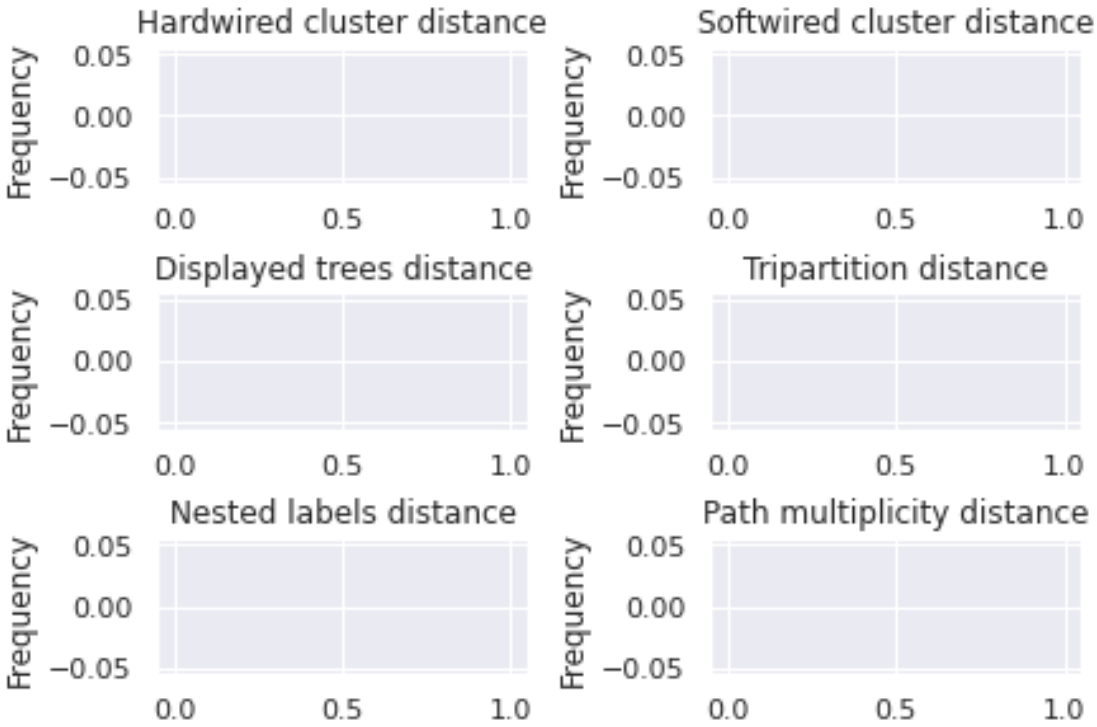
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.2 Plots for MSA_size ~ 200*n_trees

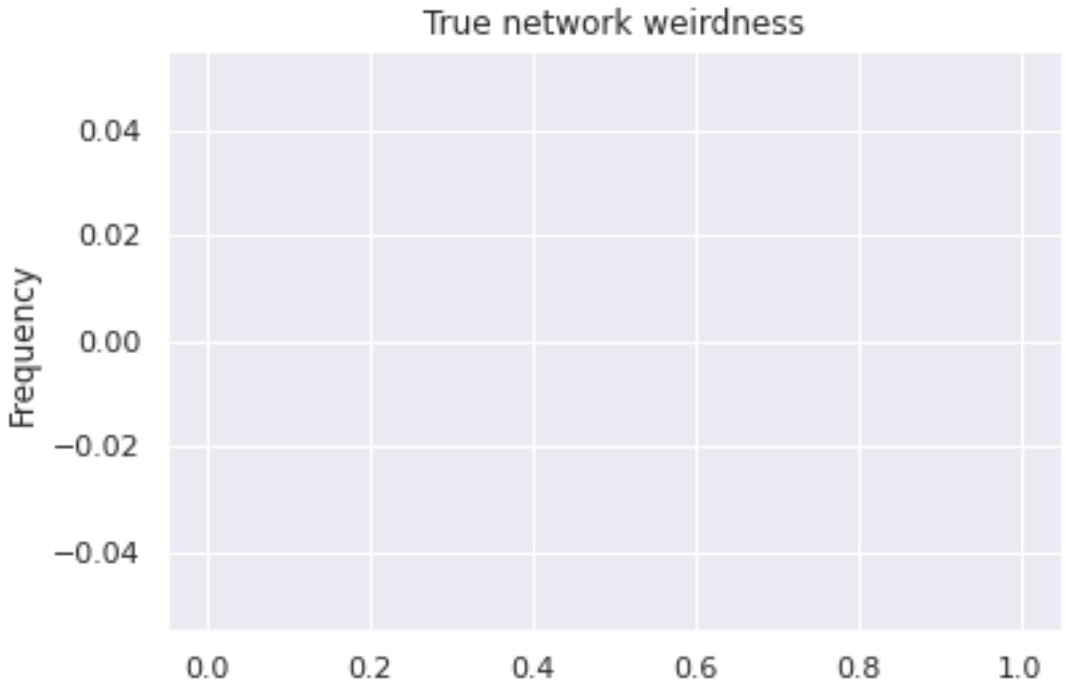
[18]:
```
df_random_msasize_200 = df_random.query('msa_size == 200')
build_stats(df_random_msasize_200)
```

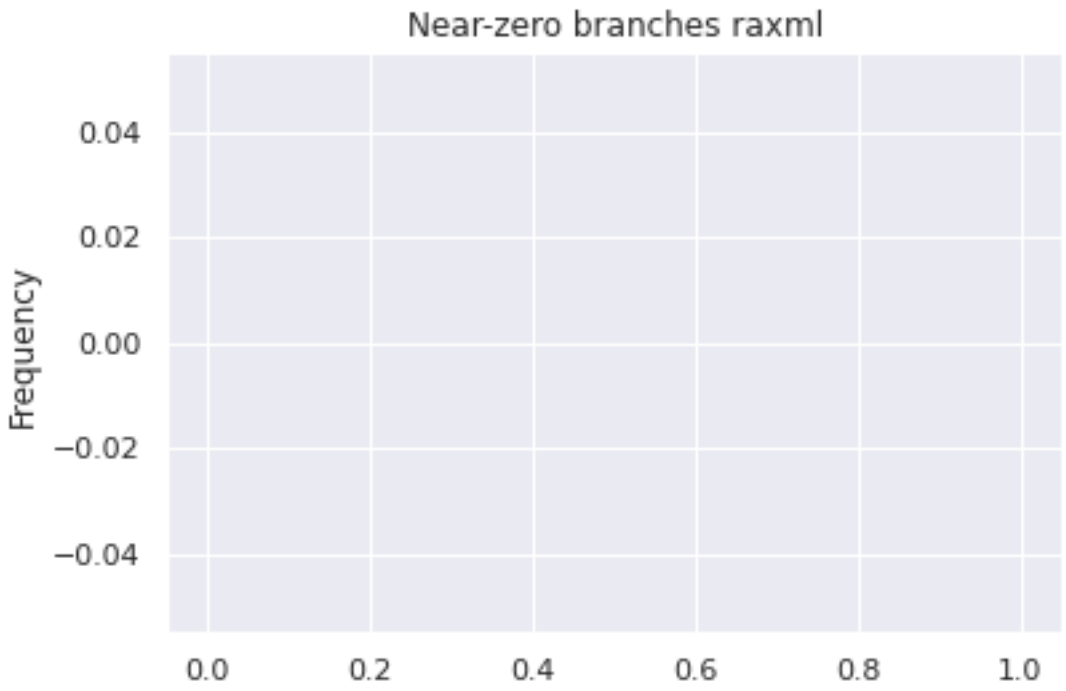
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

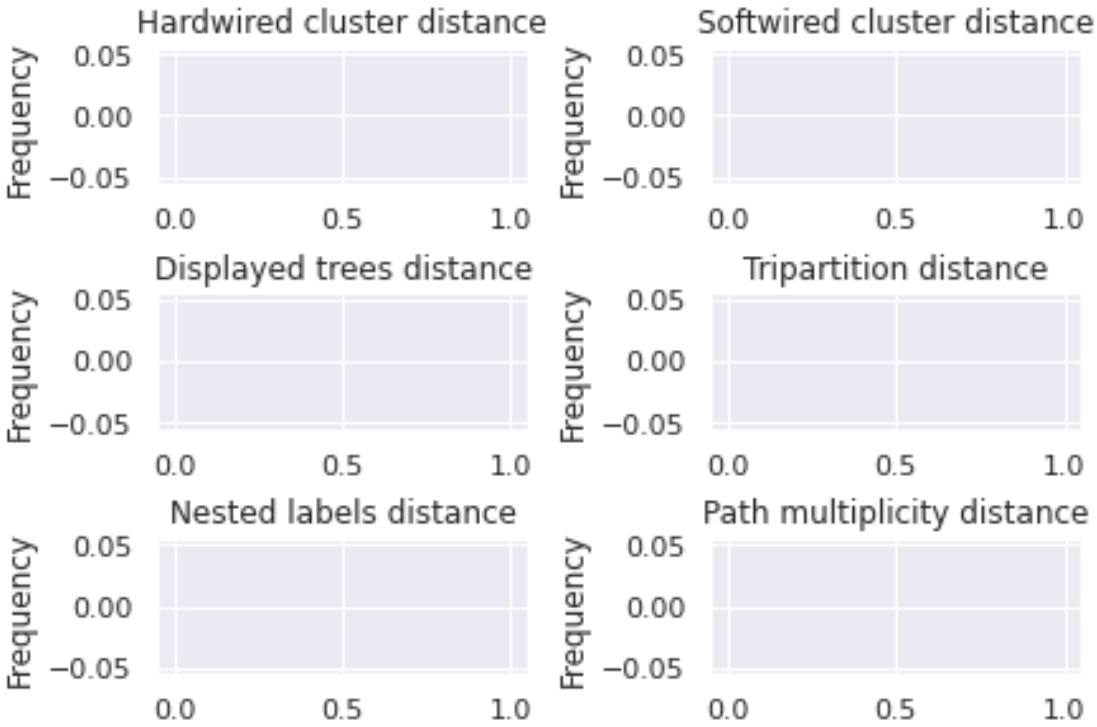
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.2.1 Plots for LikelihodType.AVERAGE

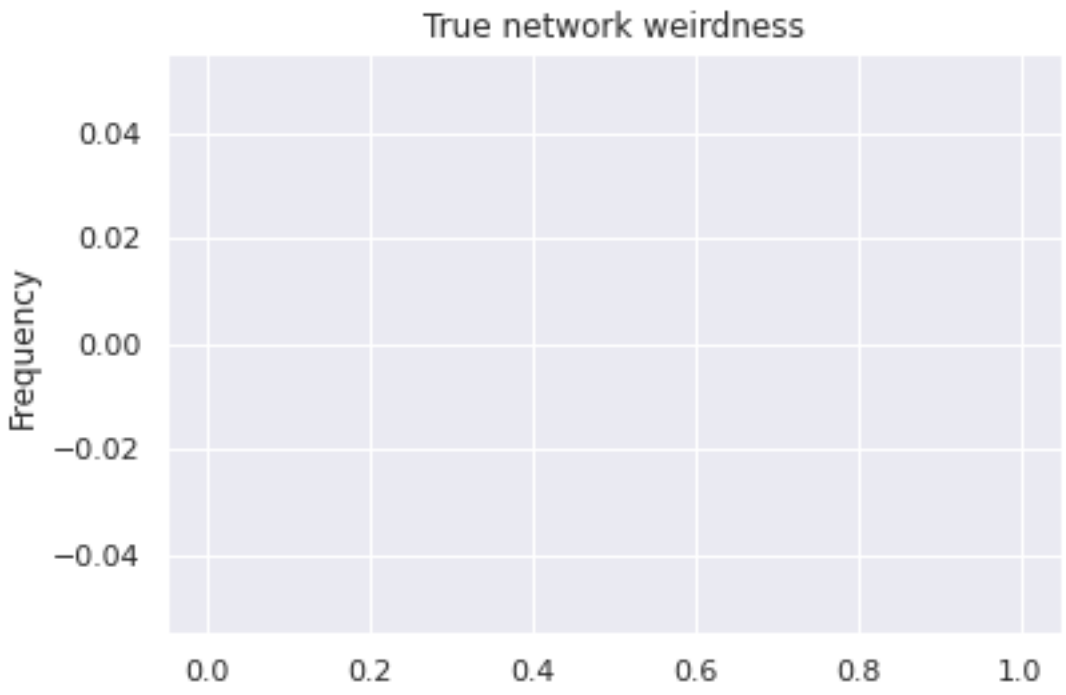
[19]:
```
df_random_msasize_200_average = df_random_msasize_200.query('likelihood_type ==␣
↪"AVERAGE"')
build_stats(df_random_msasize_200_average)
```

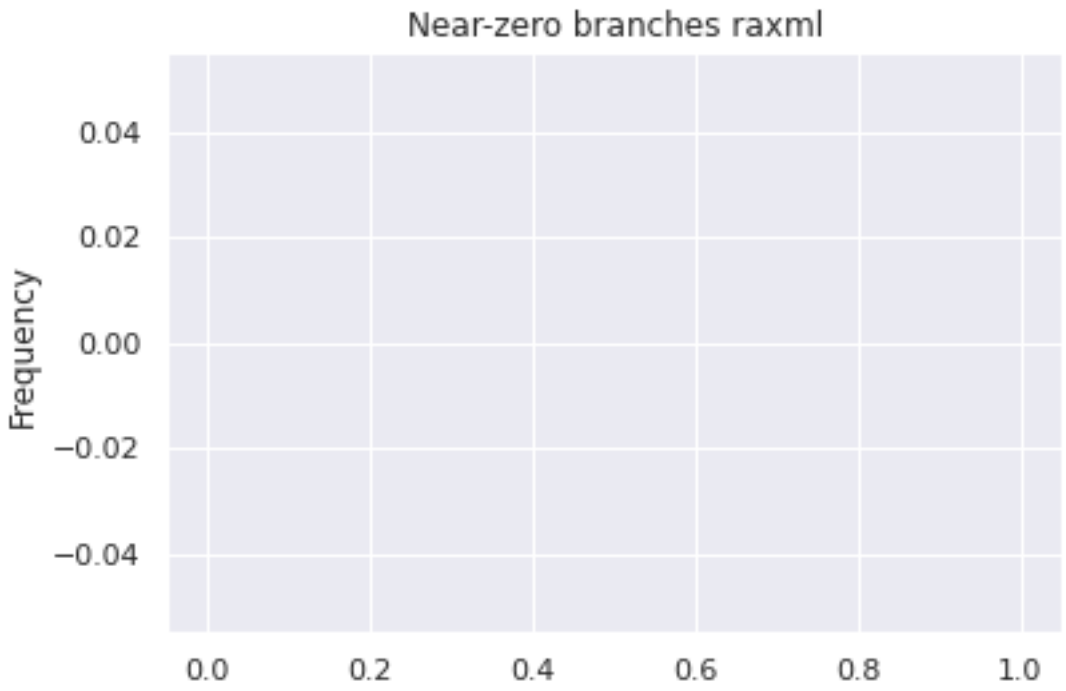
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

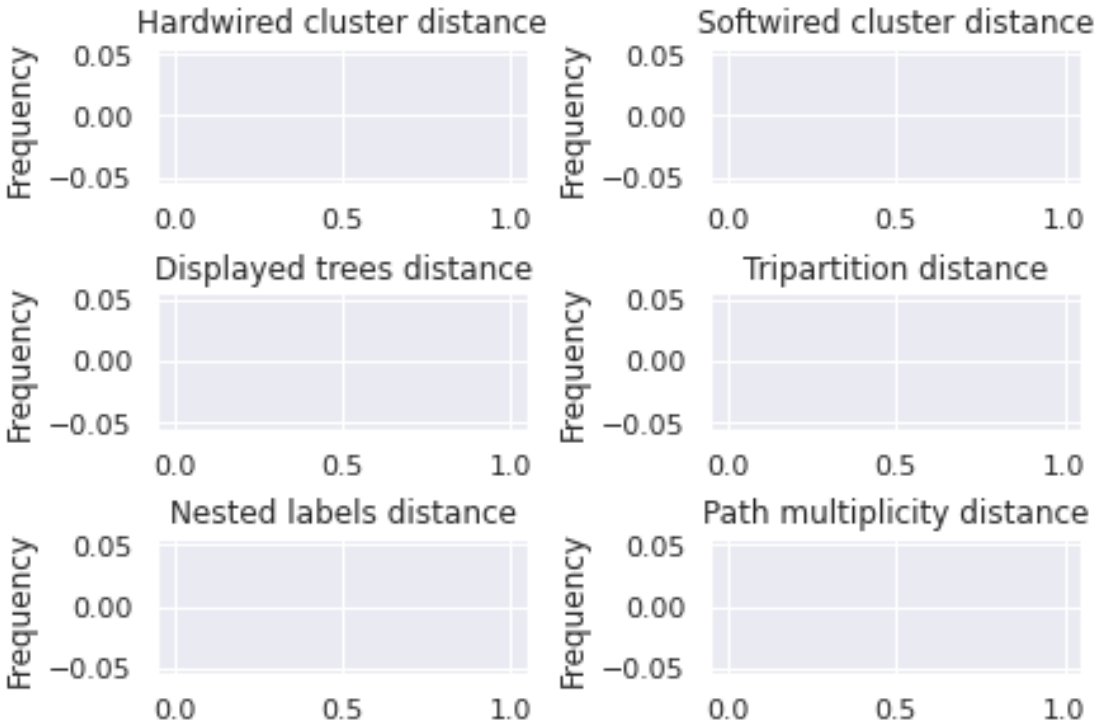
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



2.2.2 Plots for LikelihoodType.BEST

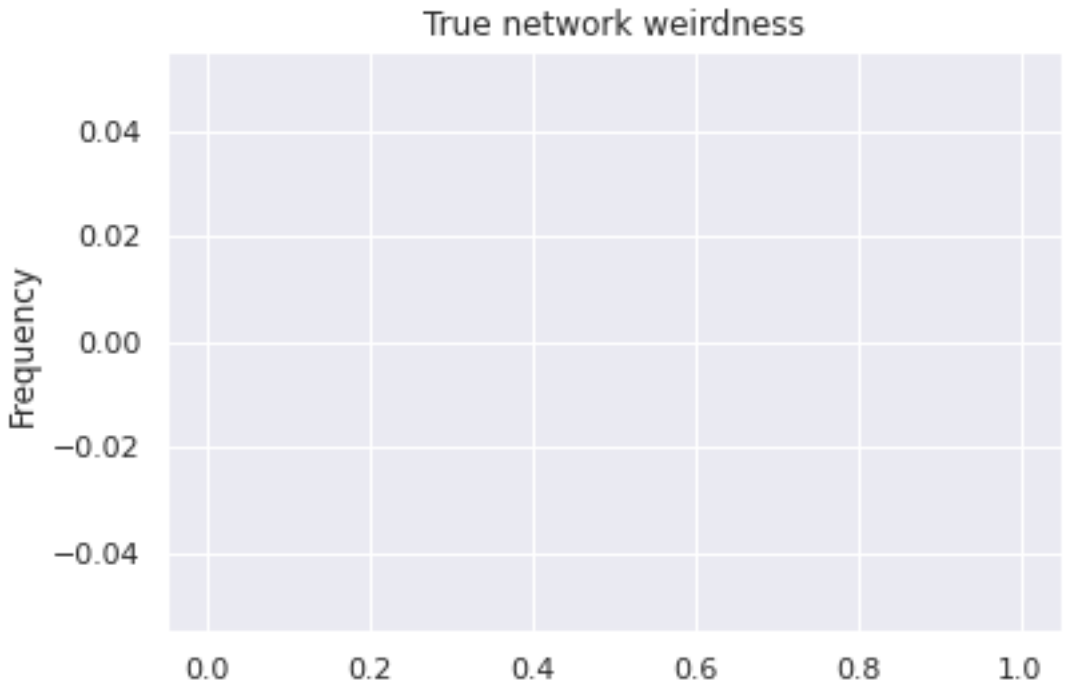
[20]:
```
df_random_msasize_200_best = df_random_msasize_200.query('likelihood_type ==␣
↪"BEST"')
build_stats(df_random_msasize_200_best)
```

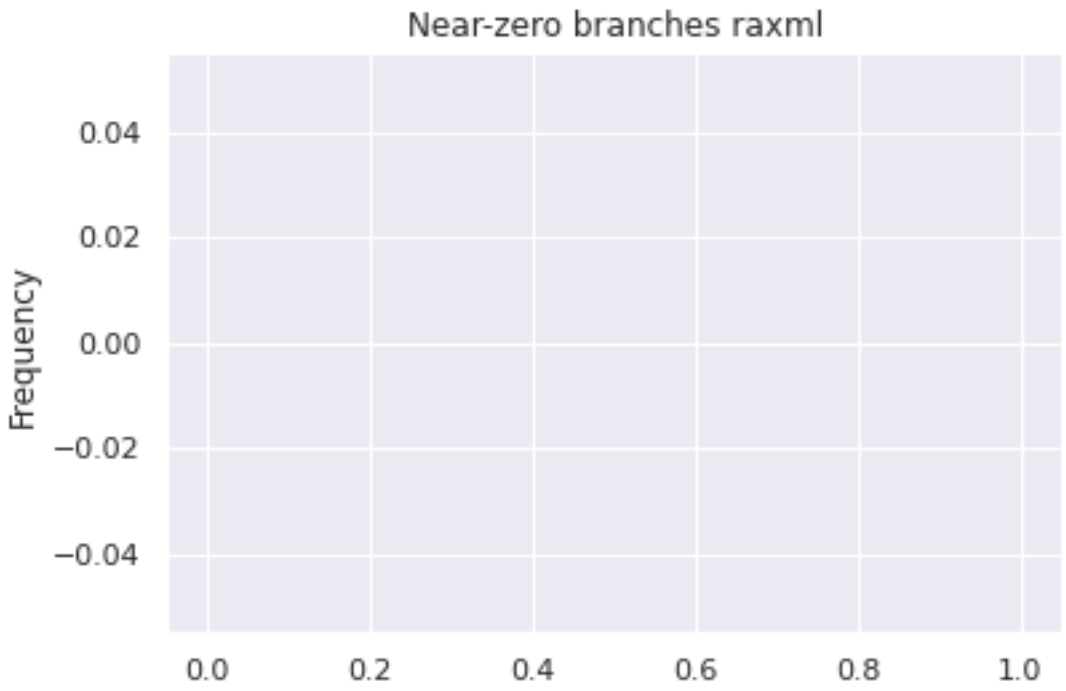
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

Inferred n_reticulations less: 0
Inferred n_reticulations equal: 0
Inferred n_reticulations more: 0
```

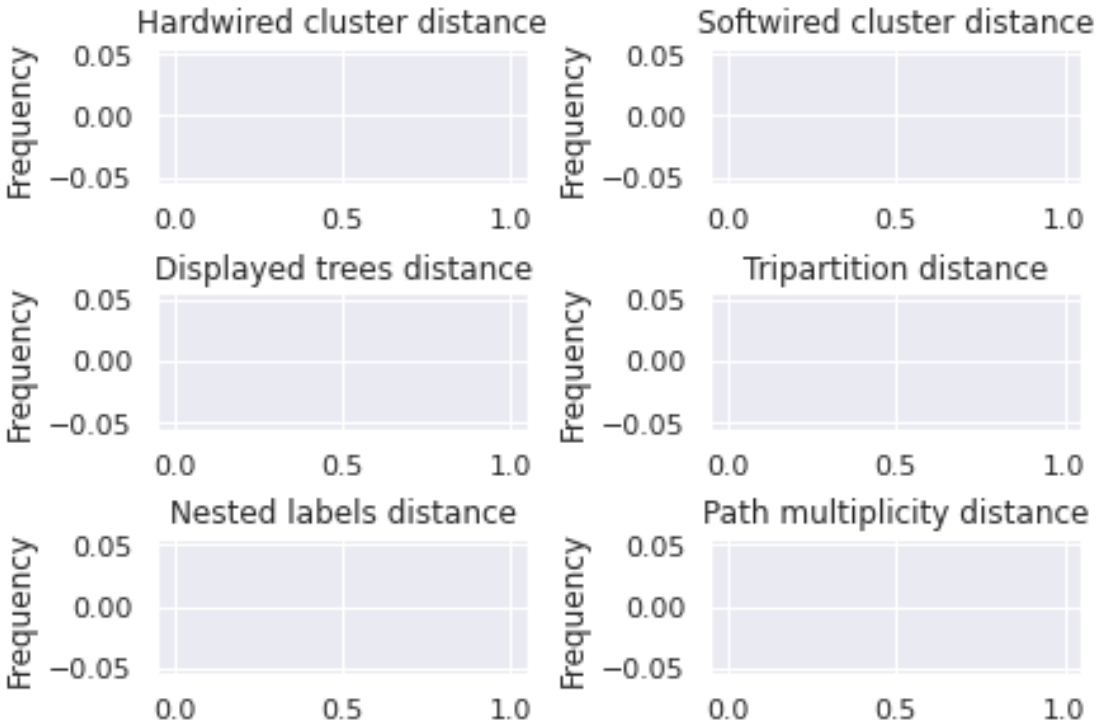
```
<Figure size 432x288 with 0 Axes>
```

```
<Figure size 432x288 with 0 Axes>
```





<Figure size 432x288 with 0 Axes>



[ ]: