NetRAX Experiment Evaluation

February 8, 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')
```

[4]:

```
pd.set_option('display.max_columns', None)
df.head()
```

[4]:

```
                                             name  n_taxa  n_trees  \
0  datasets_medium_network_norandom_0_0/0_22_taxa…      22        4
1  datasets_medium_network_norandom_0_0/0_22_taxa…      22        4
2  datasets_medium_network_norandom_0_0/0_22_taxa…      22        4
3  datasets_medium_network_norandom_0_0/0_22_taxa…      22        4
4  datasets_medium_network_norandom_0_1/0_17_taxa…      17        2

   n_reticulations  msa_size     sampling_type simulation_type  \
0                2       202  PERFECT_SAMPLING          CELINE
1                2       202  PERFECT_SAMPLING          CELINE
2                2       402  PERFECT_SAMPLING          CELINE
3                2       402  PERFECT_SAMPLING          CELINE
4                1       101  PERFECT_SAMPLING          CELINE

                                      celine_params  \
0  {'to': 0.16223186561955155| 'lambda': 21.49262…
```

```
1  {'to': 0.16223186561955155| 'lambda': 21.49262…
2  {'to': 0.16223186561955155| 'lambda': 21.49262…
3  {'to': 0.16223186561955155| 'lambda': 21.49262…
4  {'to': 0.10860342742632532| 'lambda': 21.35962…

                    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                         4

   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_0_0/0_22_taxa…
1  datasets_medium_network_norandom_0_0/0_22_taxa…
2  datasets_medium_network_norandom_0_0/0_22_taxa…
3  datasets_medium_network_norandom_0_0/0_22_taxa…
4  datasets_medium_network_norandom_0_1/0_17_taxa…

                               inferred_network_path likelihood_type  \
0  datasets_medium_network_norandom_0_0/0_22_taxa…         AVERAGE
1  datasets_medium_network_norandom_0_0/0_22_taxa…            BEST
2  datasets_medium_network_norandom_0_0/0_22_taxa…         AVERAGE
3  datasets_medium_network_norandom_0_0/0_22_taxa…            BEST
4  datasets_medium_network_norandom_0_1/0_17_taxa…         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           6334.250                         0
1                           0           1150.248                         0
2                           0           3626.096                         0
3                           0            869.273                         0
4                           0           4660.722                         1
```

```
      bic_true    logl_true  bic_inferred  logl_inferred    bic_raxml  \
0  3357.579938 -1317.619632   3291.448158   -1318.150983  3291.448158
1  3358.780892 -1318.220110   3291.448158   -1318.150983  3291.448158
2  6259.305638 -2738.890554   6238.391973   -2764.783699  6238.401624
3  6260.156175 -2739.315822   6238.391973   -2764.783699  6238.401624
4  1171.233082  -384.511527   1162.979859    -380.384915  1165.501221

    logl_raxml  hardwired_cluster_distance  softwired_cluster_distance  \
0 -1318.150983                         7.0                         5.0
1 -1318.150983                         7.0                         5.0
2 -2764.788525                         7.0                         6.0
3 -2764.788525                         7.0                         6.0
4  -396.542264                        12.0                        14.5

   displayed_trees_distance  tripartition_distance  nested_labels_distance  \
0                       2.5                    9.0                    14.0
1                       2.5                    9.0                    14.0
2                       2.5                    9.0                    12.0
3                       2.5                    9.0                    12.0
4                       1.5                   11.0                    14.0

   path_multiplicity_distance
0                        11.5
1                        11.5
2                         9.5
3                         9.5
4                        11.5
```

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

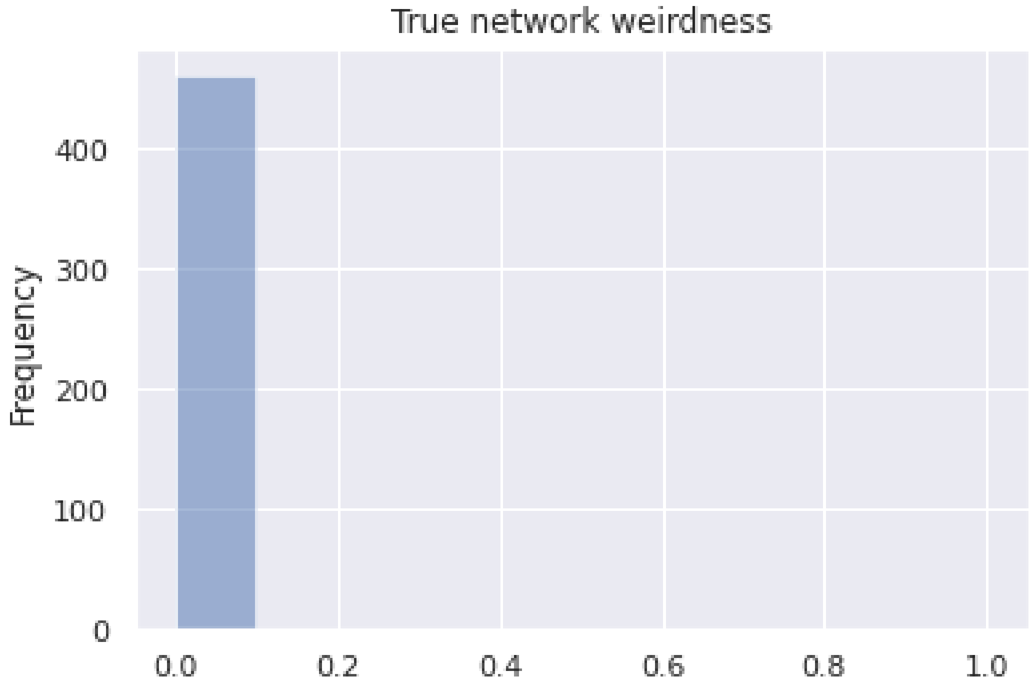
[5]:
```
Index(['name', 'n_taxa', 'n_trees', 'n_reticulations', 'msa_size',
       'sampling_type', 'simulation_type', 'celine_params', 'seqgen_params',
       'near_zero_branches_raxml', 'n_equal_tree_pairs',
       'true_network_weirdness', 'true_network_path', 'inferred_network_path',
       'likelihood_type', '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',
       'hardwired_cluster_distance', 'softwired_cluster_distance',
       'displayed_trees_distance', 'tripartition_distance',
       'nested_labels_distance', 'path_multiplicity_distance'],
      dtype='object')
```

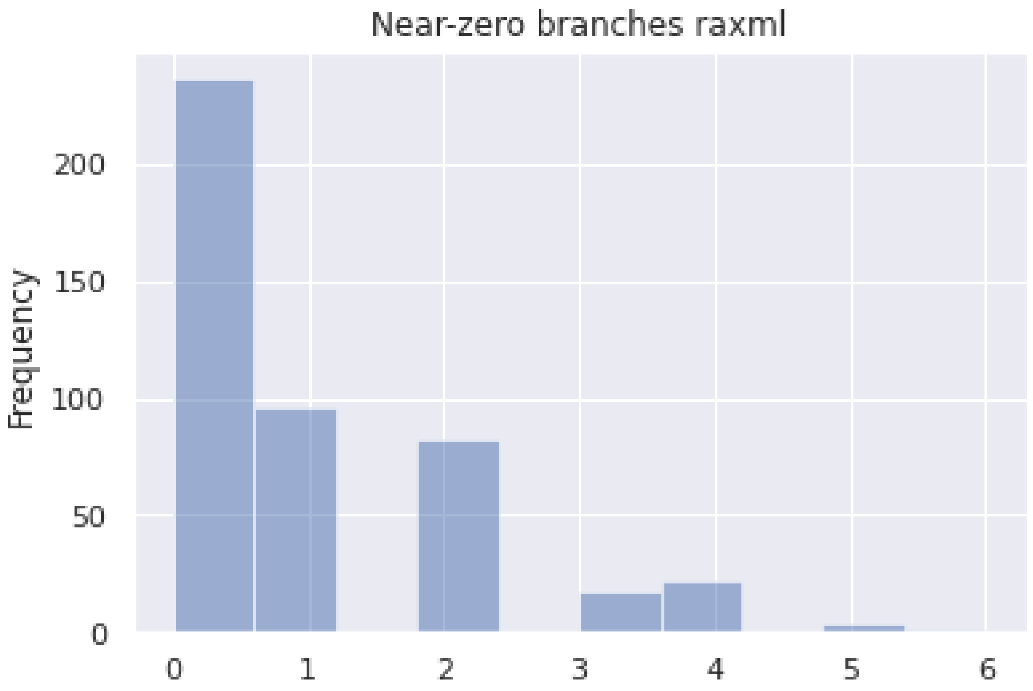
[6]:
```
build_stats(df)
```

```
Inferred BIC better or equal: 415
Inferred BIC worse: 45
Inferred n_reticulations less: 413
Inferred n_reticulations equal: 47
Inferred n_reticulations more: 0
```

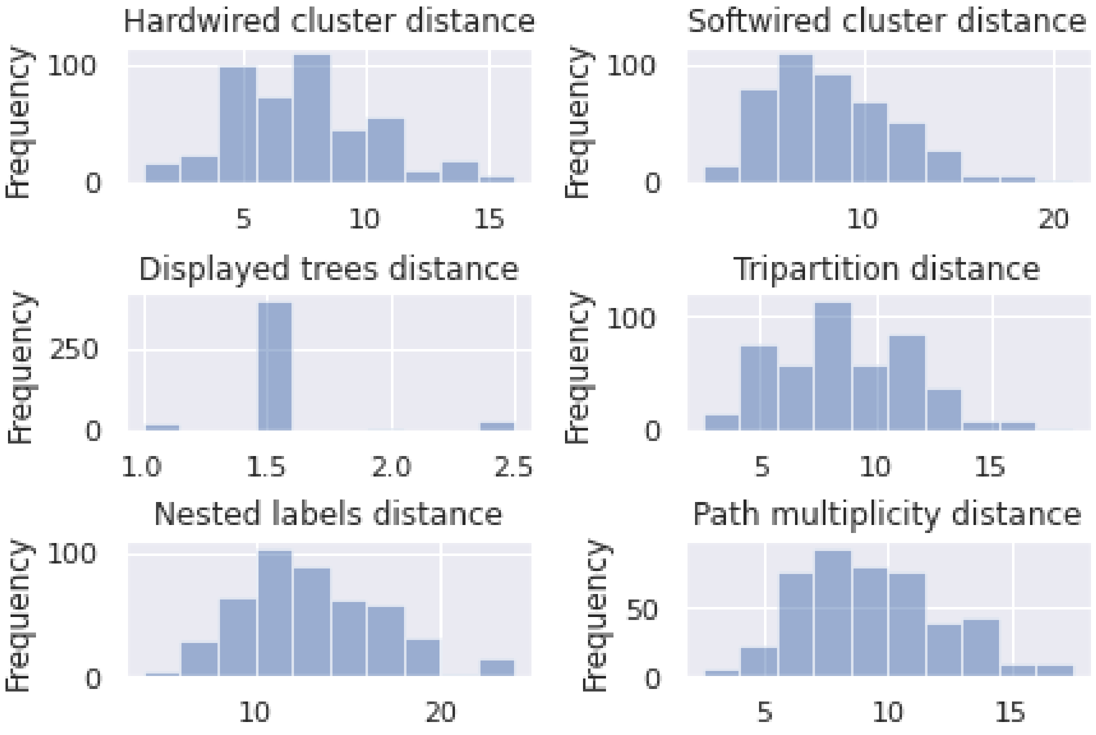
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
50
100
150
200
0
1
2
3
4
5
6

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


Hardwired cluster distance
Frequency
100
0
5
10
15
Softwired cluster distance
Frequency
100
0
10
20
Displayed trees distance
Frequency
250
0
1.0
1.5
2.0
2.5
Tripartition distance
Frequency
100
0
5
10
15
Nested labels distance
Frequency
100
0
10
20
Path multiplicity distance
Frequency
50
0
5
10
15

1 Plots for starting with raxml-ng best tree only

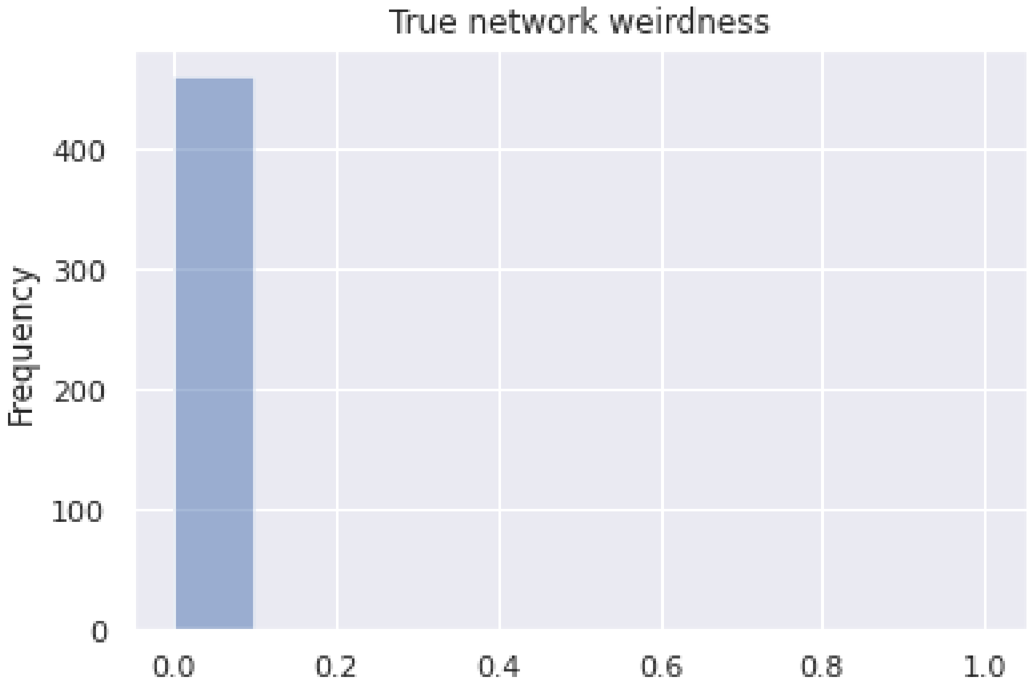
```
[7]: df_raxml_only = df.query('start_type == "FROM_RAXML"')
     build_stats(df_raxml_only)
```

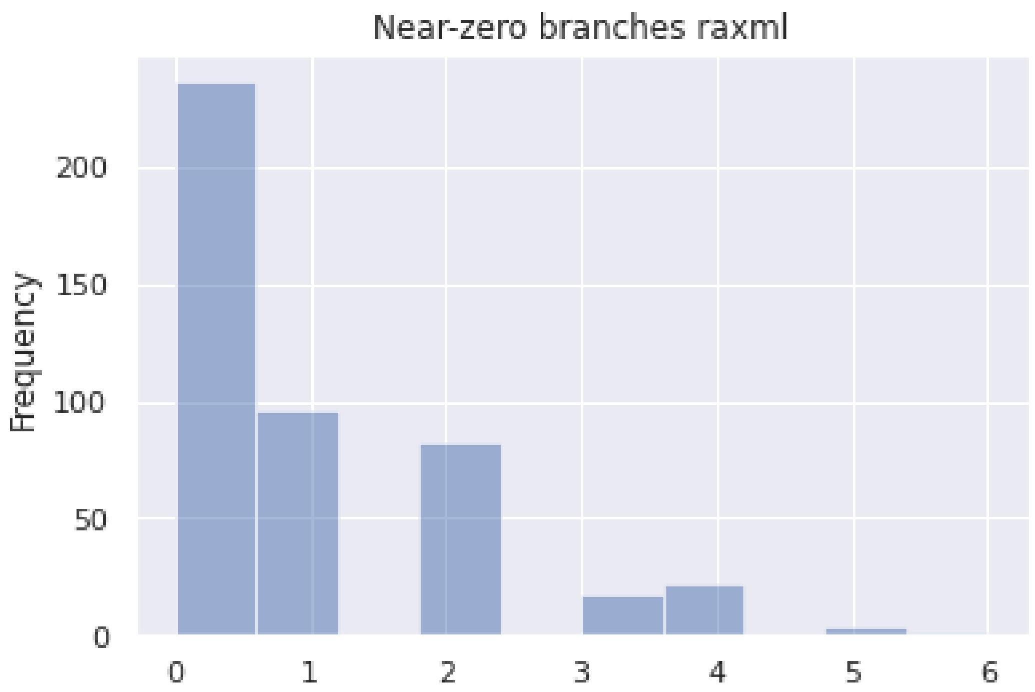
```
Inferred BIC better or equal: 415
Inferred BIC worse: 45

Inferred n_reticulations less: 413
Inferred n_reticulations equal: 47
Inferred n_reticulations more: 0
```

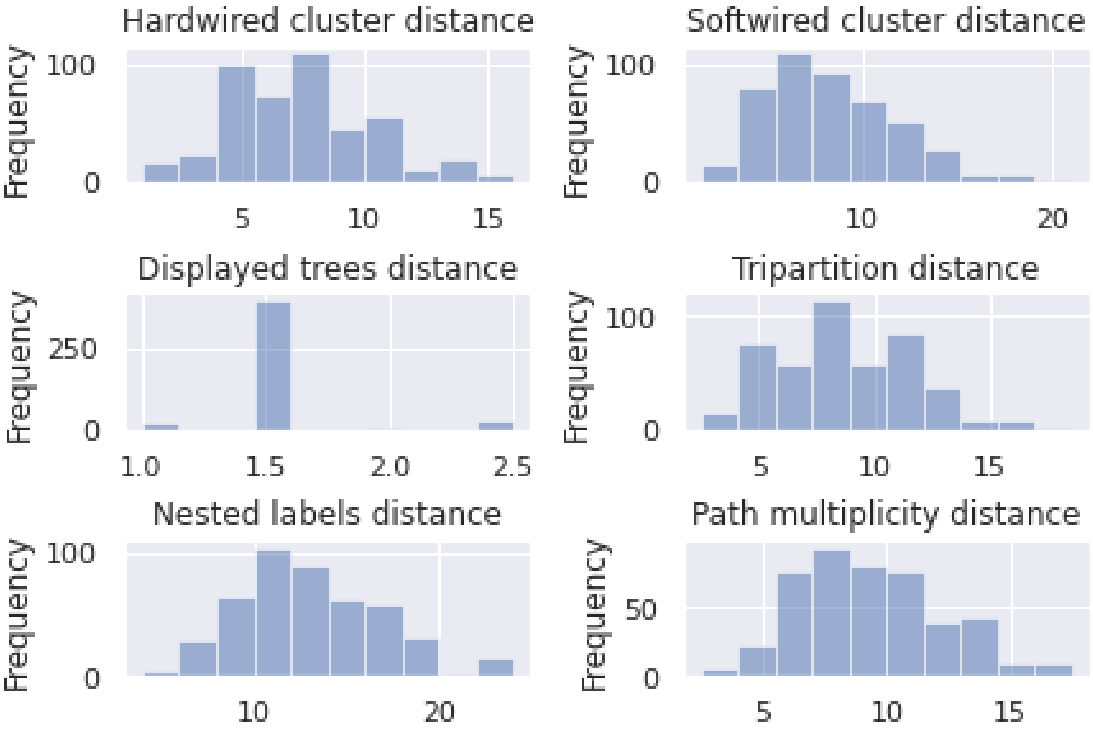
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
50
100
150
200
0
1
2
3
4
5
6

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


Hardwired cluster distance
Frequency
100
0
5
10
15
Softwired cluster distance
Frequency
100
0
10
20
Displayed trees distance
Frequency
250
0
1.0
1.5
2.0
2.5
Tripartition distance
Frequency
100
0
5
10
15
Nested labels distance
Frequency
100
0
10
20
Path multiplicity distance
Frequency
50
0
5
10
15

1.1 Plots for MSA_size ~ 100*n_trees

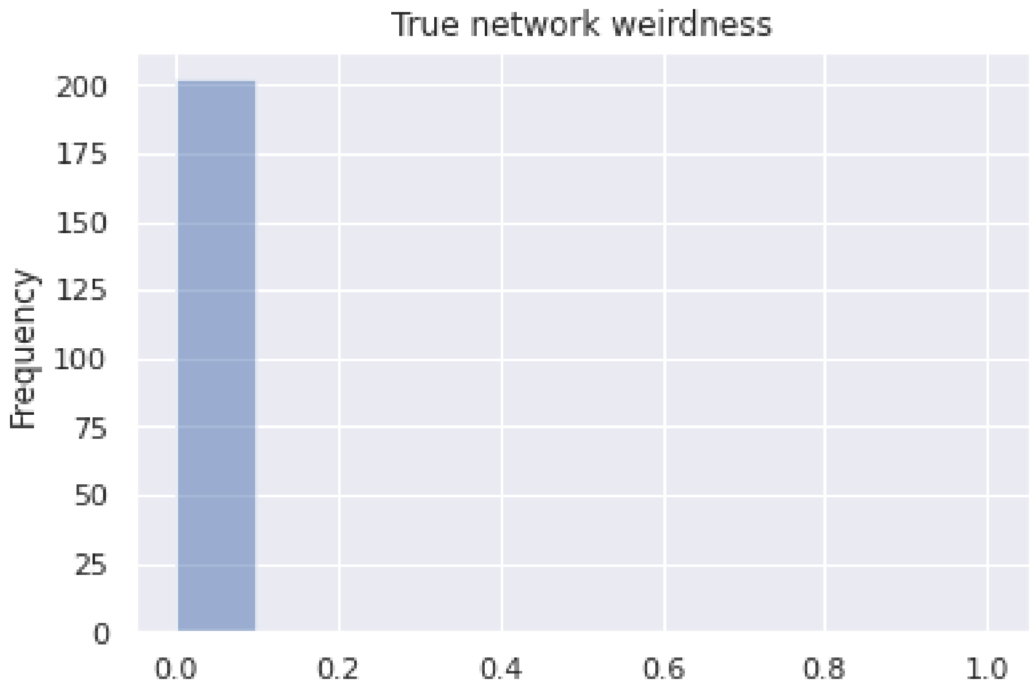
[8]:
```
df_raxml_only_msasize_100 = df_raxml_only.query('msa_size == 101')
build_stats(df_raxml_only_msasize_100)
```

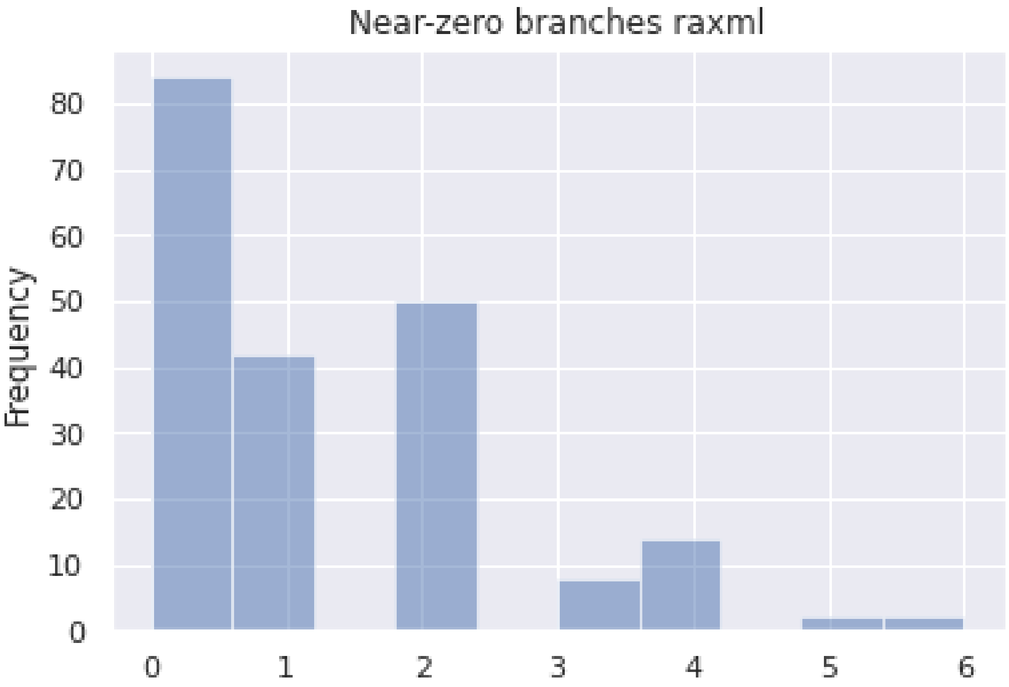
```
Inferred BIC better or equal: 193
Inferred BIC worse: 9

Inferred n_reticulations less: 182
Inferred n_reticulations equal: 20
Inferred n_reticulations more: 0
```

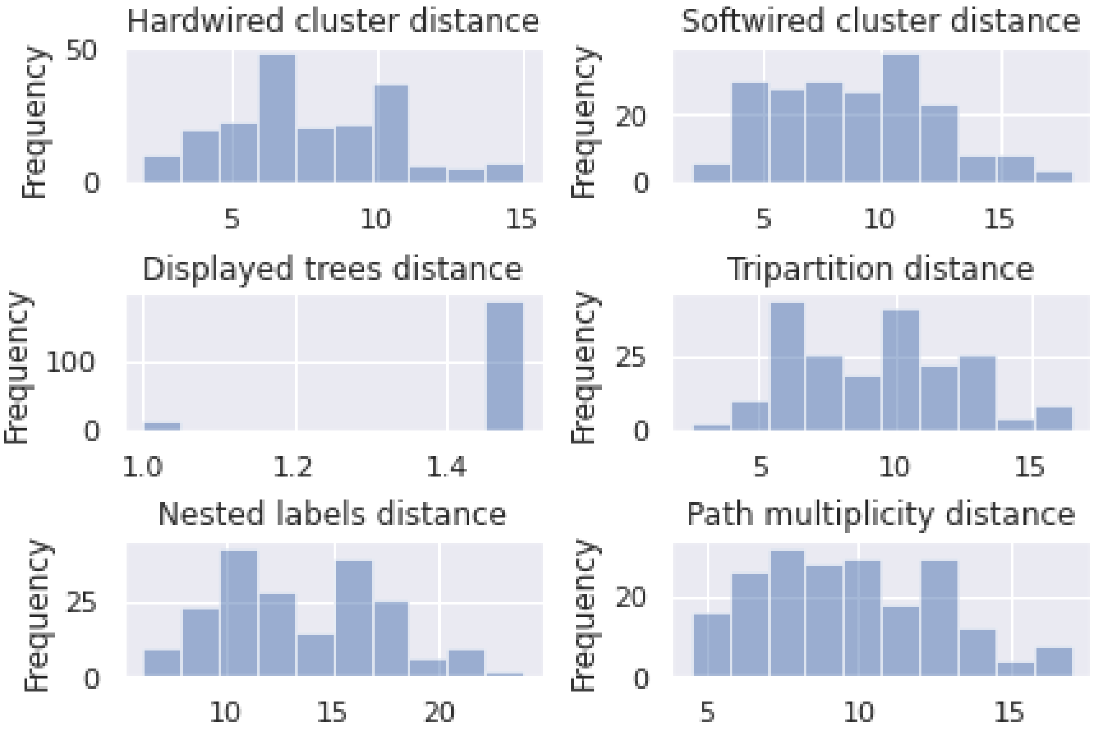
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
10
20
30
40
50
60
70
80
0
1
2
3
4
5
6

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


Hardwired cluster distance
Frequency
50
0
5
10
15
Softwired cluster distance
Frequency
20
0
5
10
15
Displayed trees distance
Frequency
100
0
1.0
1.2
1.4
Tripartition distance
Frequency
25
0
5
10
15
Nested labels distance
Frequency
25
0
10
15
20
Path multiplicity distance
Frequency
20
0
5
10
15

1.1.1 Plots for LikelihodType.AVERAGE

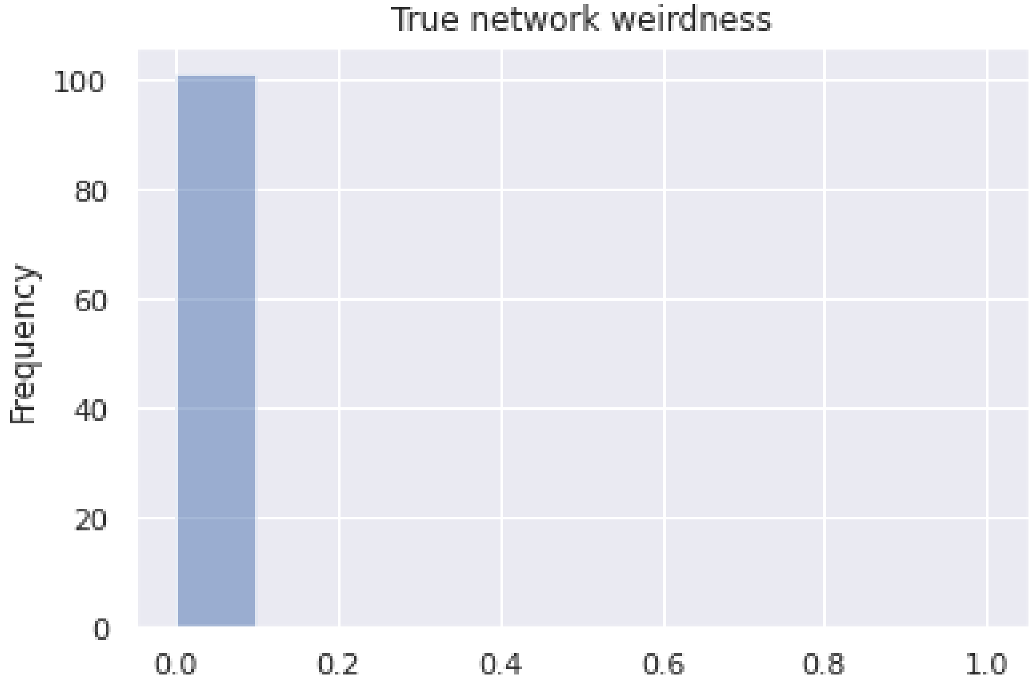
```
[9]: df_raxml_only_msasize_100_average = df_raxml_only_msasize_100.
      ↪query('likelihood_type == "AVERAGE"')
     build_stats(df_raxml_only_msasize_100_average)
```

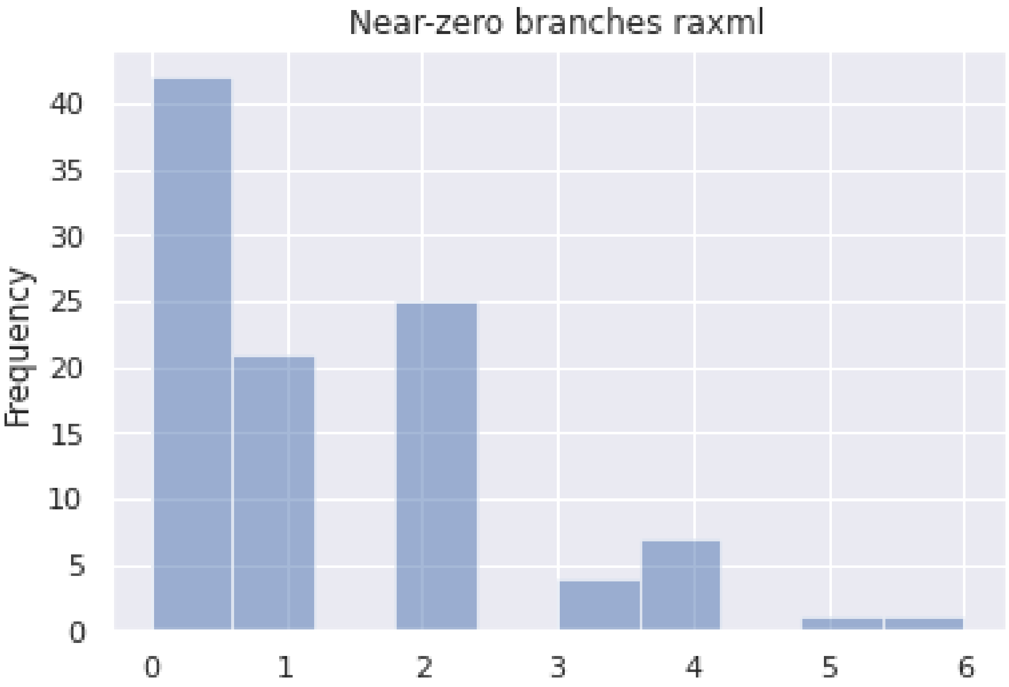
```
Inferred BIC better or equal: 97
Inferred BIC worse: 4

Inferred n_reticulations less: 91
Inferred n_reticulations equal: 10
Inferred n_reticulations more: 0
```

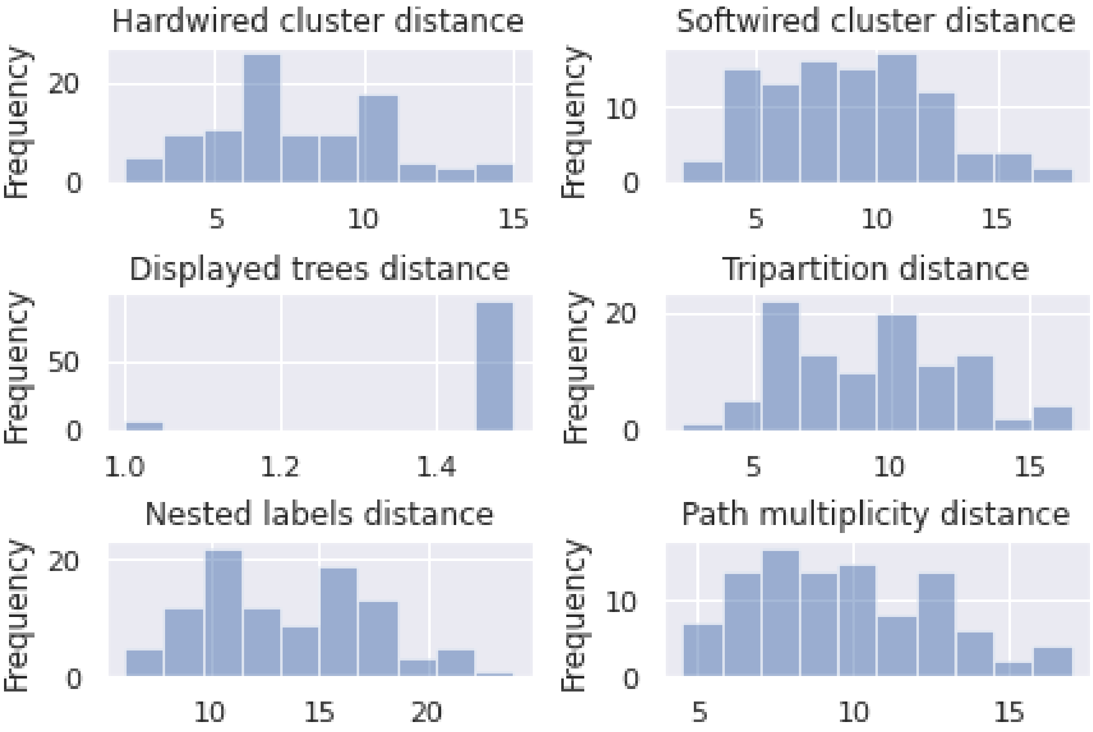
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
5
10
15
20
25
30
35
40
0
1
2
3
4
5
6

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


Hardwired cluster distance
Frequency
0
20
5
10
15
Softwired cluster distance
Frequency
0
10
5
10
15
Displayed trees distance
Frequency
0
50
1.0
1.2
1.4
Tripartition distance
Frequency
0
20
5
10
15
Nested labels distance
Frequency
0
20
10
15
20
Path multiplicity distance
Frequency
0
10
5
10
15

1.1.2 Plots for LikelihoodType.BEST

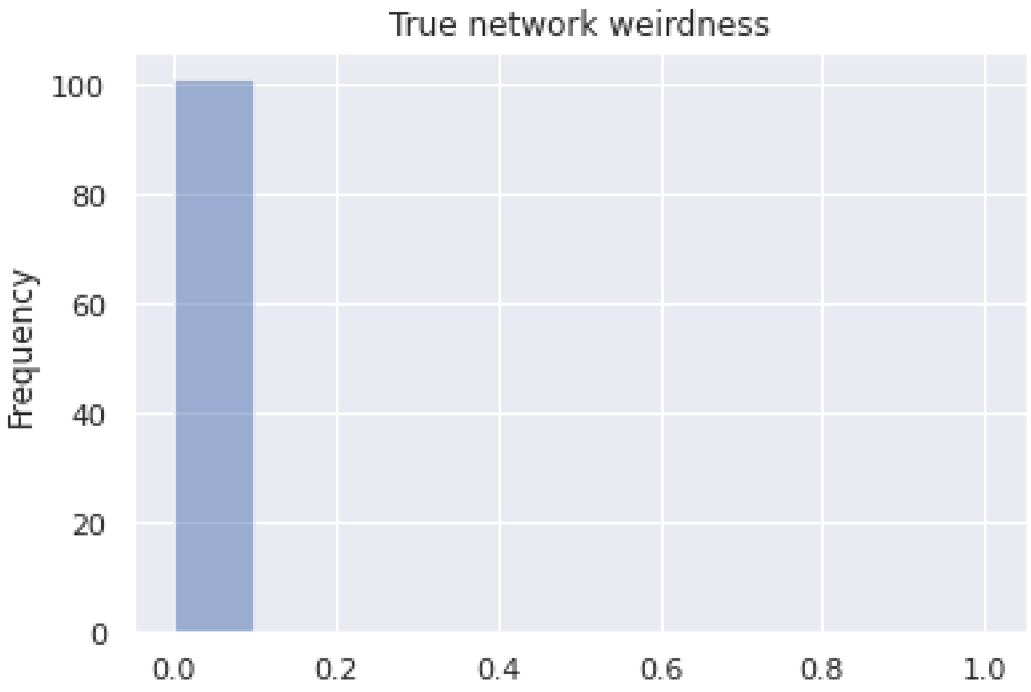
```
[10]: df_raxml_only_msasize_100_best = df_raxml_only_msasize_100.
       ↪query('likelihood_type == "BEST"')
      build_stats(df_raxml_only_msasize_100_best)
```

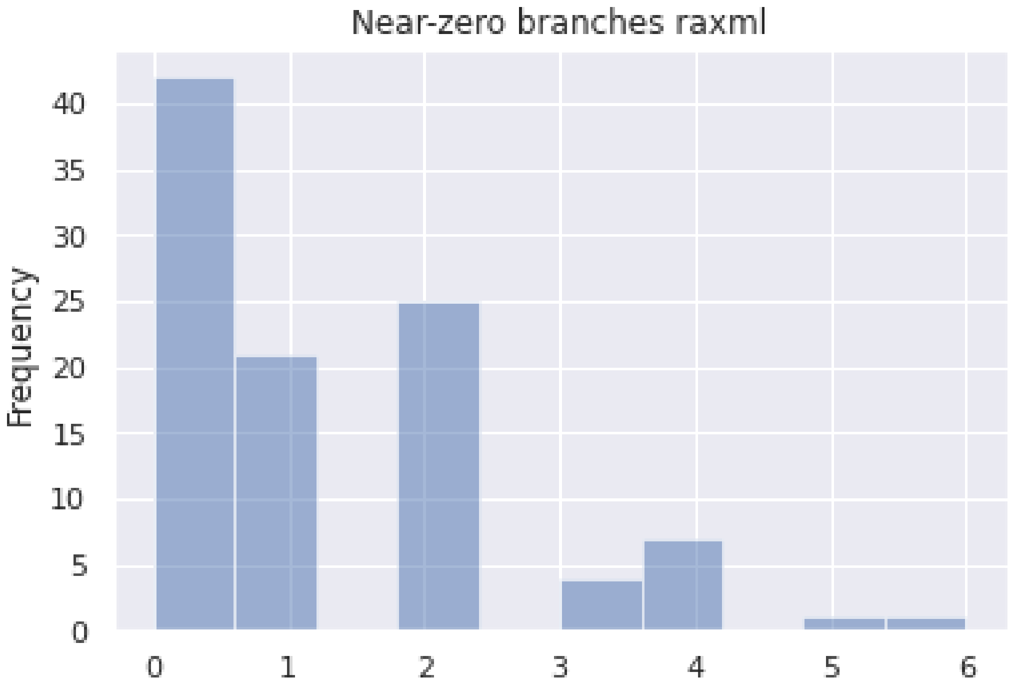
```
Inferred BIC better or equal: 96
Inferred BIC worse: 5

Inferred n_reticulations less: 91
Inferred n_reticulations equal: 10
Inferred n_reticulations more: 0
```

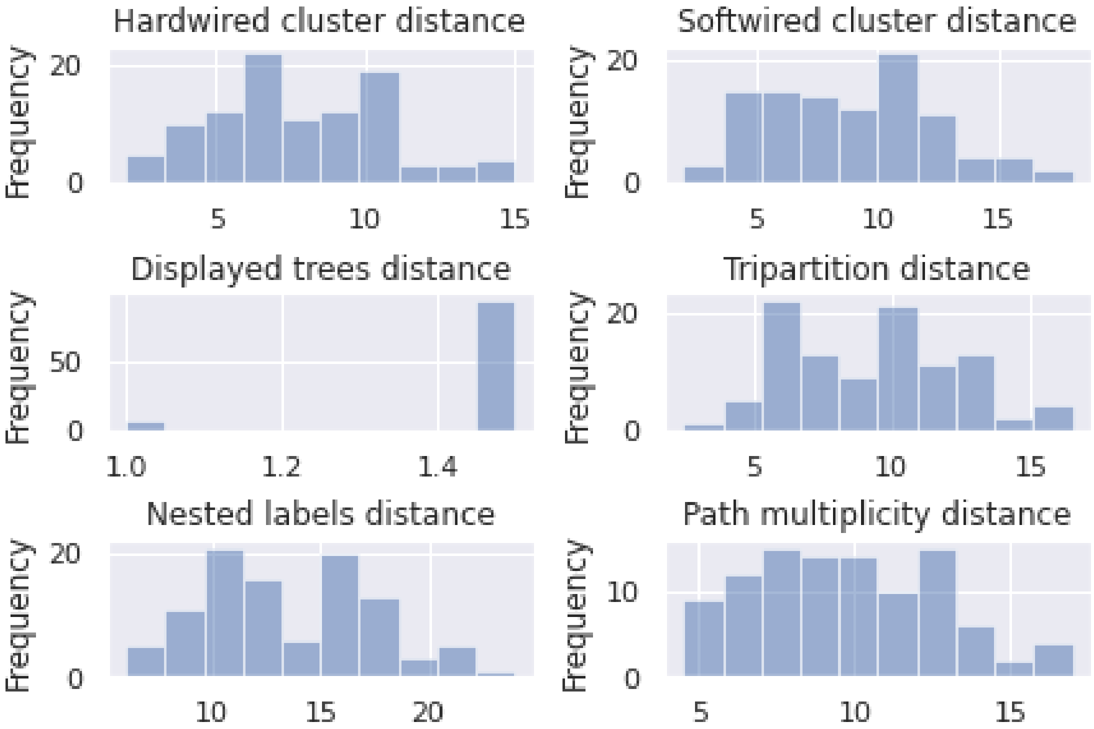
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
5
10
15
20
25
30
35
40
0
1
2
3
4
5
6

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


Hardwired cluster distance
Frequency
0
20
5
10
15
Softwired cluster distance
Frequency
0
20
5
10
15
Displayed trees distance
Frequency
0
50
1.0
1.2
1.4
Tripartition distance
Frequency
0
20
5
10
15
Nested labels distance
Frequency
0
20
10
15
20
Path multiplicity distance
Frequency
0
10
5
10
15

1.2 Plots for MSA_size ~ 200*n_trees

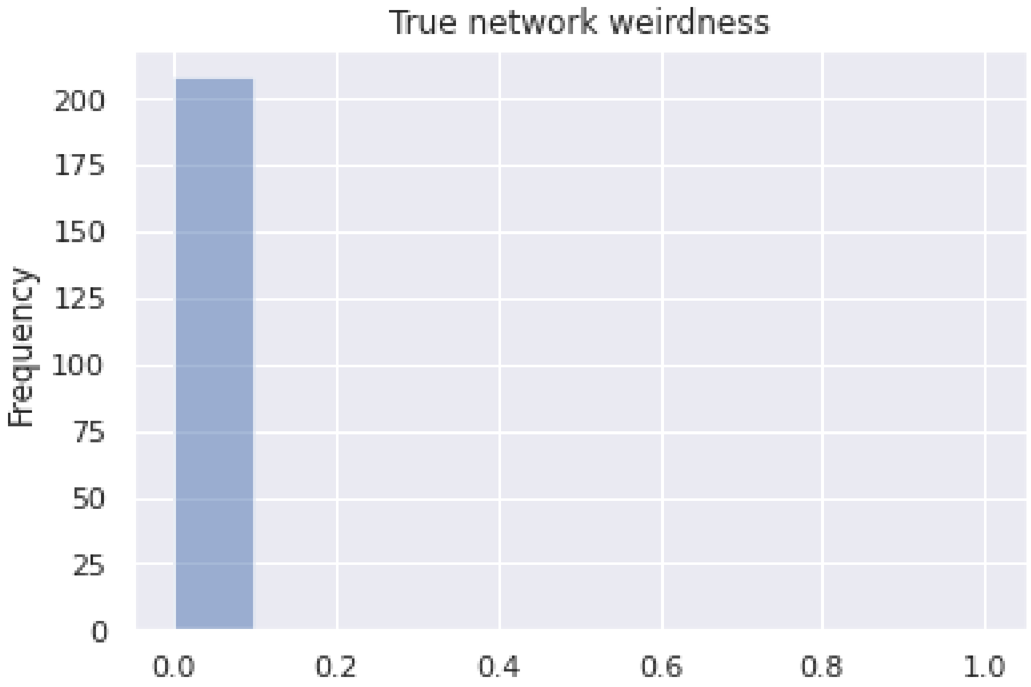
[11]:
```
df_raxml_only_msasize_200 = df_raxml_only.query('msa_size == 201')
build_stats(df_raxml_only_msasize_200)
```

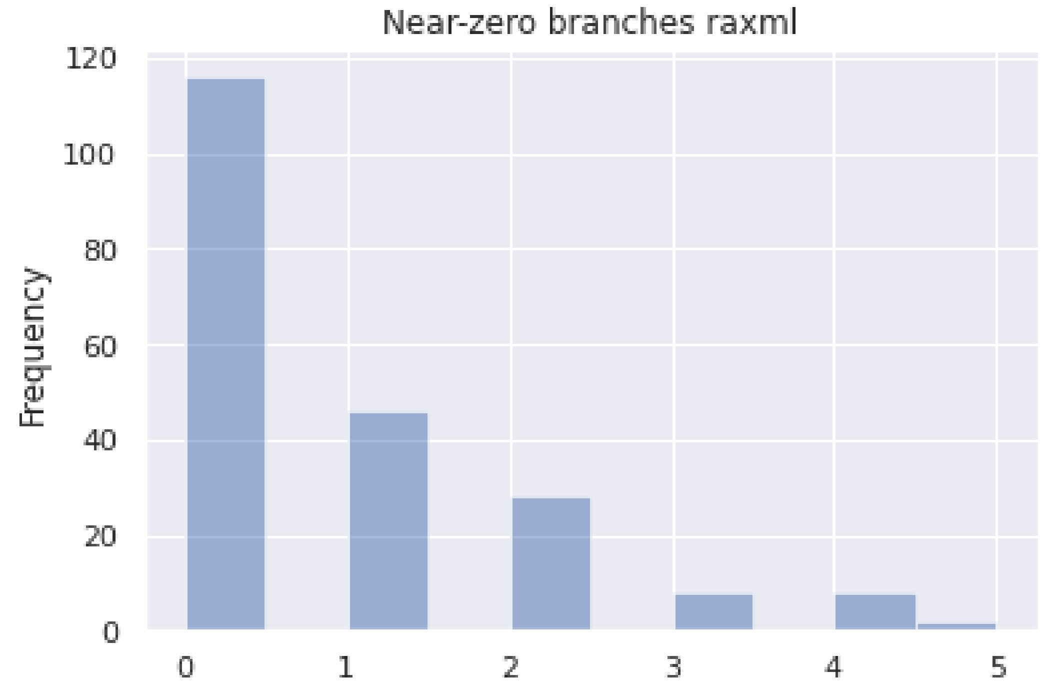
```
Inferred BIC better or equal: 185
Inferred BIC worse: 23

Inferred n_reticulations less: 182
Inferred n_reticulations equal: 26
Inferred n_reticulations more: 0
```

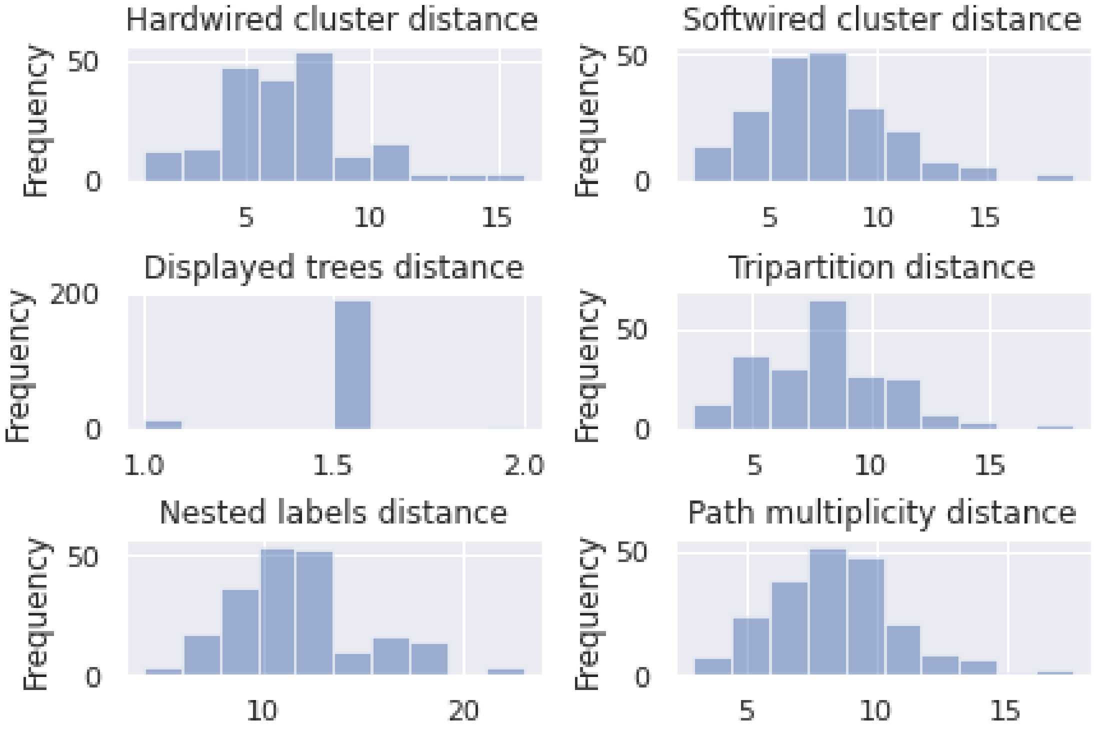
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
120
100
80
60
40
20
0
0
1
2
3
4
5

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


Hardwired cluster distance
Frequency
50
0
5
10
15
Softwired cluster distance
Frequency
50
0
5
10
15
Displayed trees distance
Frequency
200
0
1.0
1.5
2.0
Tripartition distance
Frequency
50
0
5
10
15
Nested labels distance
Frequency
50
0
10
20
Path multiplicity distance
Frequency
50
0
5
10
15

1.2.1 Plots for LikelihodType.AVERAGE

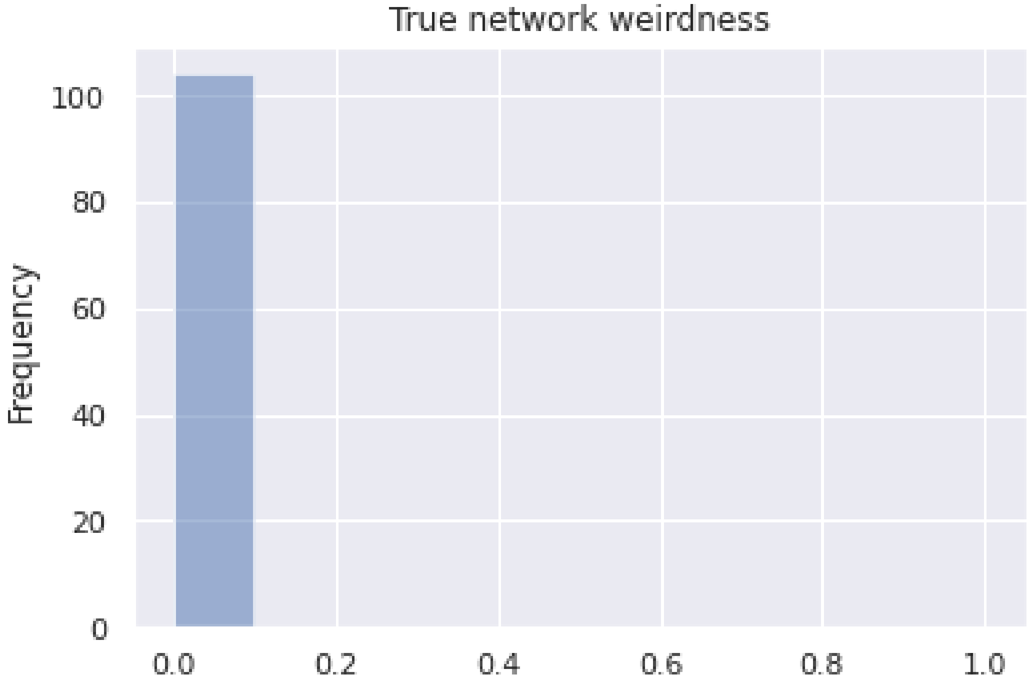
```
[12]: df_raxml_only_msasize_200_average = df_raxml_only_msasize_200.
       ↪query('likelihood_type == "AVERAGE"')
      build_stats(df_raxml_only_msasize_200_average)
```

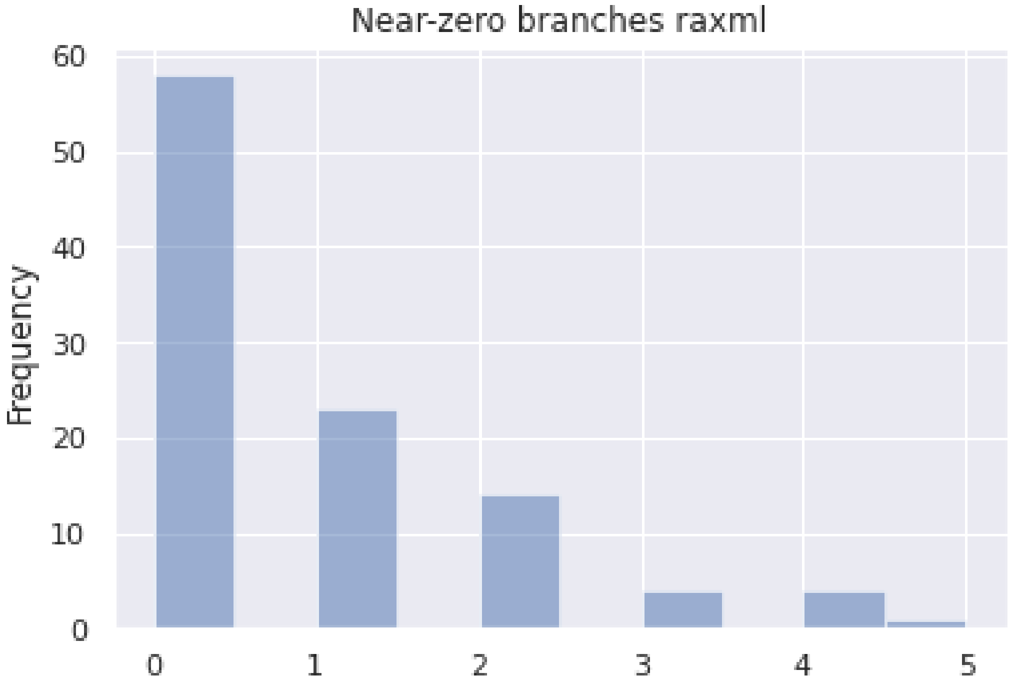
```
Inferred BIC better or equal: 96
Inferred BIC worse: 8

Inferred n_reticulations less: 88
Inferred n_reticulations equal: 16
Inferred n_reticulations more: 0
```

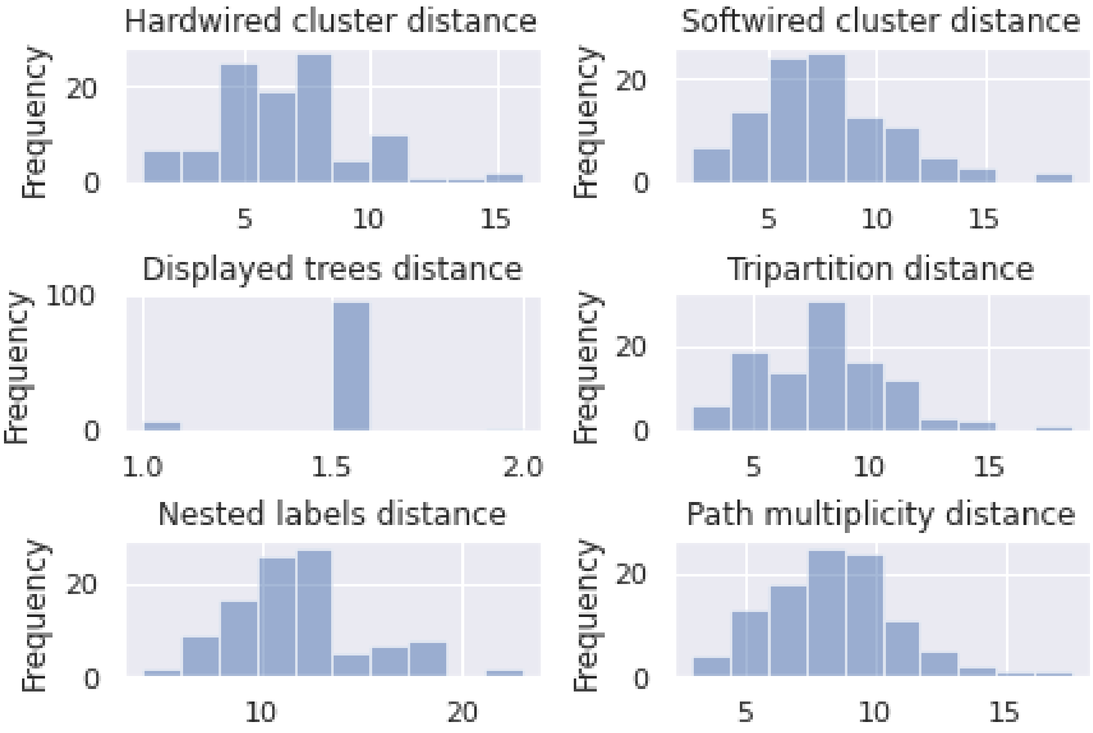
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
60
50
40
30
20
10
0
0
1
2
3
4
5

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


Hardwired cluster distance
Frequency
20
0
5
10
15
Softwired cluster distance
Frequency
20
0
5
10
15
Displayed trees distance
Frequency
100
0
1.0
1.5
2.0
Tripartition distance
Frequency
20
0
5
10
15
Nested labels distance
Frequency
20
0
10
20
Path multiplicity distance
Frequency
20
0
5
10
15

1.2.2 Plots for LikelihoodType.BEST

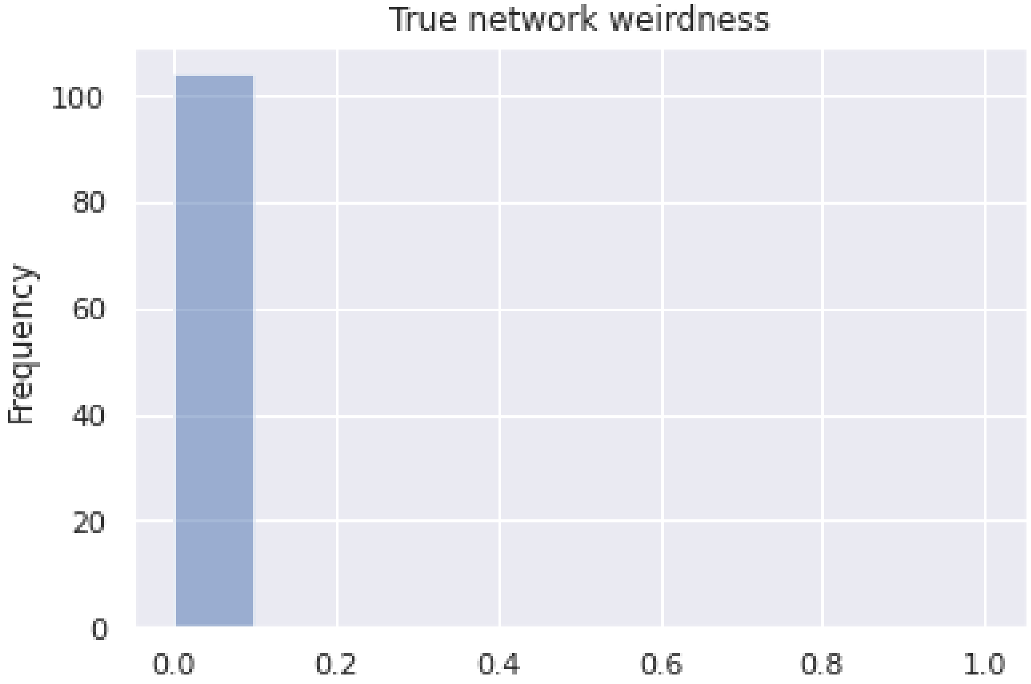
[13]:
```
df_raxml_only_msasize_200_best = df_raxml_only_msasize_200.
 ↪query('likelihood_type == "BEST"')
build_stats(df_raxml_only_msasize_200_best)
```

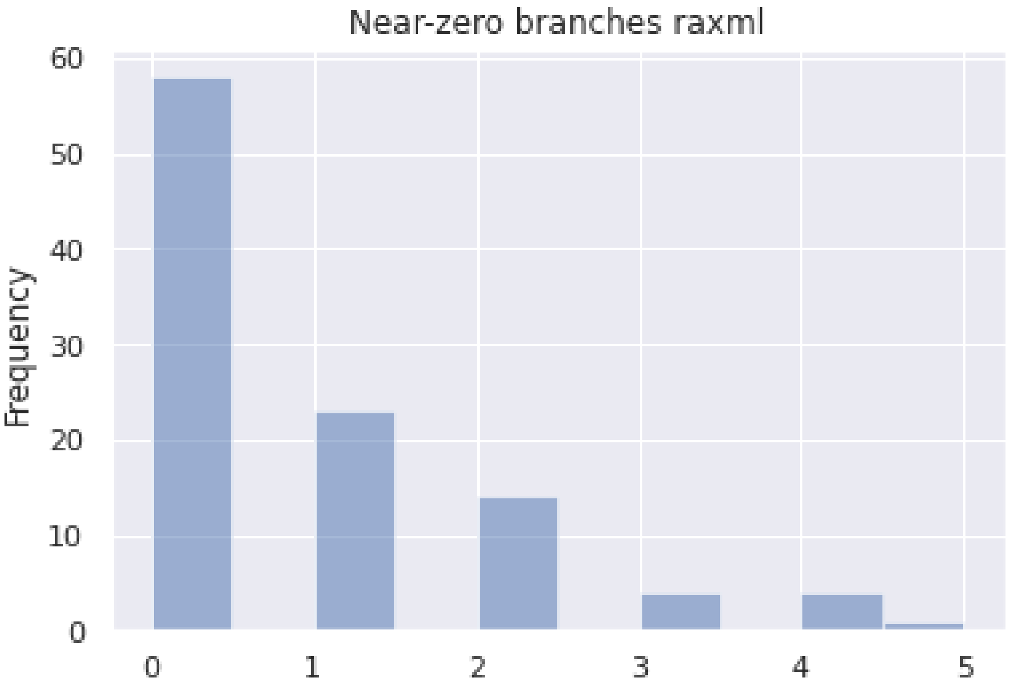
```
Inferred BIC better or equal: 89
Inferred BIC worse: 15

Inferred n_reticulations less: 94
Inferred n_reticulations equal: 10
Inferred n_reticulations more: 0
```

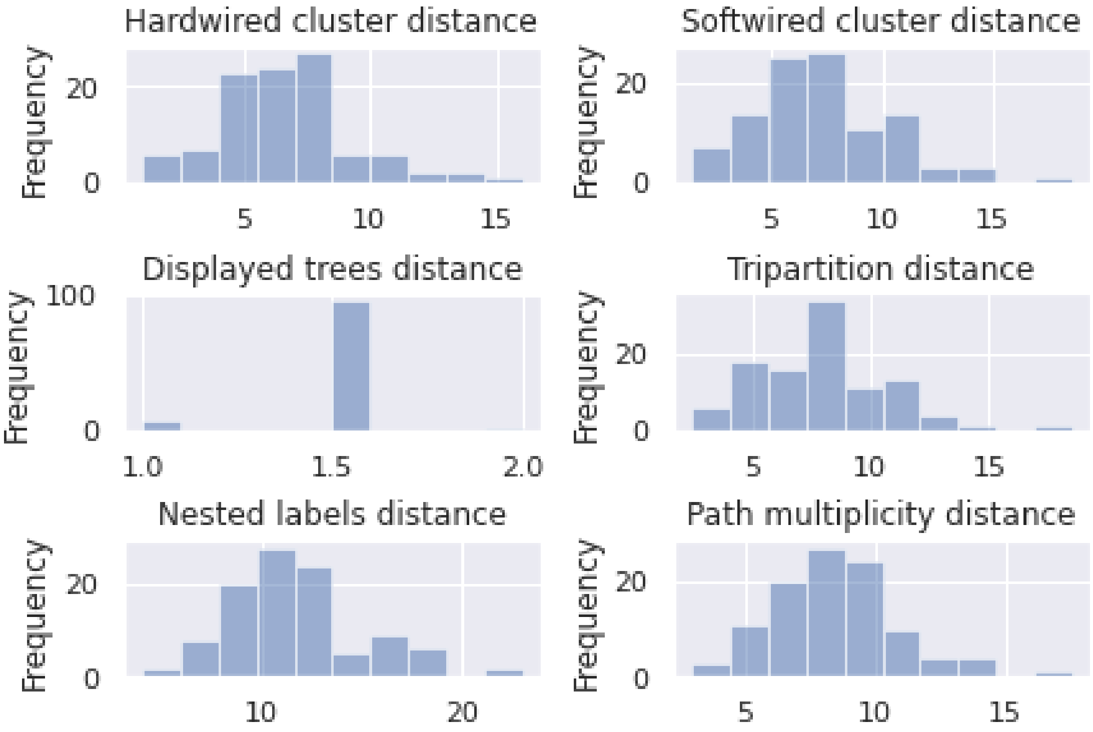
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0
10
20
30
40
50
60
0
1
2
3
4
5

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


Hardwired cluster distance
Frequency
0
20
5
10
15
Softwired cluster distance
Frequency
0
20
5
10
15
Displayed trees distance
Frequency
0
100
1.0
1.5
2.0
Tripartition distance
Frequency
0
20
5
10
15
Nested labels distance
Frequency
0
20
10
20
Path multiplicity distance
Frequency
0
20
5
10
15

2 Plots for starting with 5 random, 5 parsimony trees

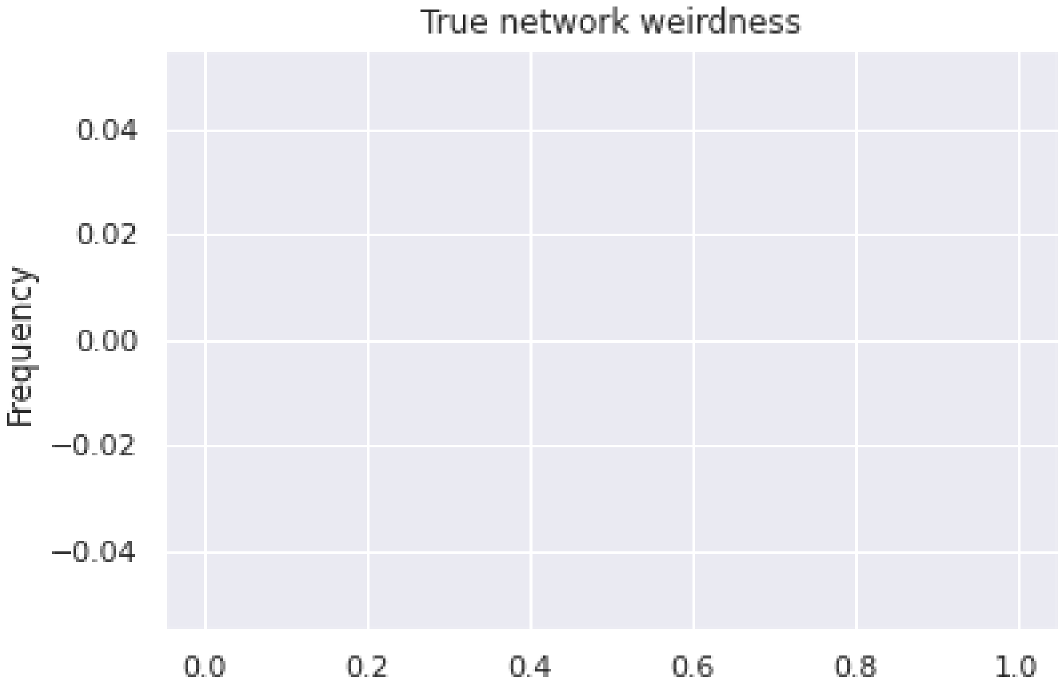
```
[14]: df_random = df.query('start_type == "RANDOM"')
      build_stats(df_random)
```

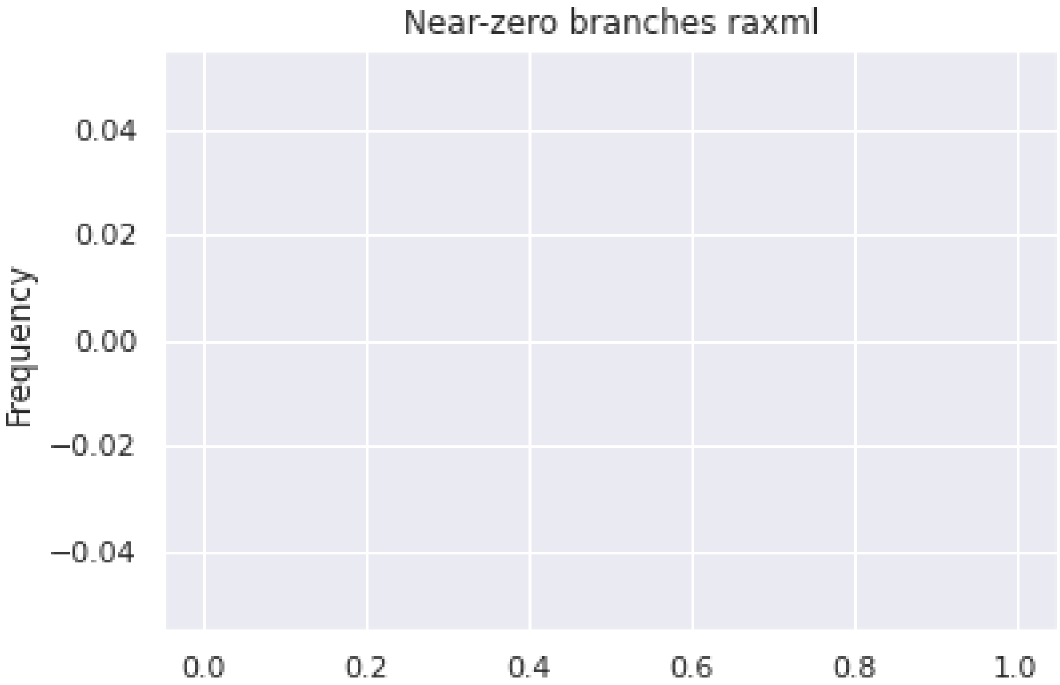
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

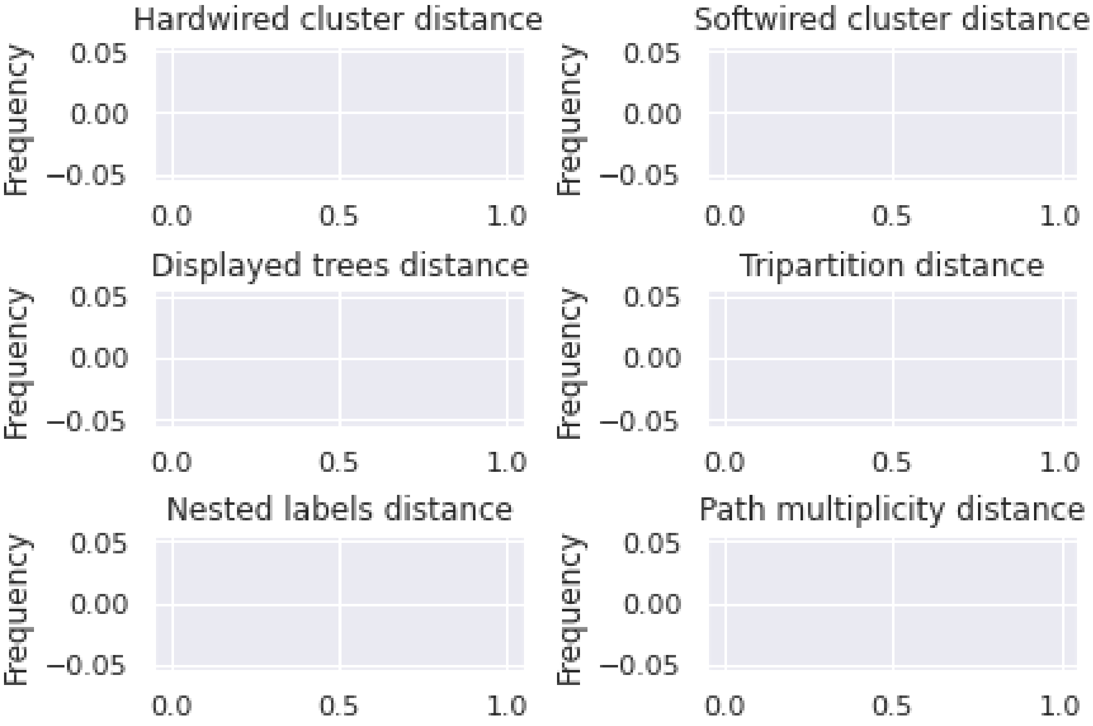
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.1 Plots for MSA_size ~ 100*n_trees

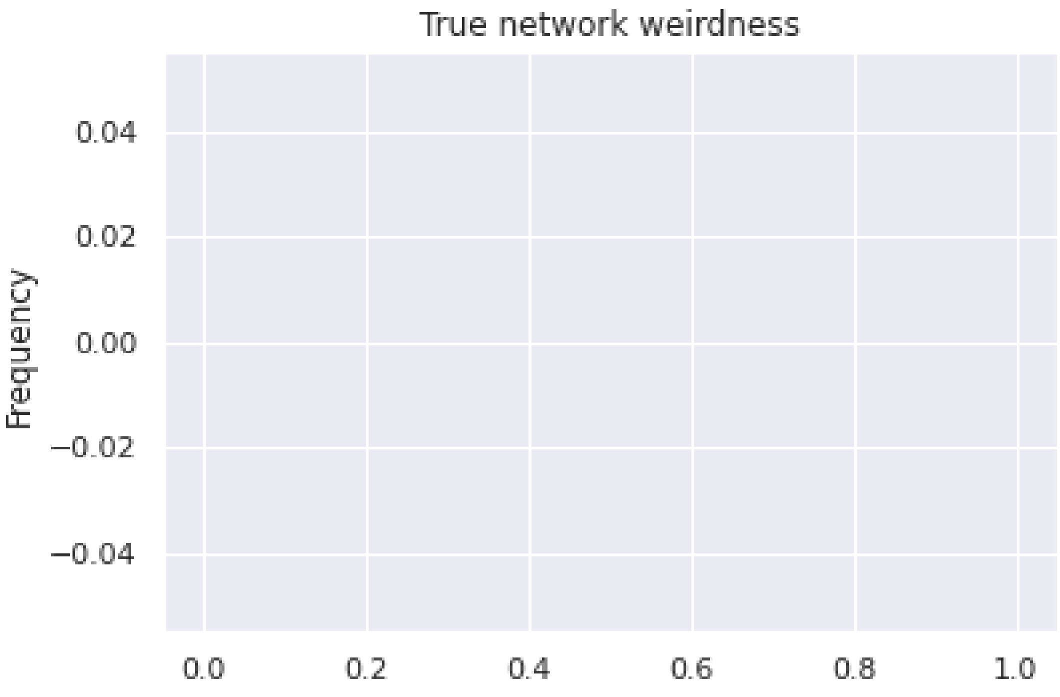
[15]:
```
df_random_msasize_100 = df_random.query('msa_size == 101')
build_stats(df_random_msasize_100)
```

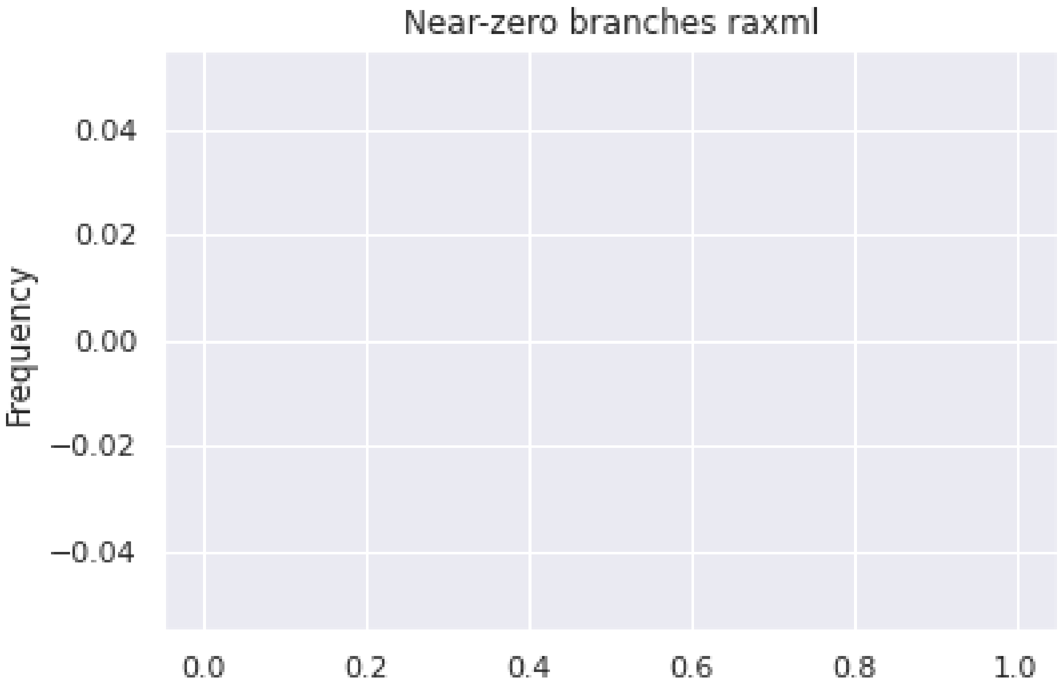
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

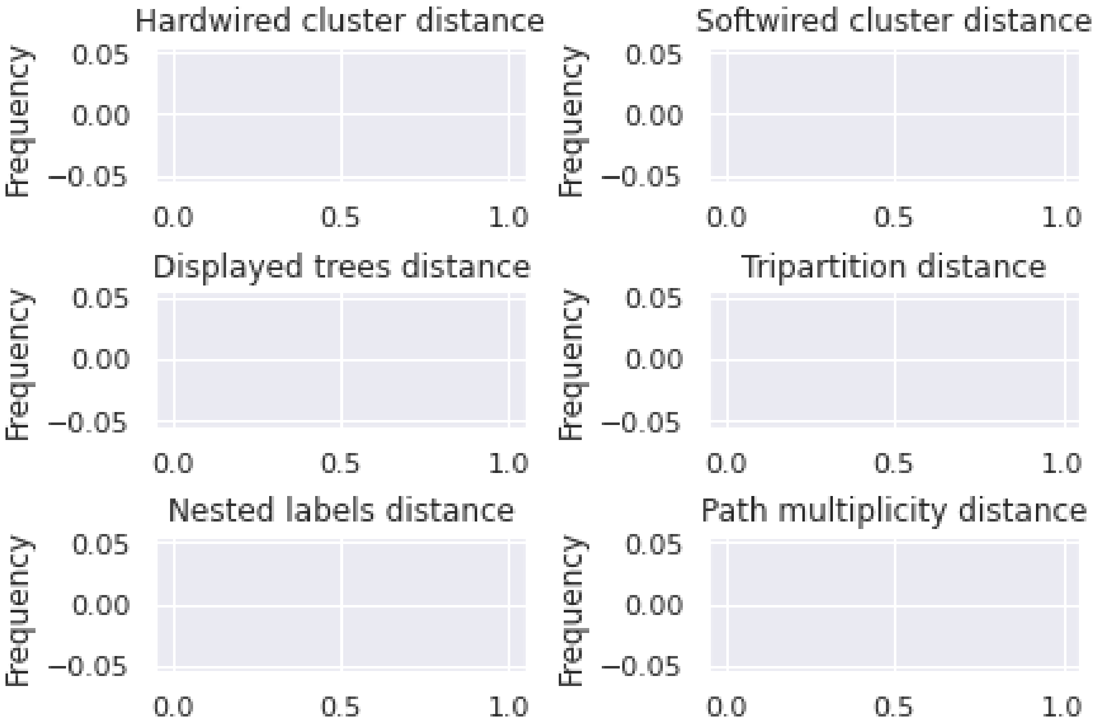
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.1.1 Plots for LikelihodType.AVERAGE

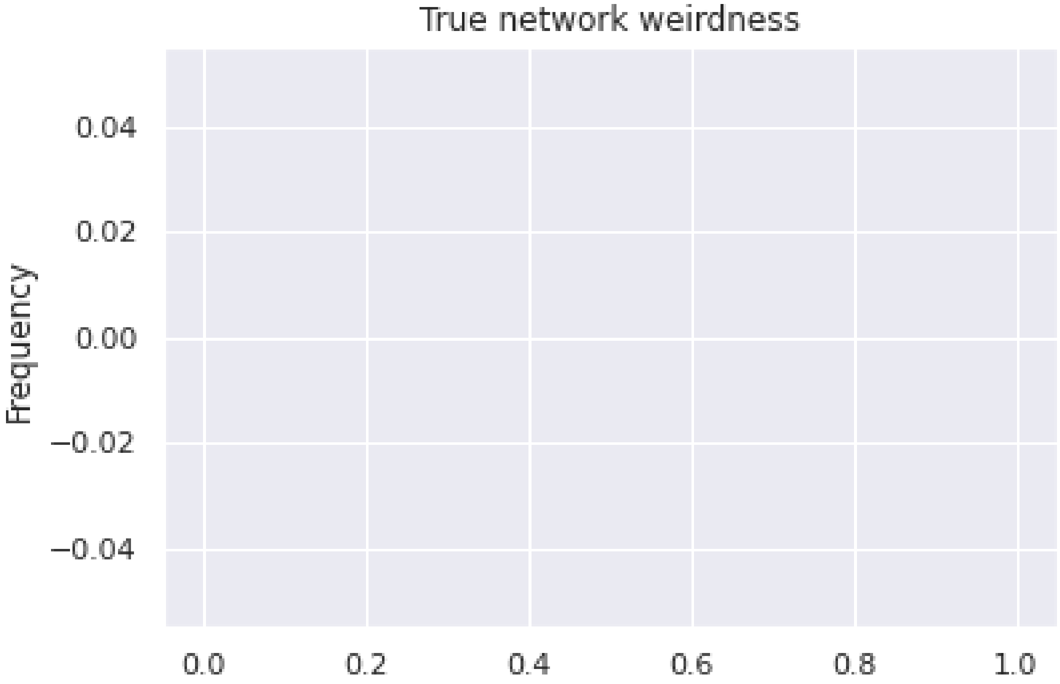
```
[16]: df_random_msasize_100_average = df_random_msasize_100.query('likelihood_type ==␣
       ↪"AVERAGE"')
      build_stats(df_random_msasize_100_average)
```

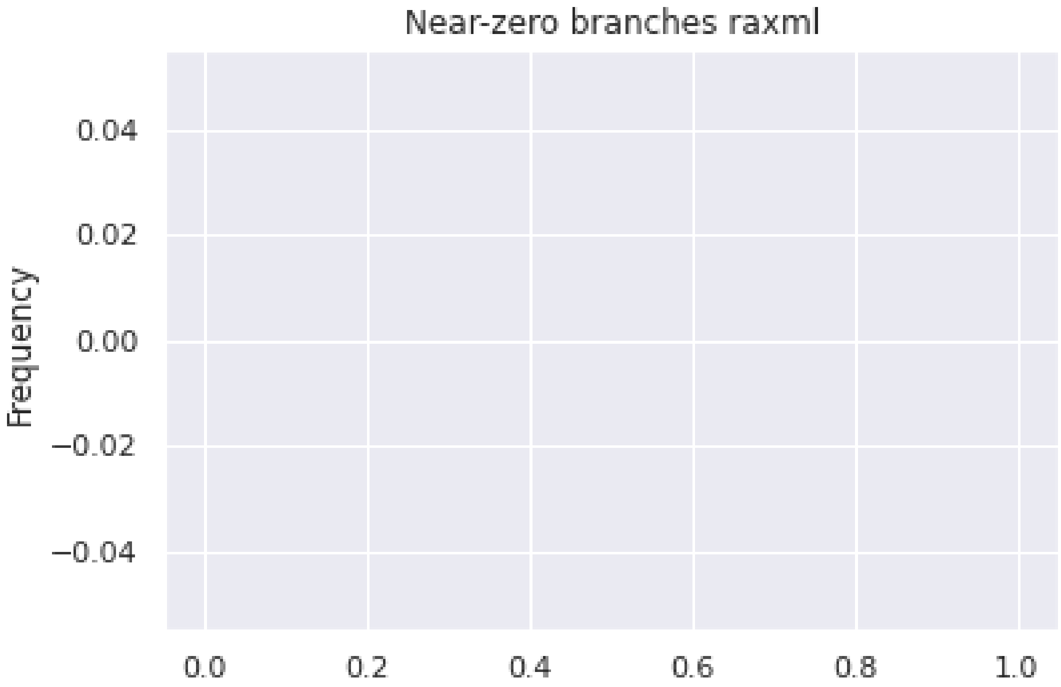
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

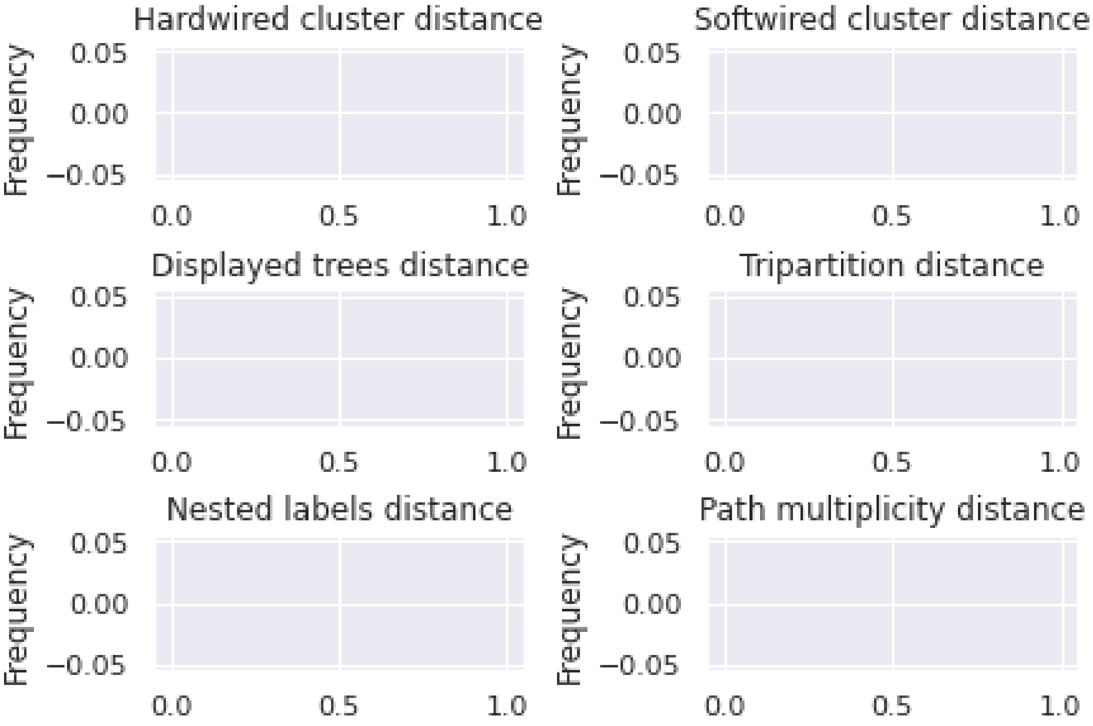
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.1.2 Plots for LikelihoodType.BEST

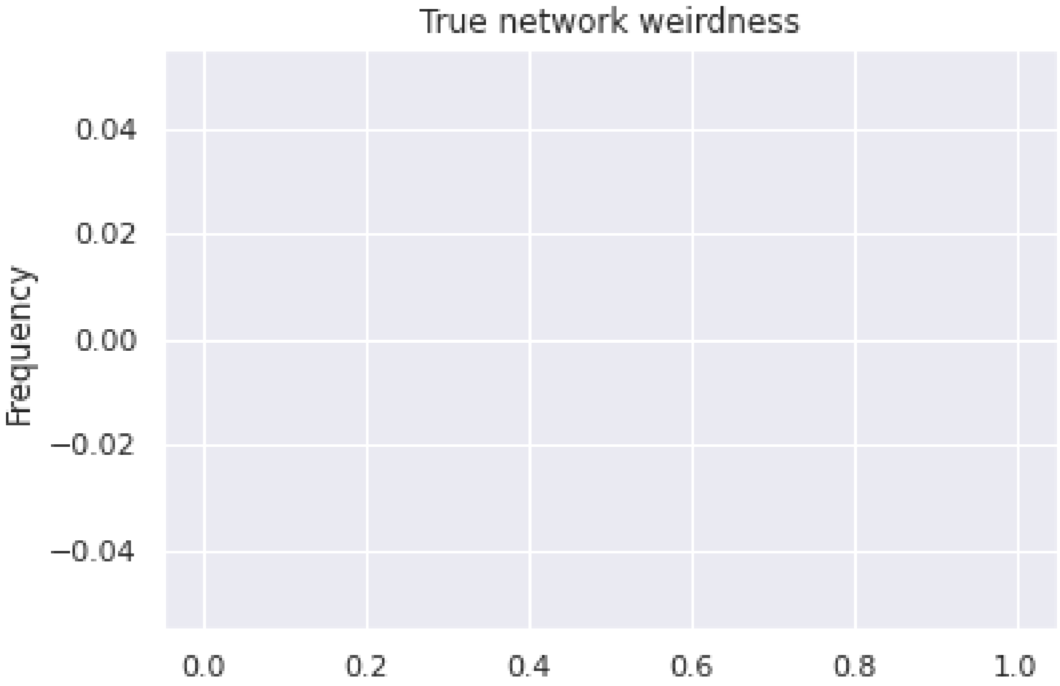
```
[17]: df_random_msasize_100_best = df_random_msasize_100.query('likelihood_type ==␣
      ↪"BEST"')
      build_stats(df_random_msasize_100_best)
```

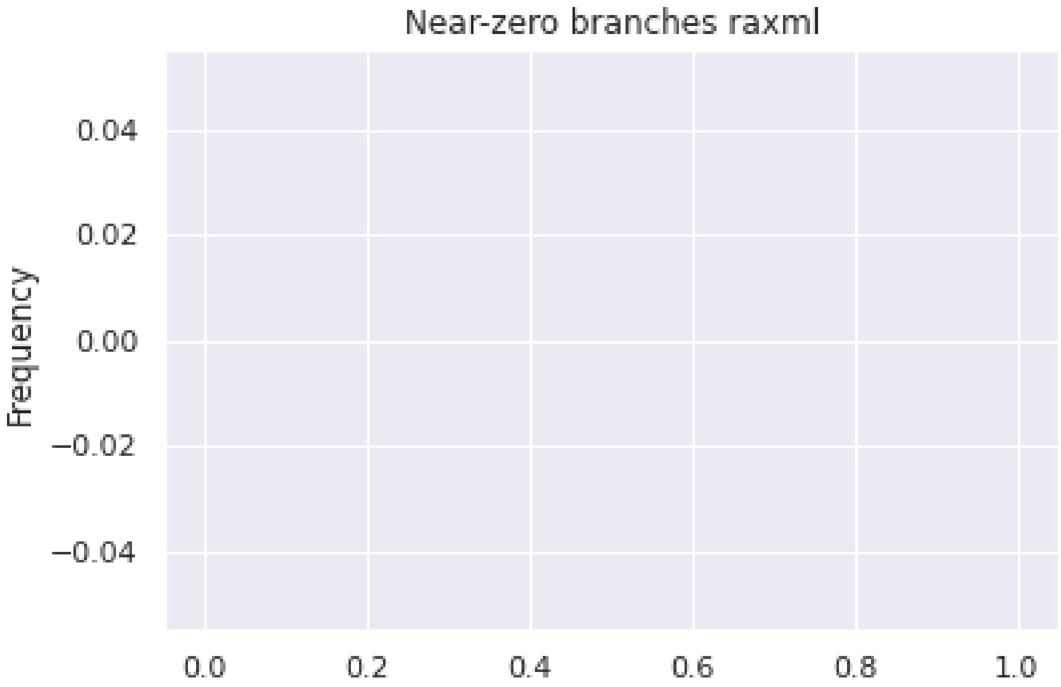
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

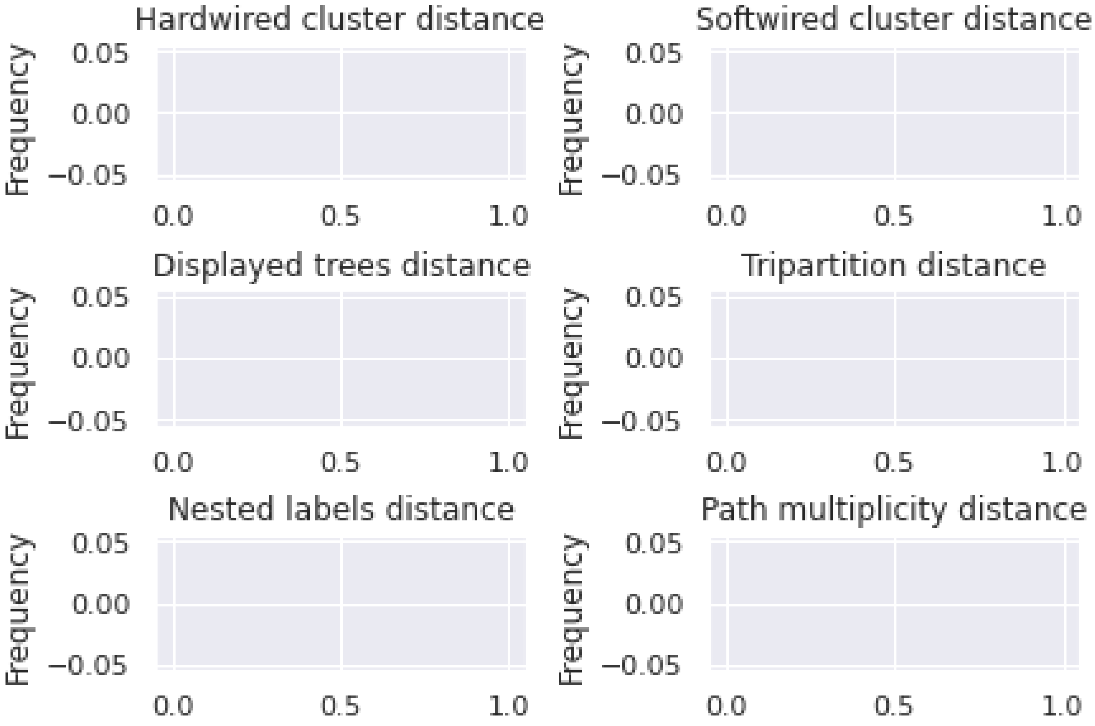
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.2 Plots for MSA_size ~ 200*n_trees

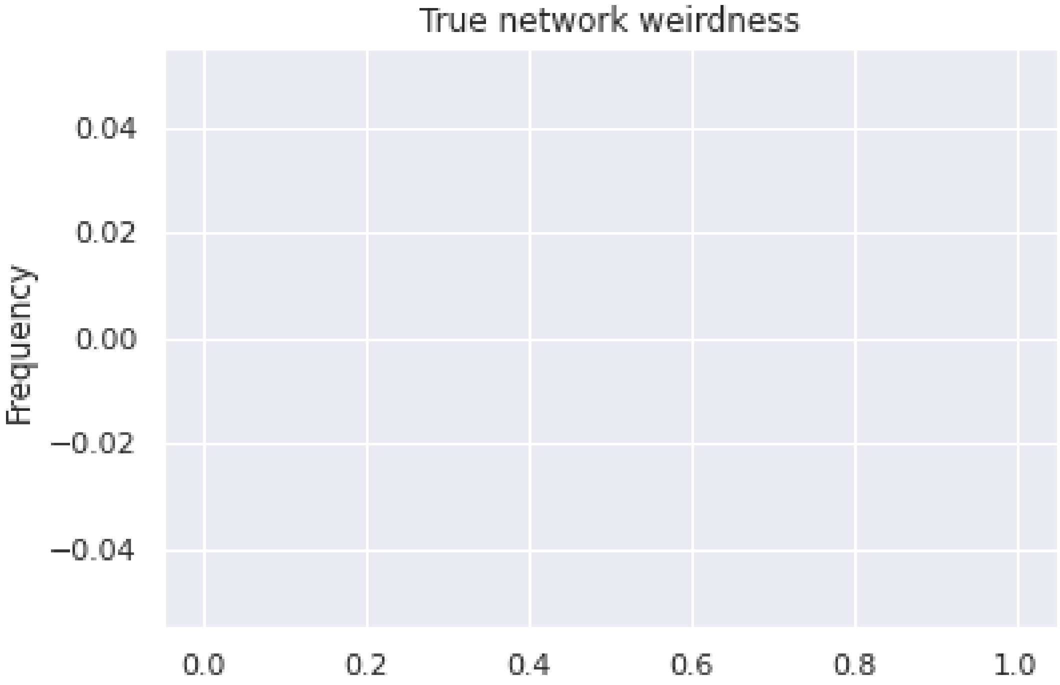
[18]:
```
df_random_msasize_200 = df_random.query('msa_size == 201')
build_stats(df_random_msasize_200)
```

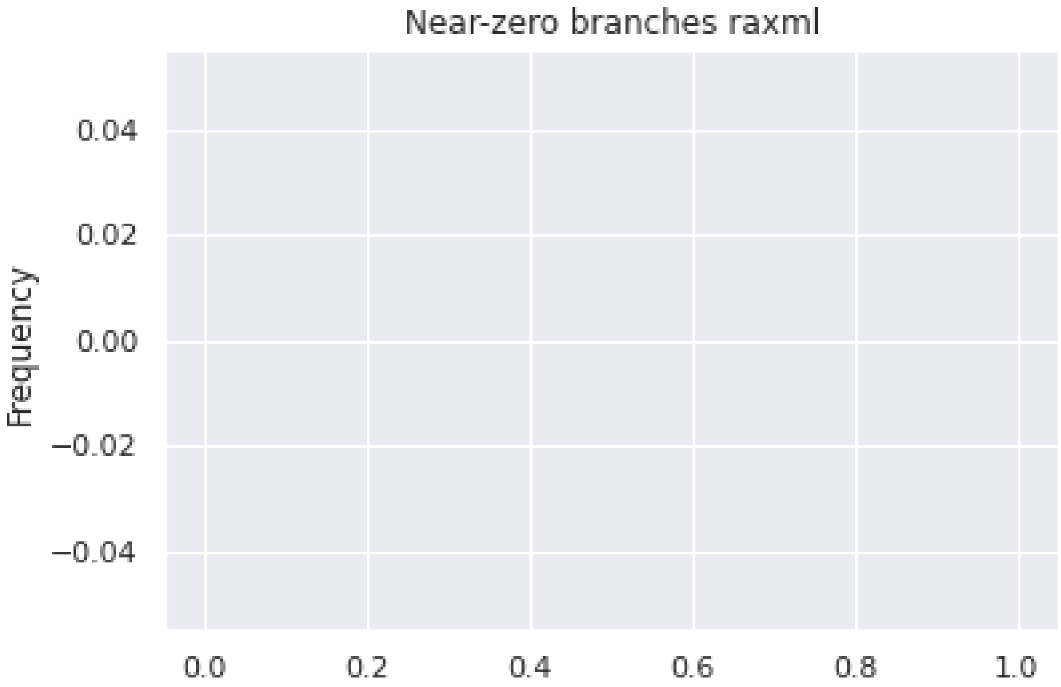
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

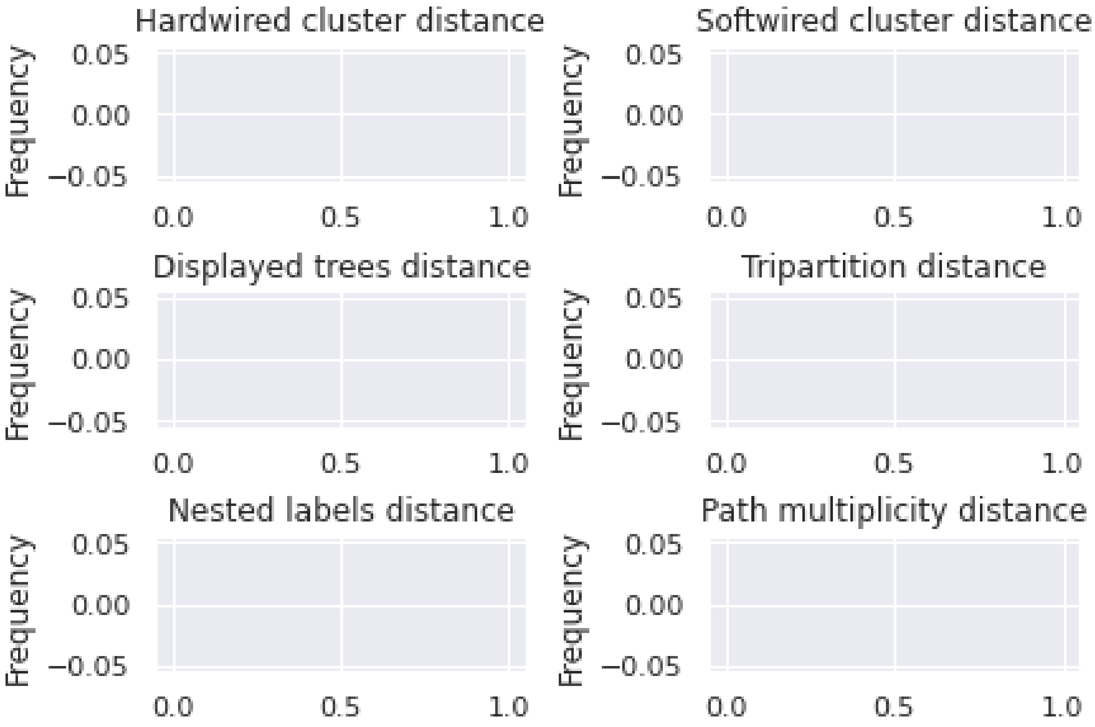
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.2.1 Plots for LikelihodType.AVERAGE

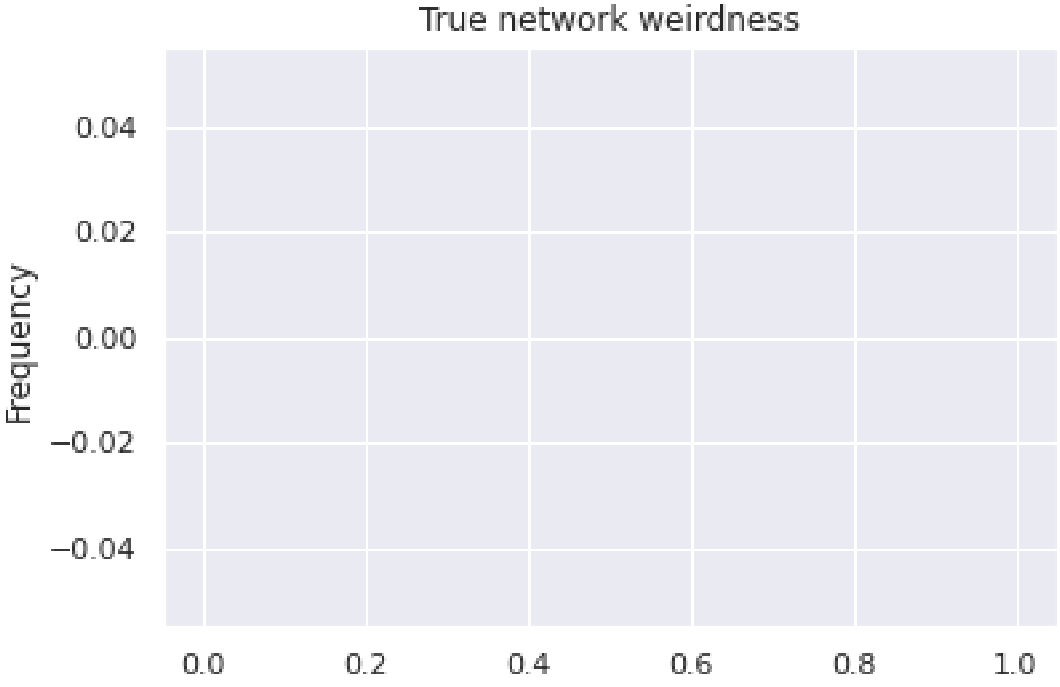
```
[19]: df_random_msasize_200_average = df_random_msasize_200.query('likelihood_type ==␣
       ↪"AVERAGE"')
      build_stats(df_random_msasize_200_average)
```

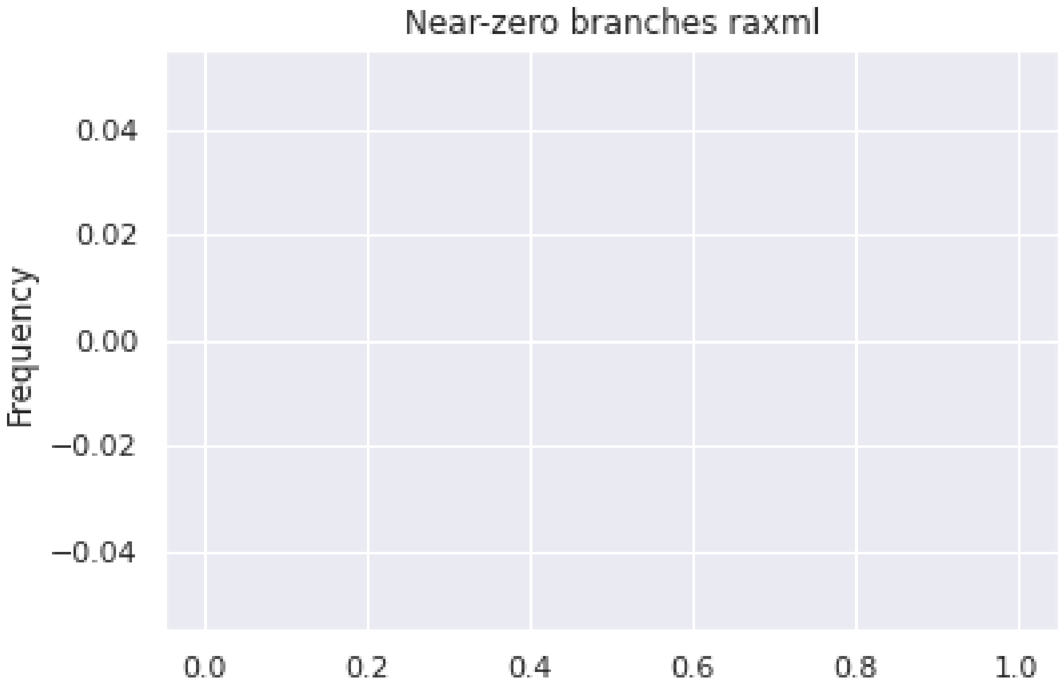
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

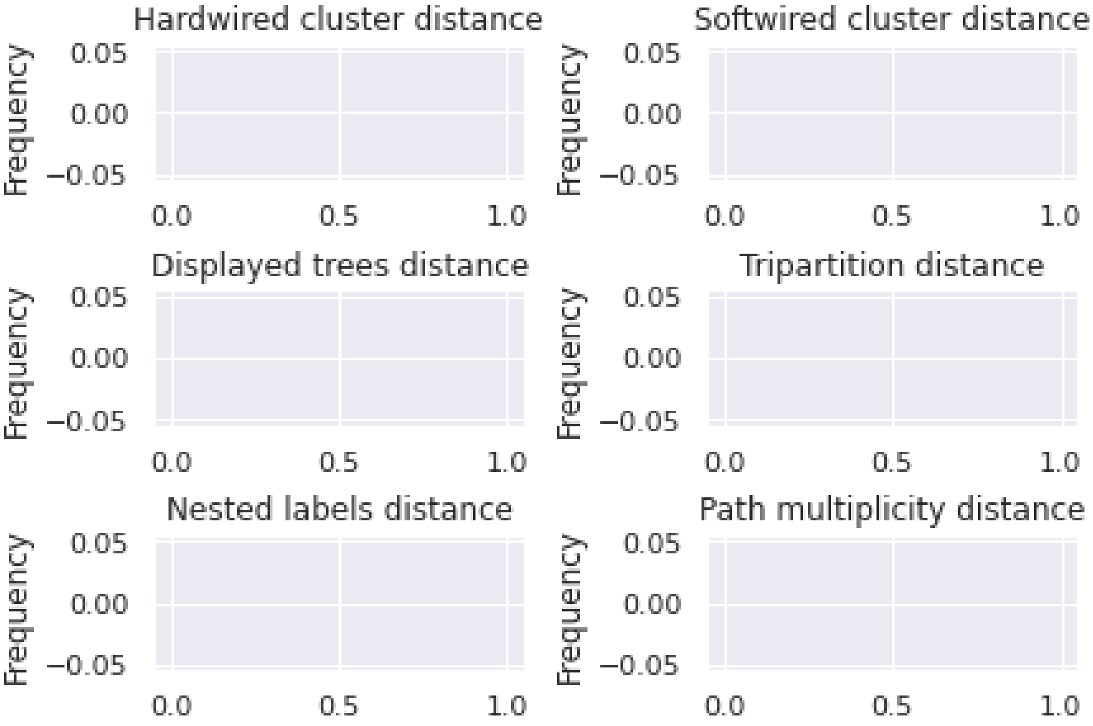
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

2.2.2 Plots for LikelihoodType.BEST

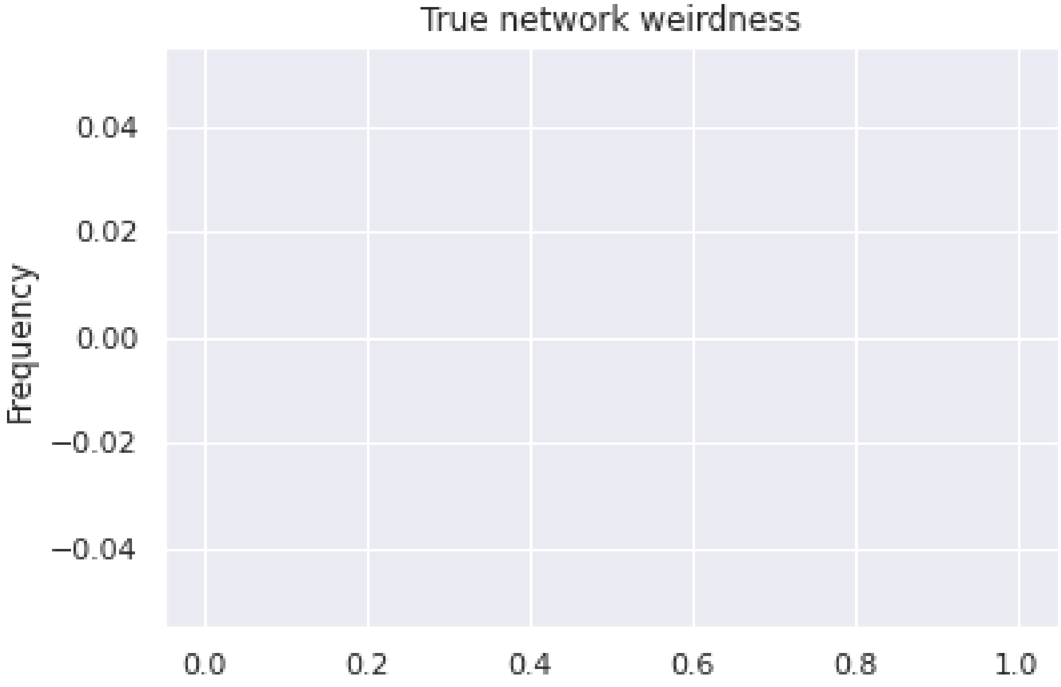
```
[20]: df_random_msasize_200_best = df_random_msasize_200.query('likelihood_type ==␣
       ↪"BEST"')
      build_stats(df_random_msasize_200_best)
```

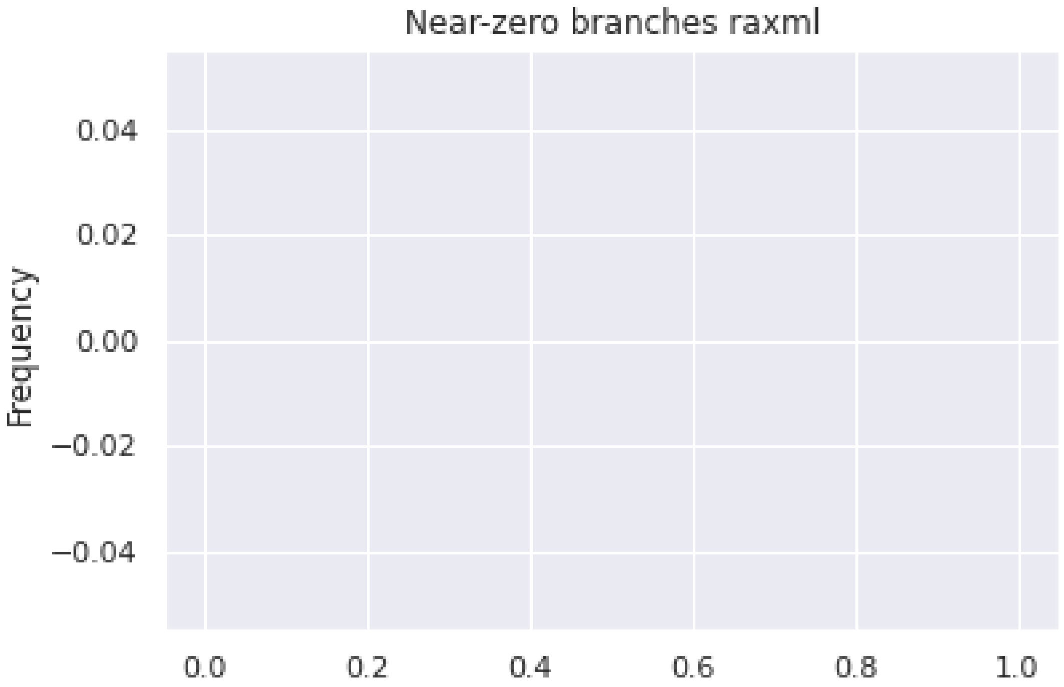
```
Inferred BIC better or equal: 0
Inferred BIC worse: 0

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

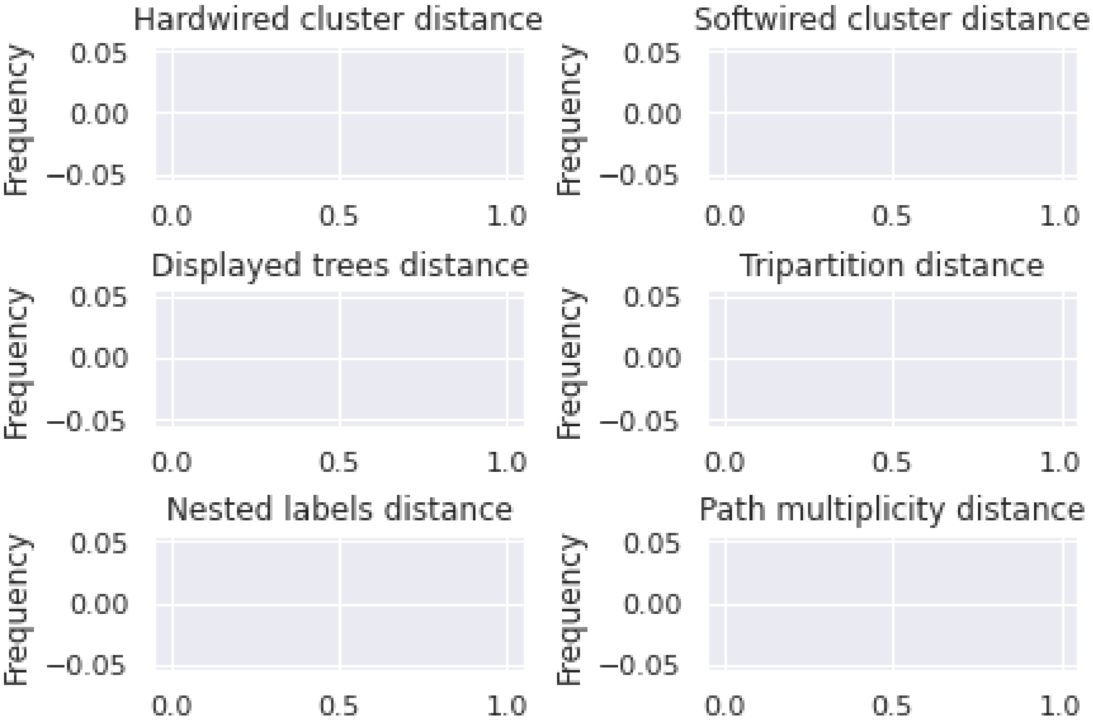
```
<Figure size 432x288 with 0 Axes>
```

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




Near-zero branches raxml
Frequency
0.04
0.02
0.00
−0.02
−0.04
0.0
0.2
0.4
0.6
0.8
1.0

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


Hardwired cluster distance
Softwired cluster distance
Displayed trees distance
Tripartition distance
Nested labels distance
Path multiplicity distance
Frequency
0.05
0.00
−0.05
0.0
0.5
1.0

[ ]:

```
```