

NetRAX Experiment Evaluation

February 10, 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']]))))
    df['bic_diff'].plot.hist(bins=100, alpha=0.5, title='(bic_true -
    ↳bic_inferred) / bic_true\n value >0 means inferred BIC was better')

def logl_stats(df):
    print("Inferred loglh better or equal: " + str(len(df[df['logl_inferred']
    ↳>= df['logl_true']]))))
    print("Inferred loglh worse: " + str(len(df[df['logl_inferred'] <
    ↳df['logl_true']]))))
    df['logl_diff'].plot.hist(bins=100, alpha=0.5, title='(logl_true -
    ↳logl_inferred) / logl_true\n value <0 means inferred logl was better')

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')
```

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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)
    logl_stats(df)
    print("")
    plt.figure(2)
    reticulation_stats(df)
    print("")
    plt.figure(3)
    weirdness_stats(df)
    print("")
    plt.figure(4)
    zero_branches_stats(df)
    print("")
    plt.figure(5)
    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')

      df['bic_diff'] = (df['bic_true'] - df['bic_inferred']) / df['bic_true']
      df['logl_diff'] = (df['logl_true'] - df['logl_inferred']) / df['logl_true']

```

```

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

```

[4]:

```

                                name  n_taxa  n_trees  \
0  datasets_medium_network_norandom_uniform_0_0/0...      26      4
1  datasets_medium_network_norandom_uniform_0_0/0...      26      4
2  datasets_medium_network_norandom_uniform_0_0/0...      26      4
3  datasets_medium_network_norandom_uniform_0_0/0...      26      4
4  datasets_medium_network_norandom_uniform_0_1/0...      22      2

n_reticulations  msa_size      sampling_type  simulation_type  \
0                2        200  PERFECT_SAMPLING  CELINE
1                2        200  PERFECT_SAMPLING  CELINE
2                2        400  PERFECT_SAMPLING  CELINE
3                2        400  PERFECT_SAMPLING  CELINE
4                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

	bic_diff	logl_diff
0	-0.012717	-0.027015
1	-0.018216	-0.044945
2	-0.025225	-0.040128
3	-0.025225	-0.040128
4	0.011293	-0.011257

```
[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', 'bic_diff', 'logl_diff'],
         dtype='object')
```

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

Inferred BIC better or equal: 382

Inferred BIC worse: 122

Inferred loglh better or equal: 168

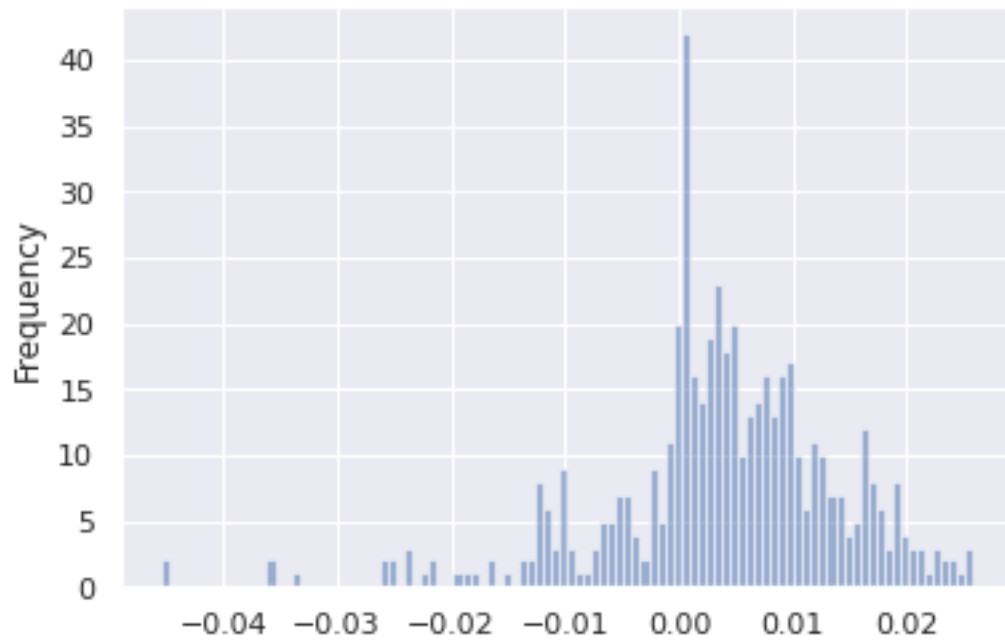
Inferred loglh worse: 336

Inferred n_reticulations less: 415

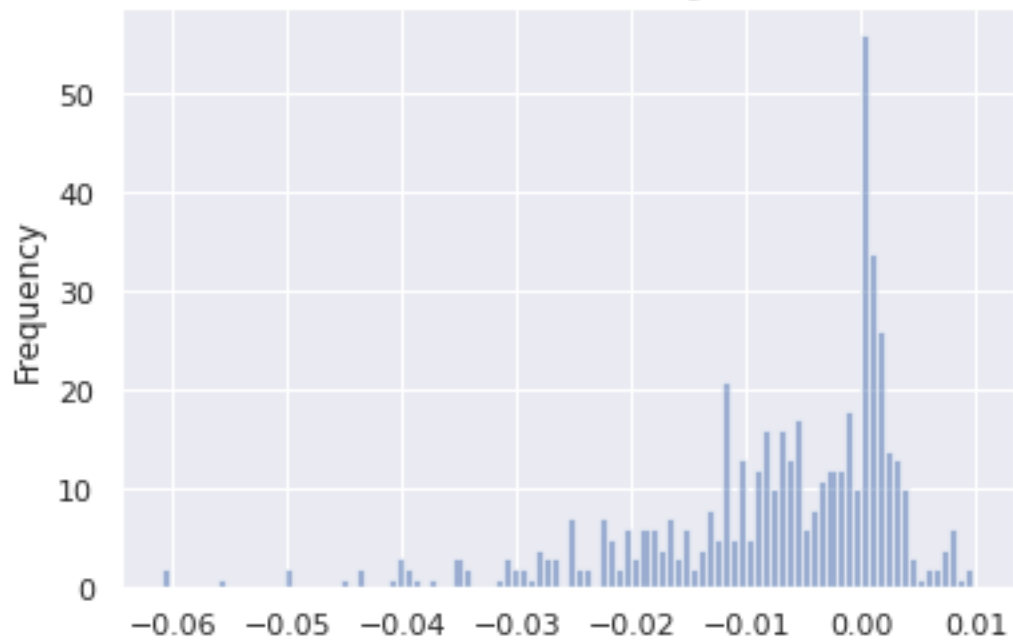
Inferred n_reticulations equal: 89

Inferred n_reticulations more: 0

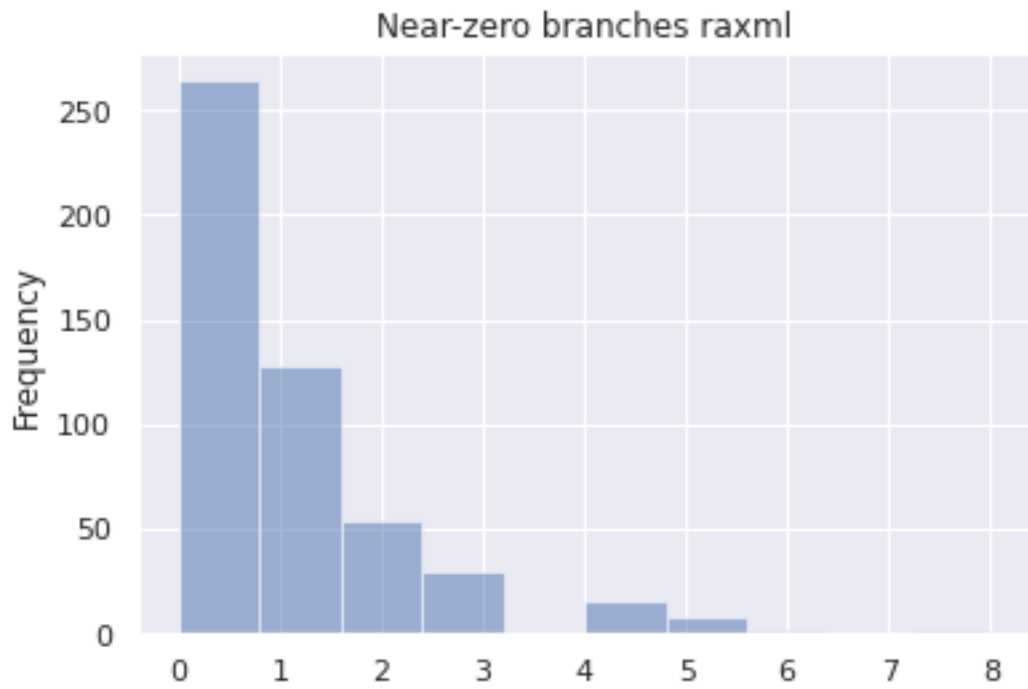
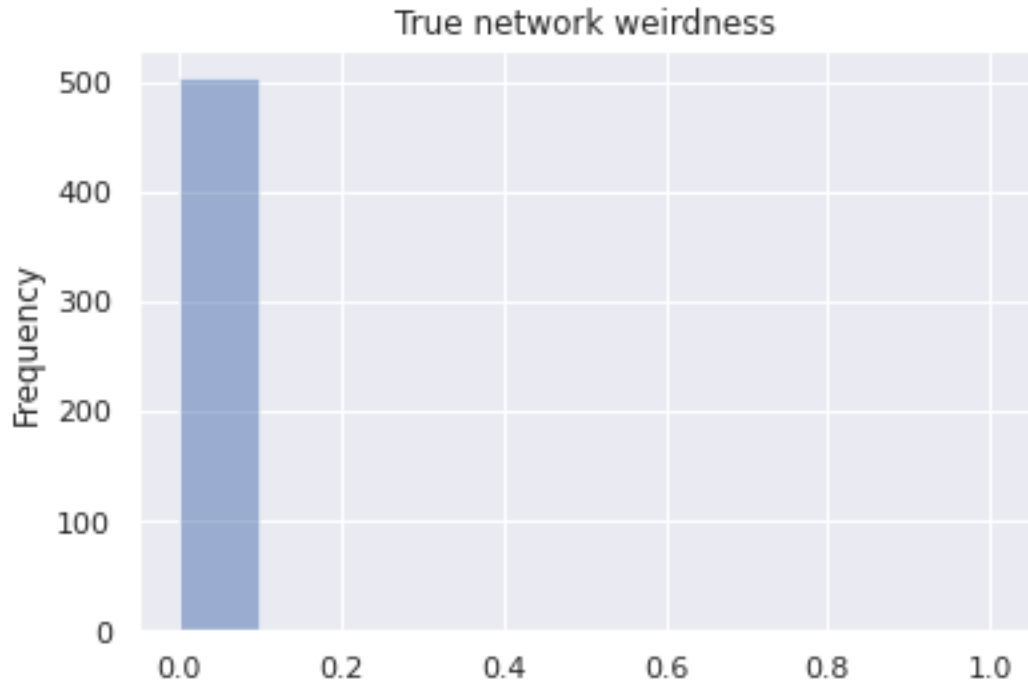
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



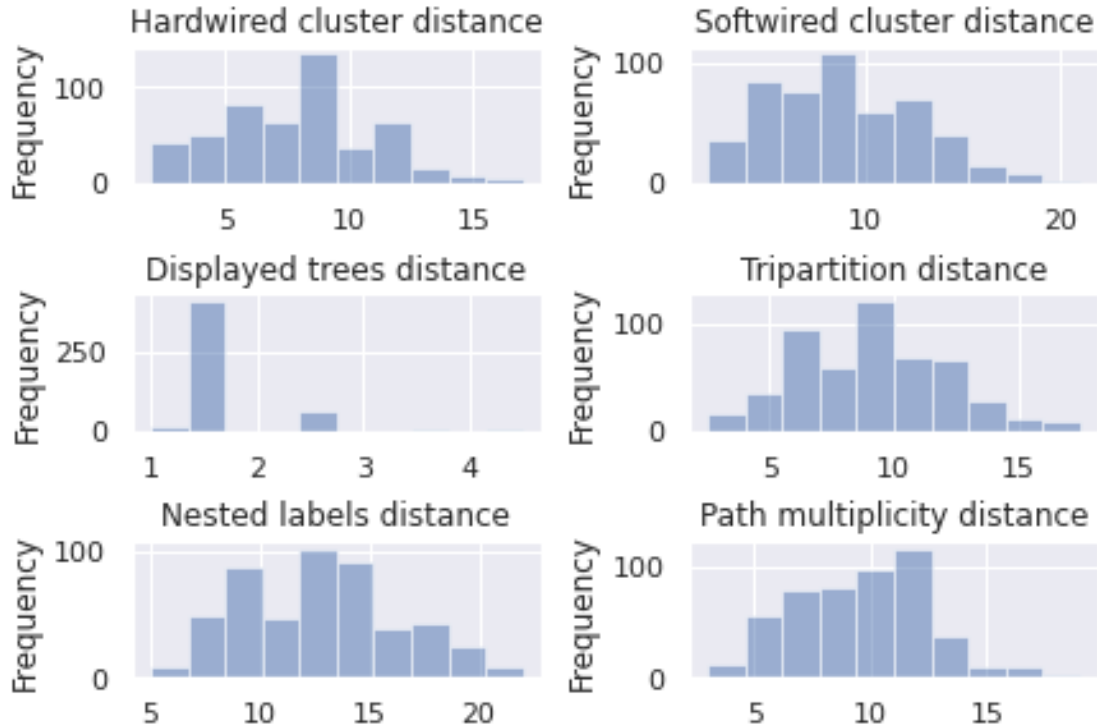
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



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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 loglh better or equal: 168

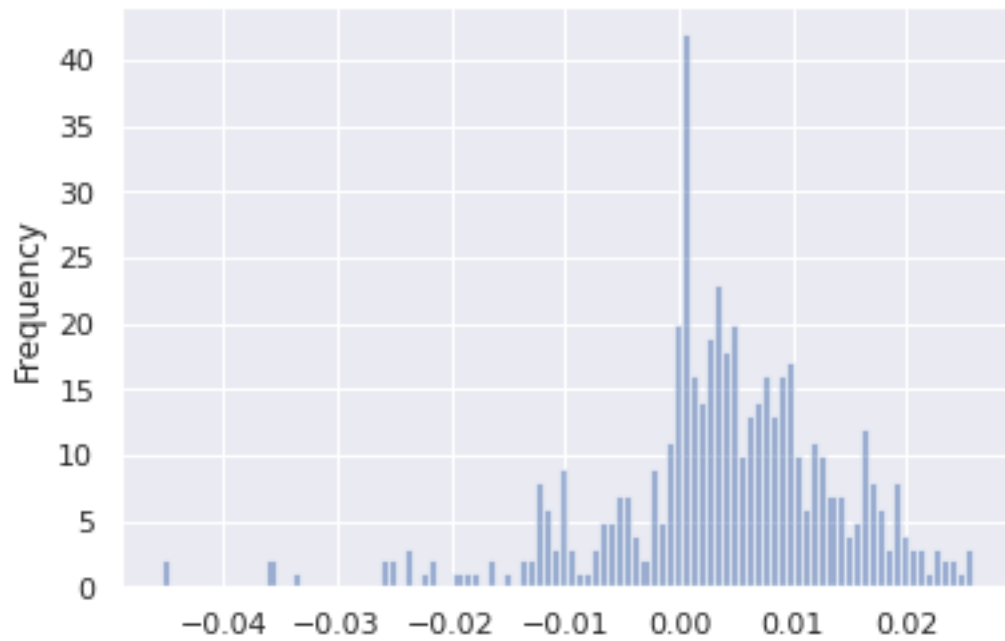
Inferred loglh worse: 336

Inferred n_reticulations less: 415

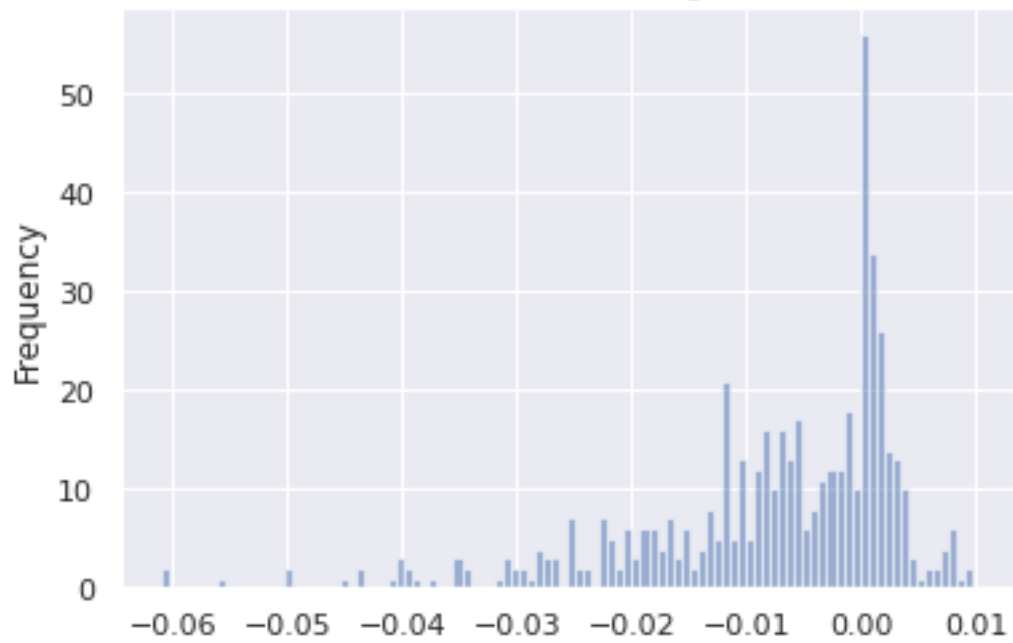
Inferred n_reticulations equal: 89

Inferred n_reticulations more: 0

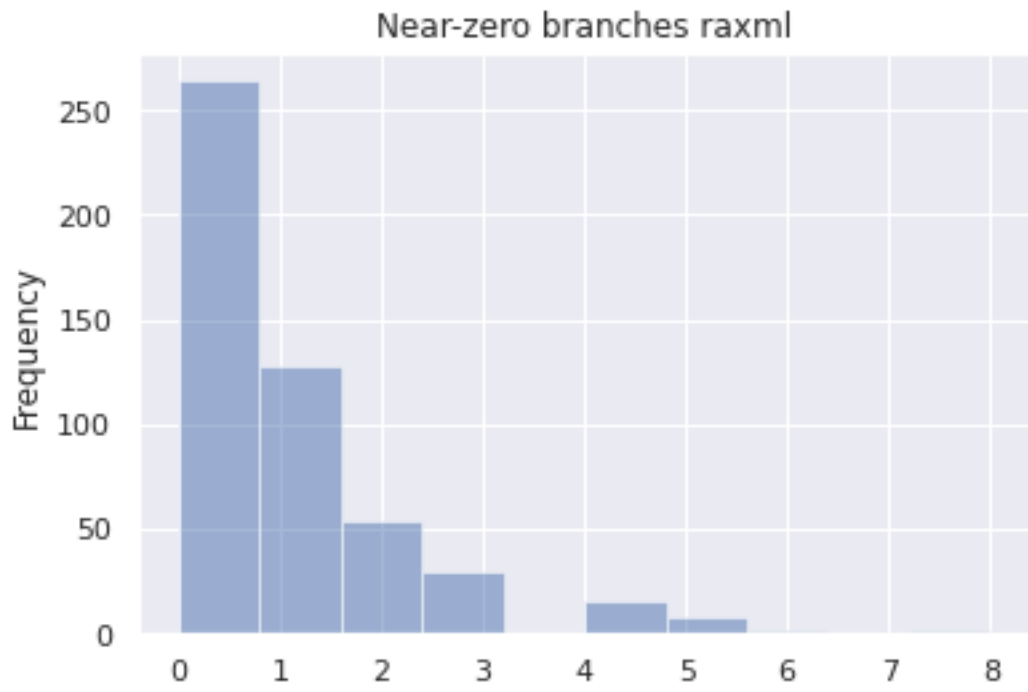
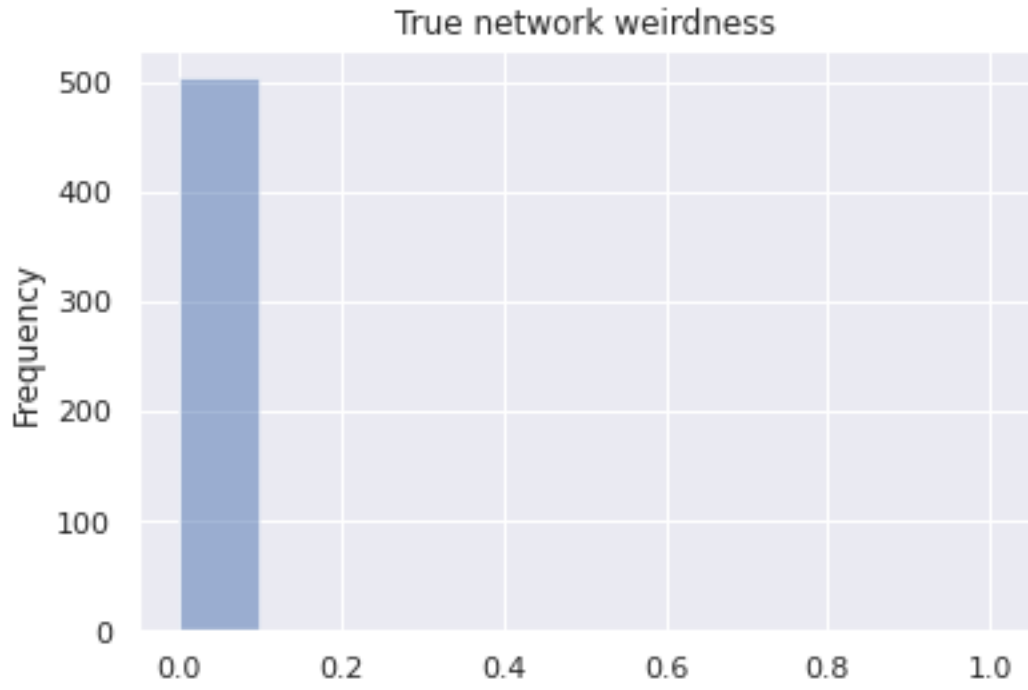
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



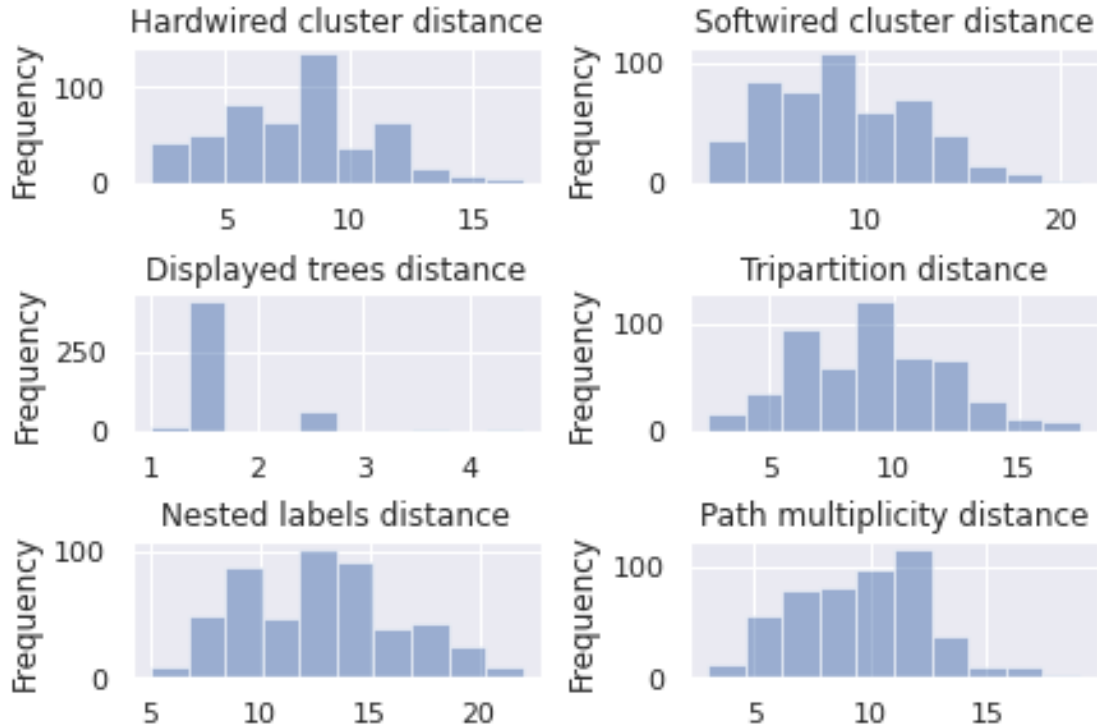
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



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1.1 Plots for MSA_size ~ 100*n_trees

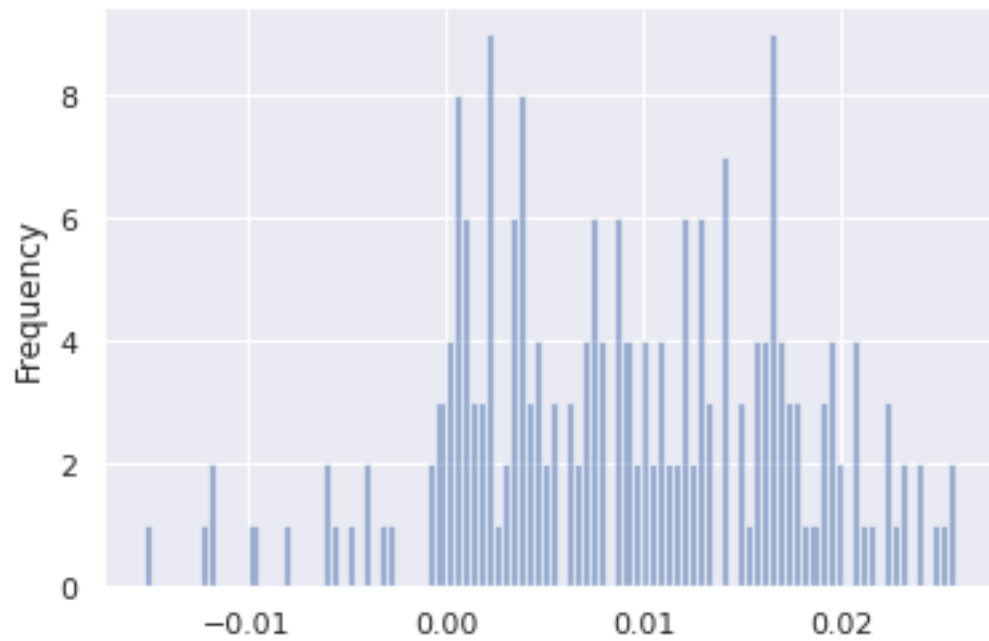
```
[8]: df_raxml_only_msasize_100 = df_raxml_only.query('msa_size == 100')  
      build_stats(df_raxml_only_msasize_100)
```

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

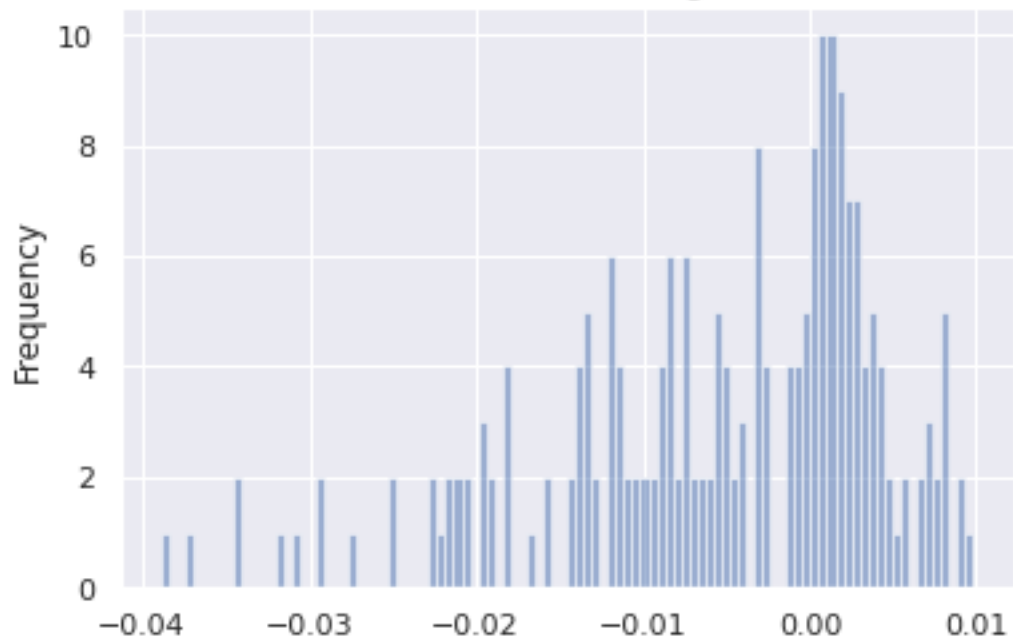
Inferred loglh better or equal: 87
Inferred loglh worse: 123

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

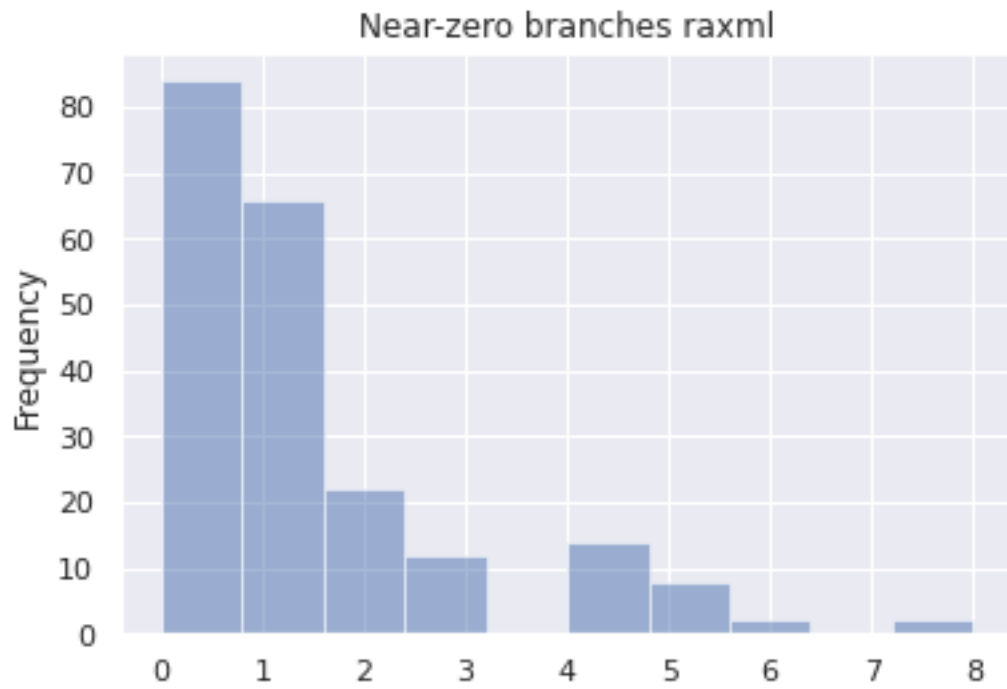
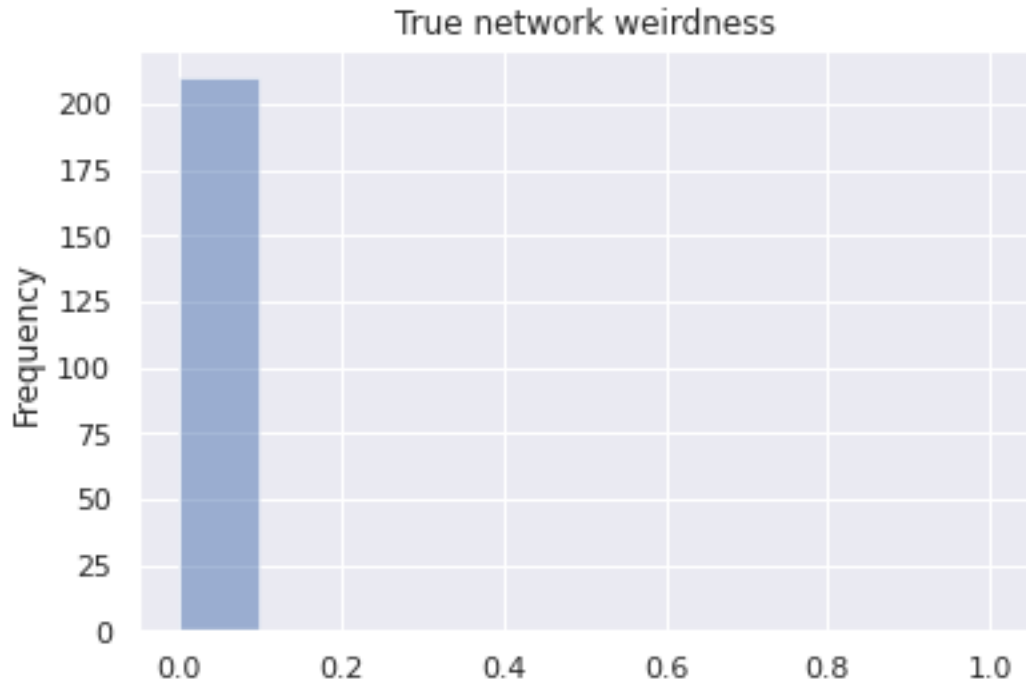
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



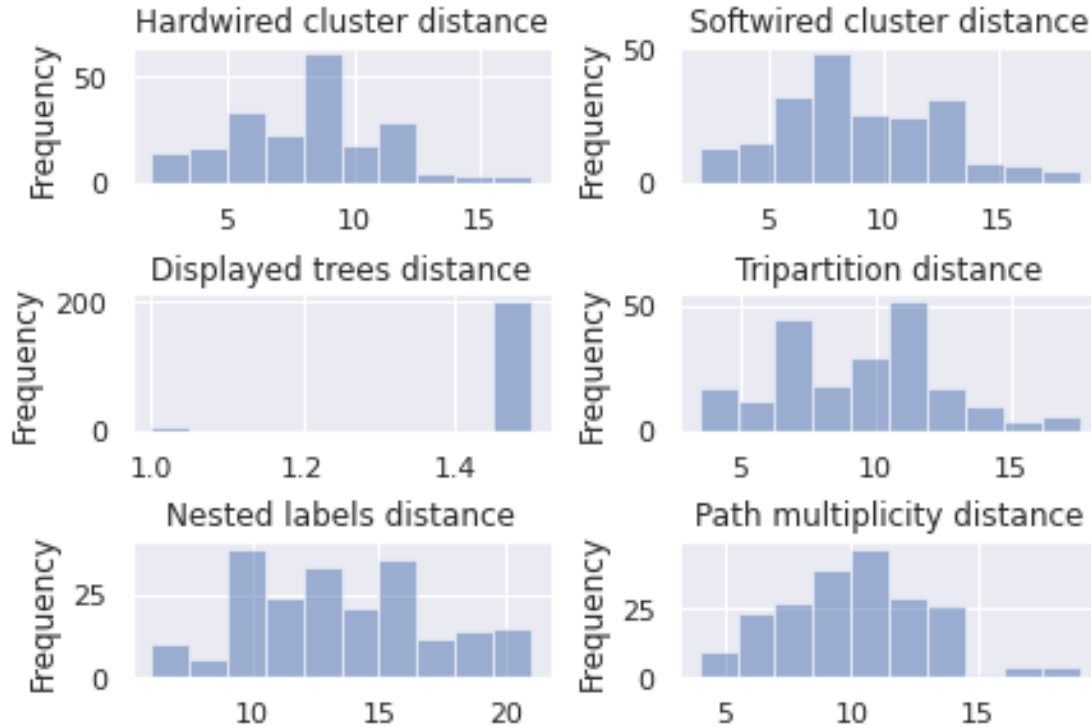
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



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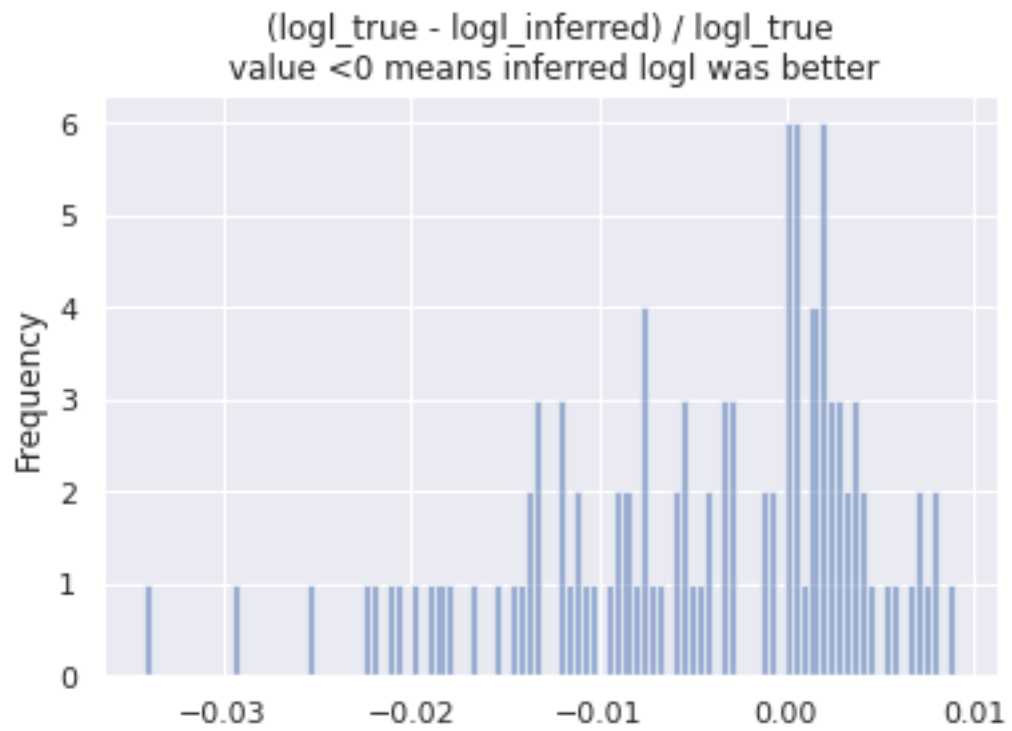
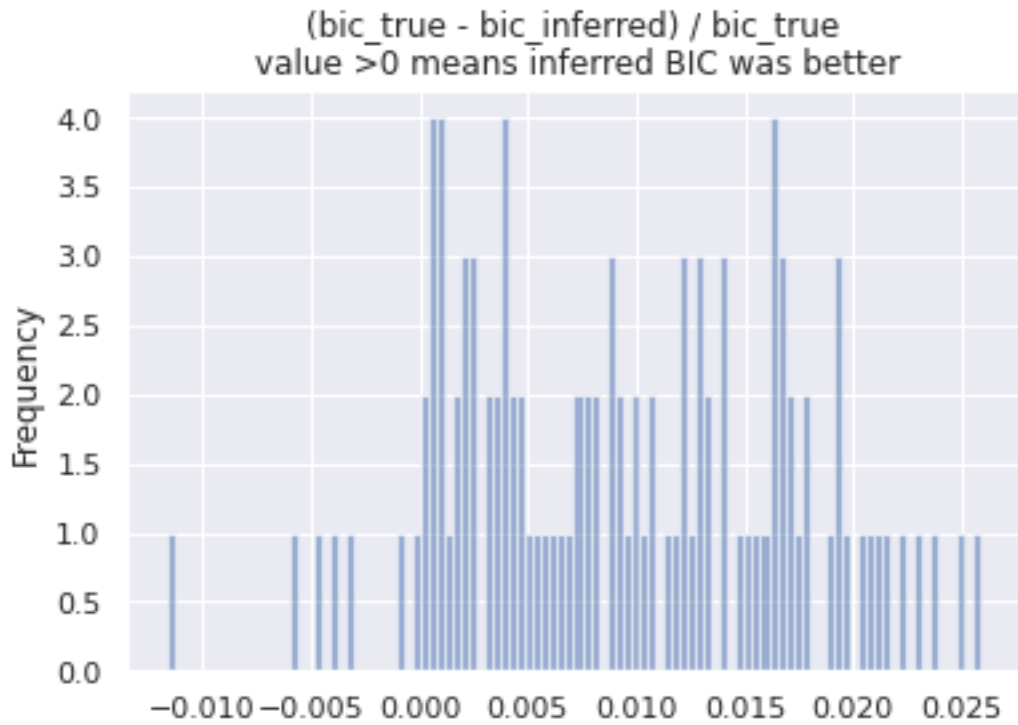
1.1.1 Plots for LikelihoodType.AVERAGE

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

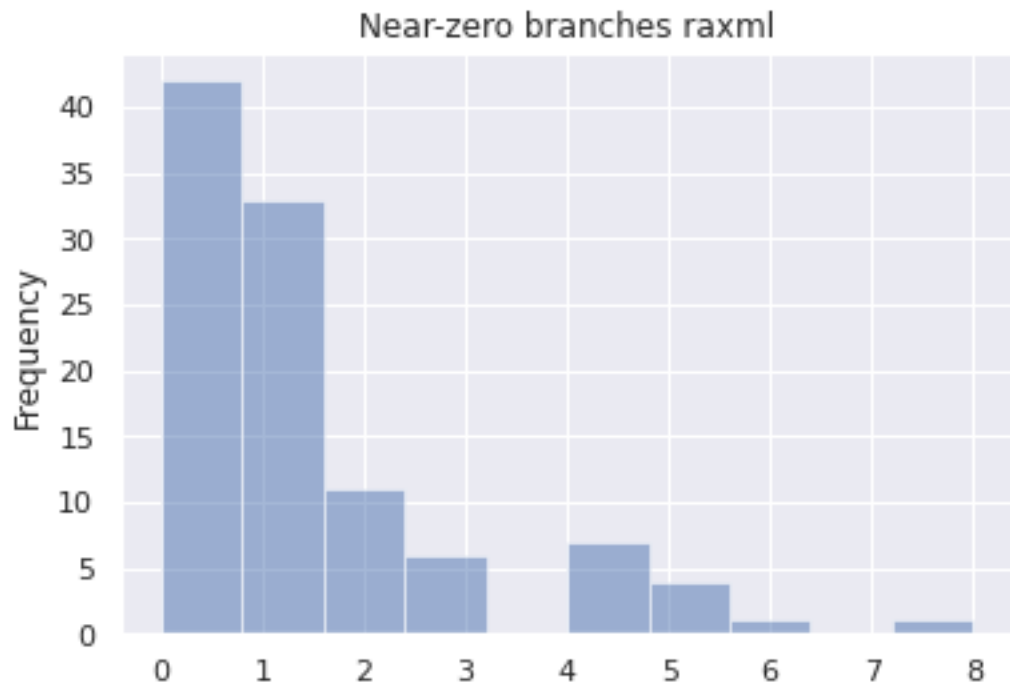
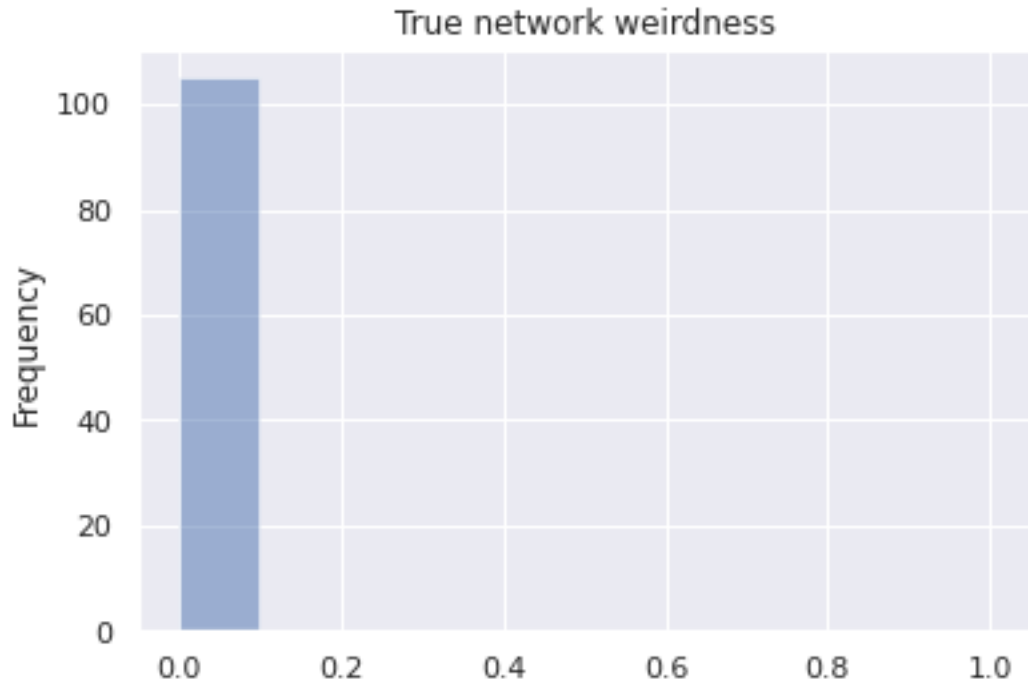
Inferred BIC better or equal: 98
Inferred BIC worse: 7

Inferred loglh better or equal: 45
Inferred loglh worse: 60

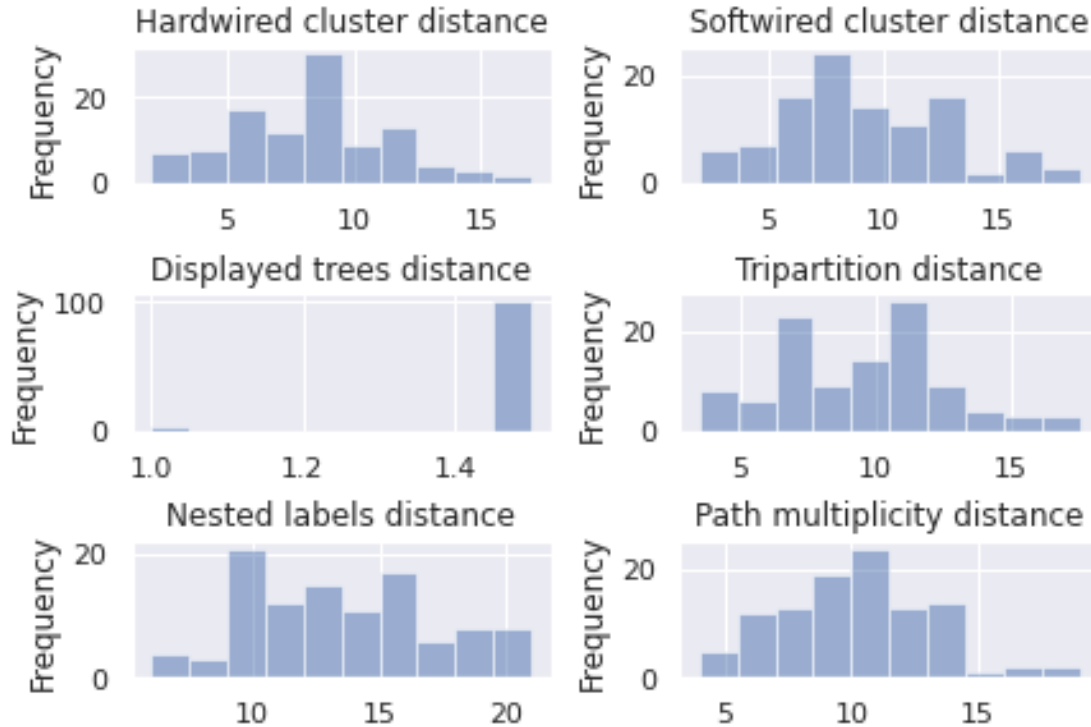
Inferred n_reticulations less: 87
Inferred n_reticulations equal: 18
Inferred n_reticulations more: 0



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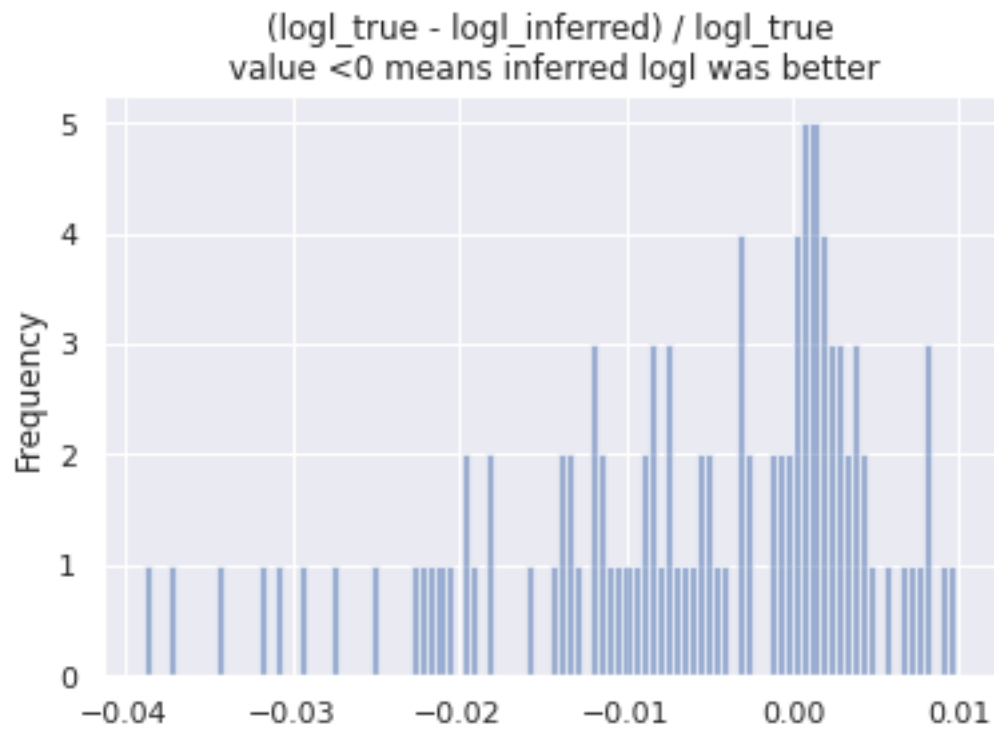
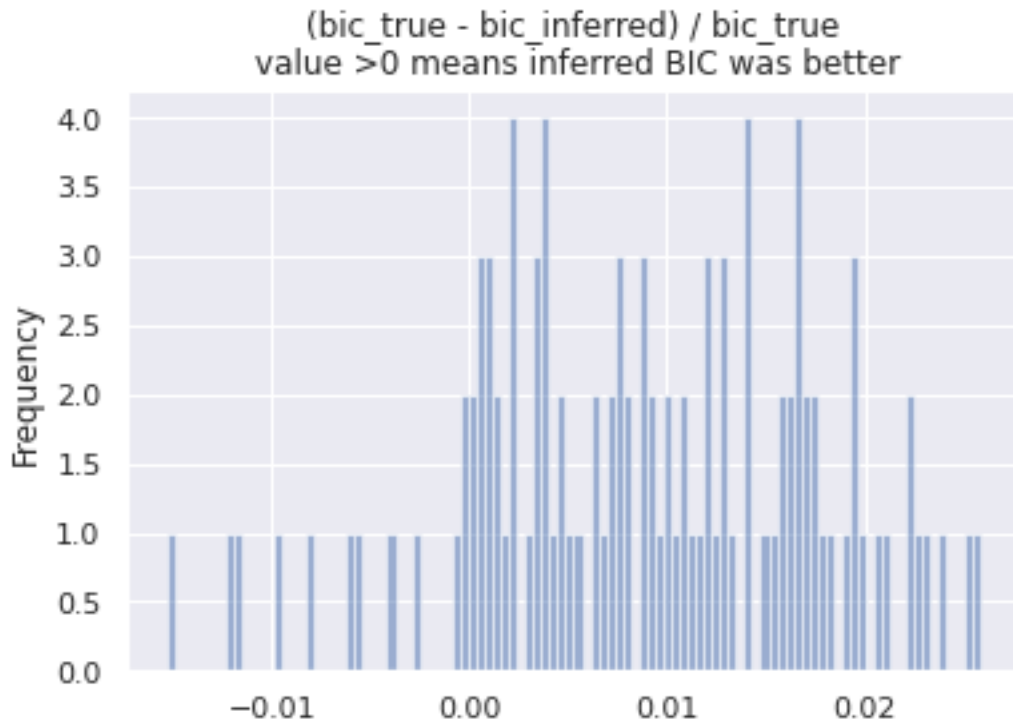
1.1.2 Plots for LikelihoodType.BEST

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

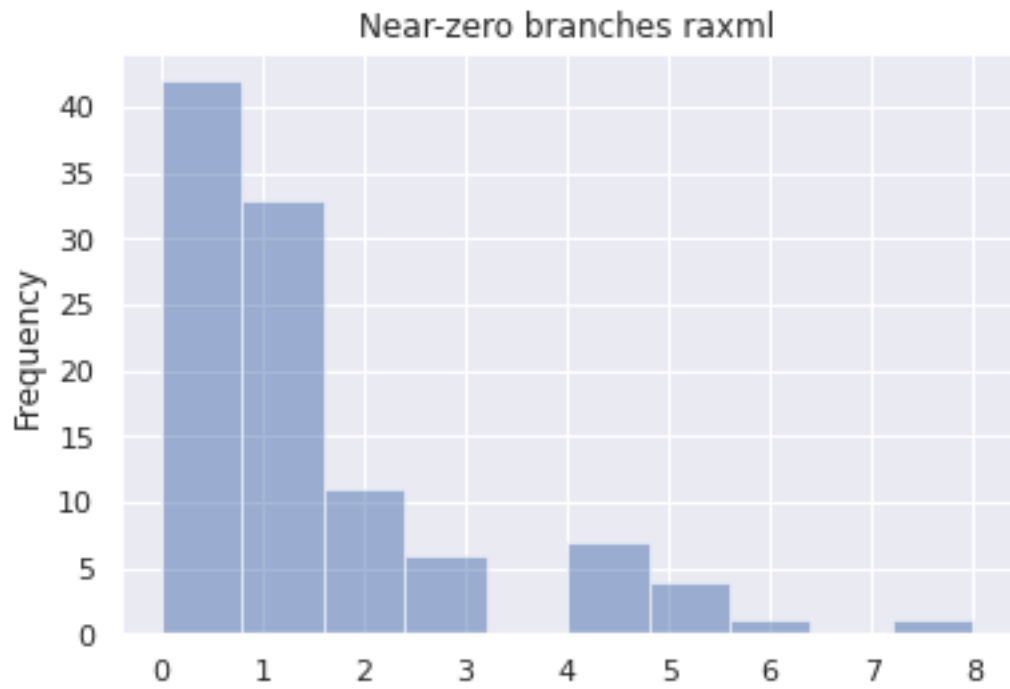
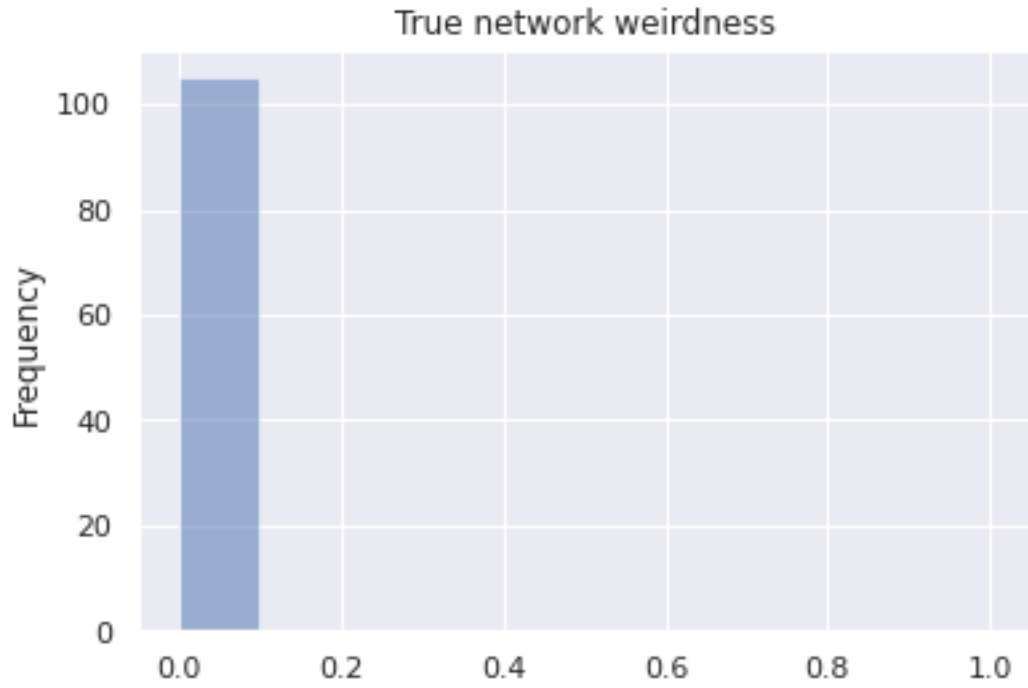
Inferred BIC better or equal: 92
Inferred BIC worse: 13

Inferred loglh better or equal: 42
Inferred loglh worse: 63

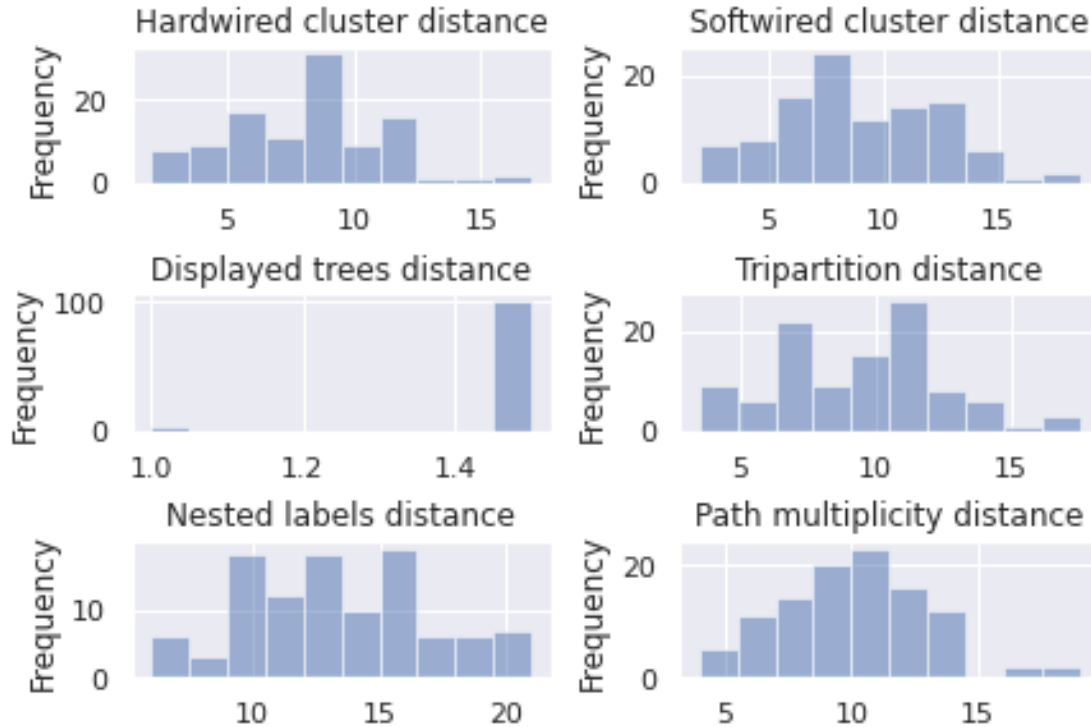
Inferred n_reticulations less: 92
Inferred n_reticulations equal: 13
Inferred n_reticulations more: 0



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1.2 Plots for MSA_size ~ 200*n_trees

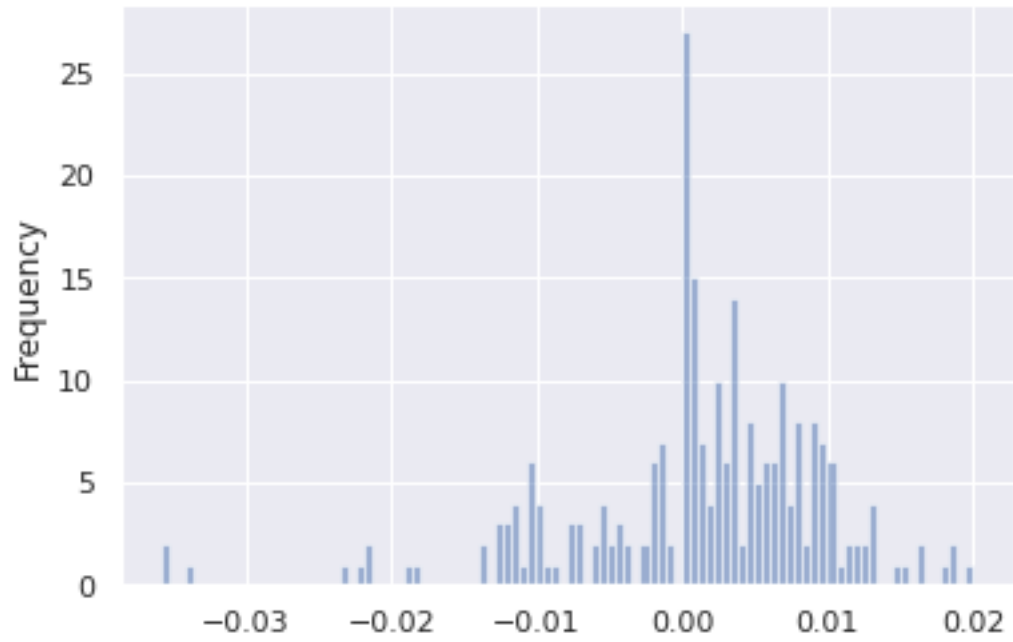
```
[11]: df_raxml_only_msasize_200 = df_raxml_only.query('msa_size == 200')  
      build_stats(df_raxml_only_msasize_200)
```

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

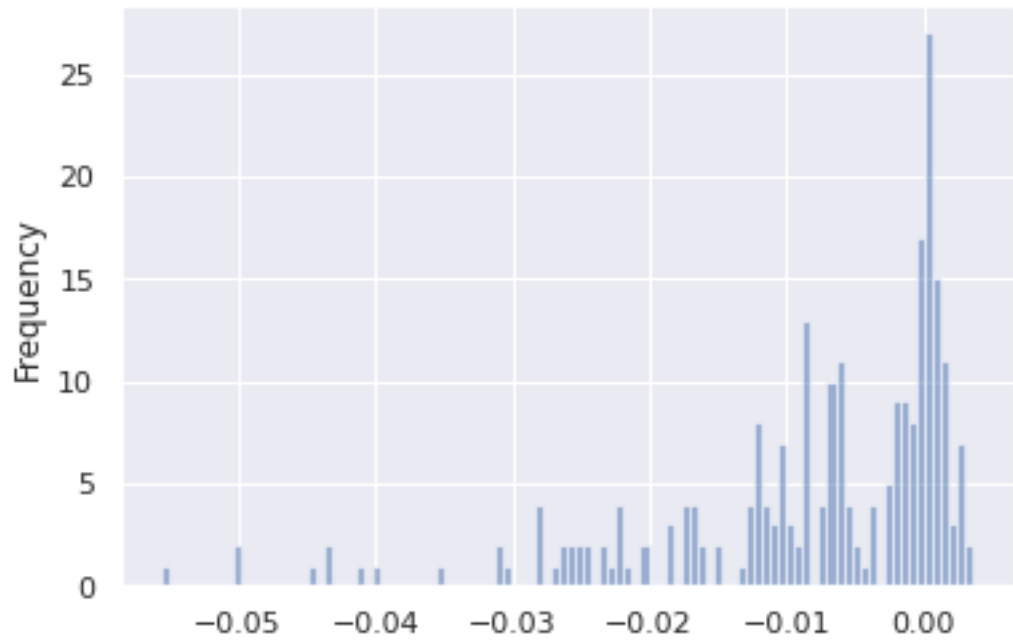
Inferred loglh better or equal: 75
Inferred loglh worse: 169

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

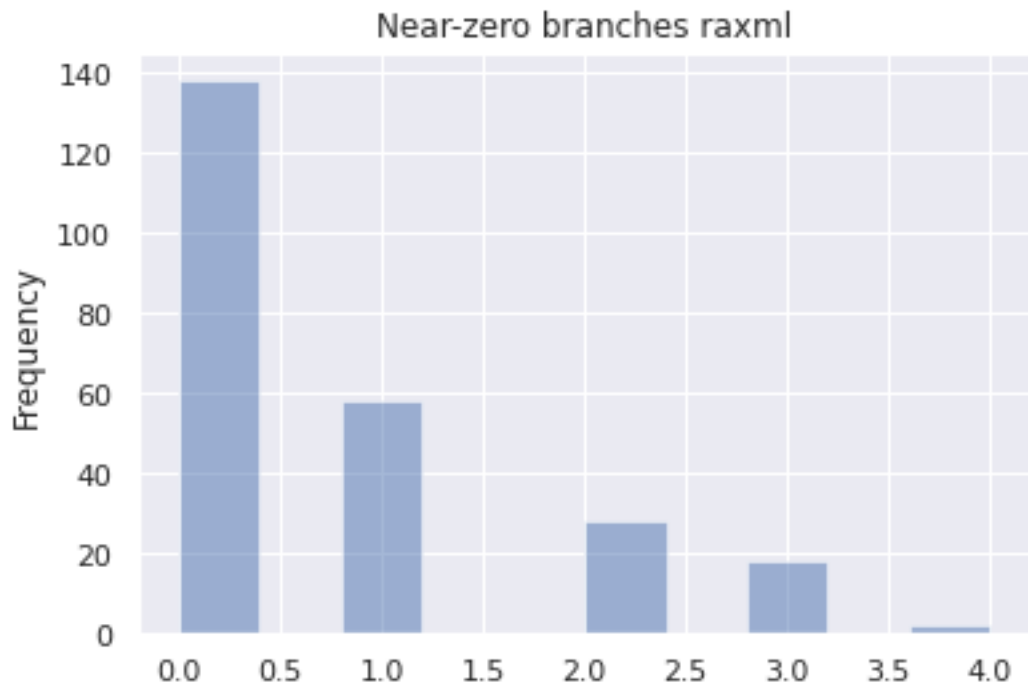
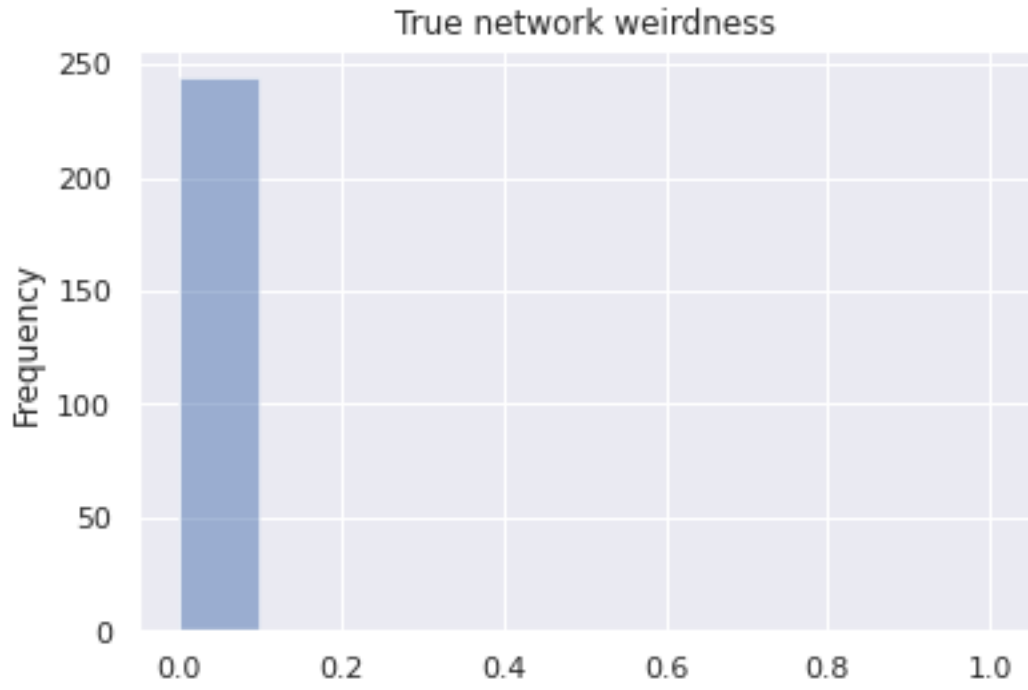
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



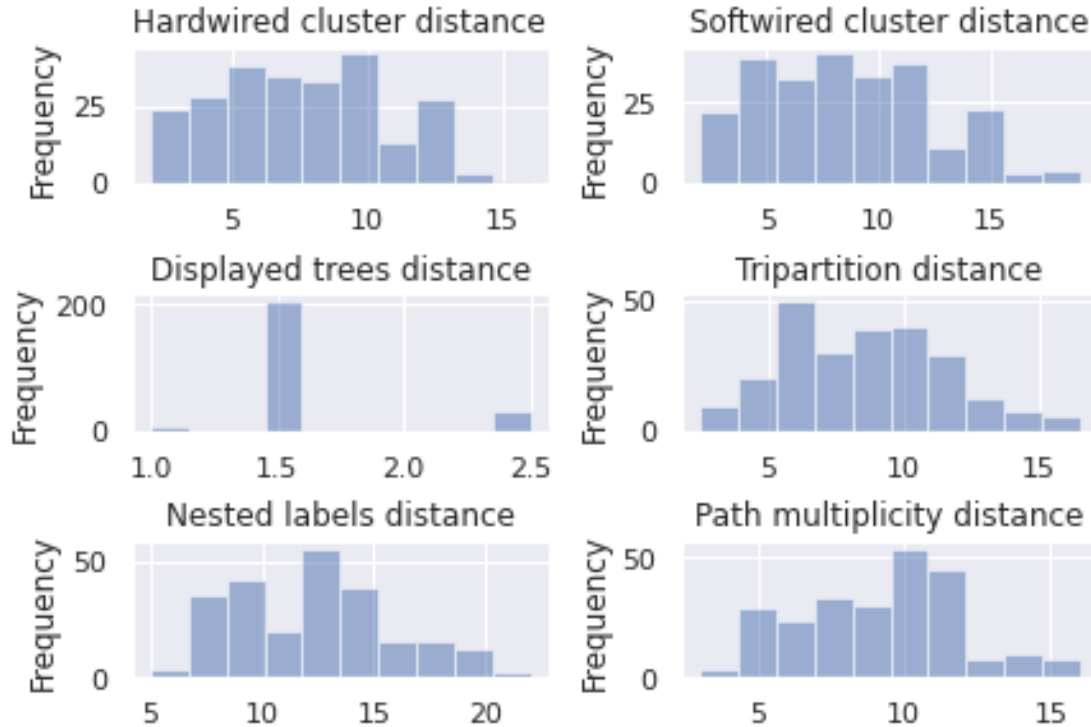
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



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1.2.1 Plots for LikelihoodType.AVERAGE

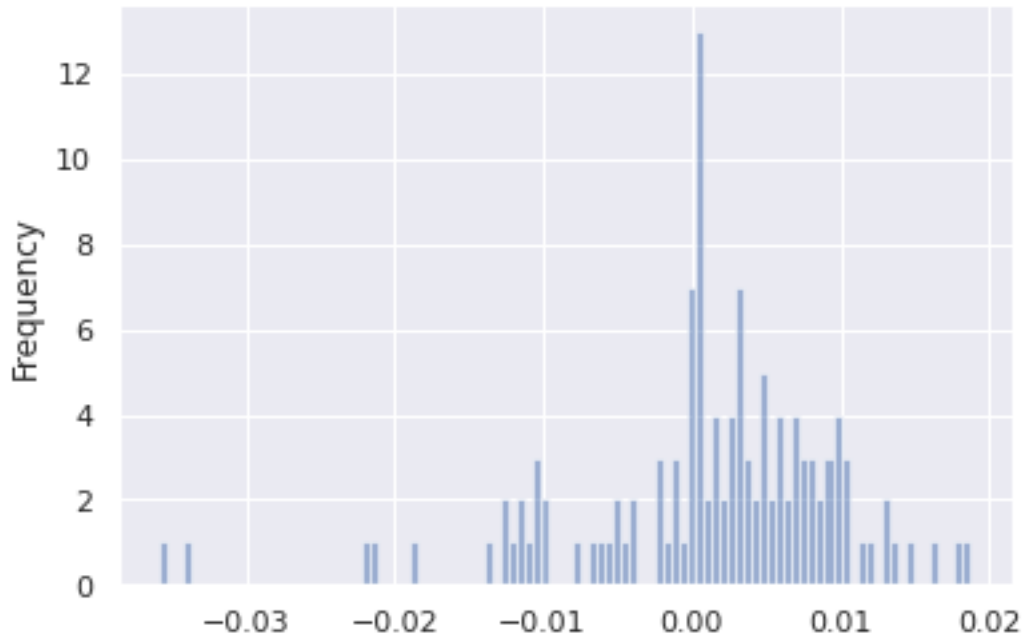
```
[12]: df_raxml_only_msasize_200_average = df_raxml_only_msasize_200.  
      ↪query('likelihood_type == "AVERAGE"')  
      build_stats(df_raxml_only_msasize_200_average)
```

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

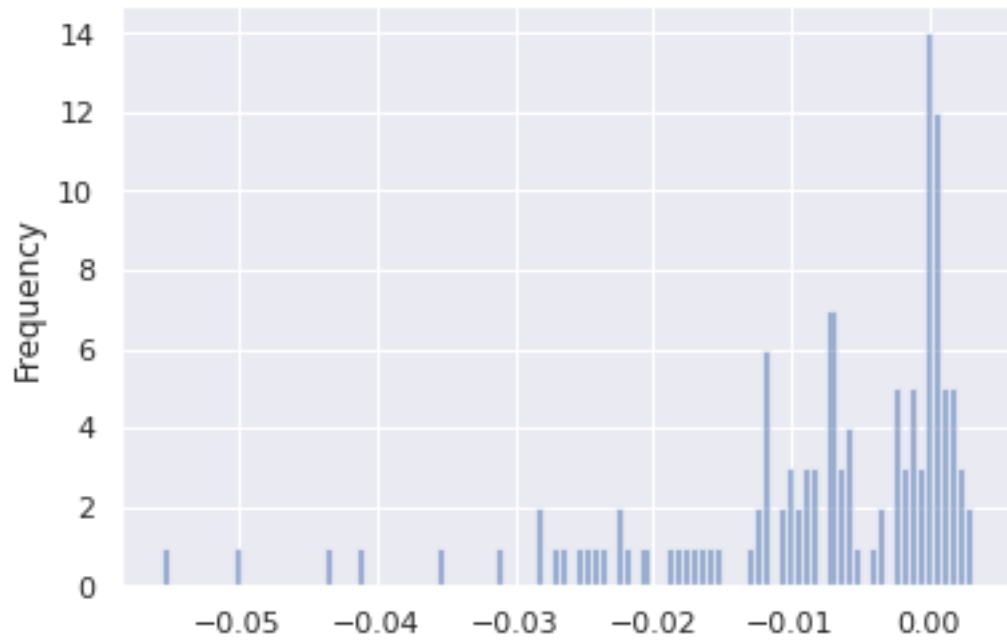
Inferred loglh better or equal: 37
Inferred loglh worse: 85

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

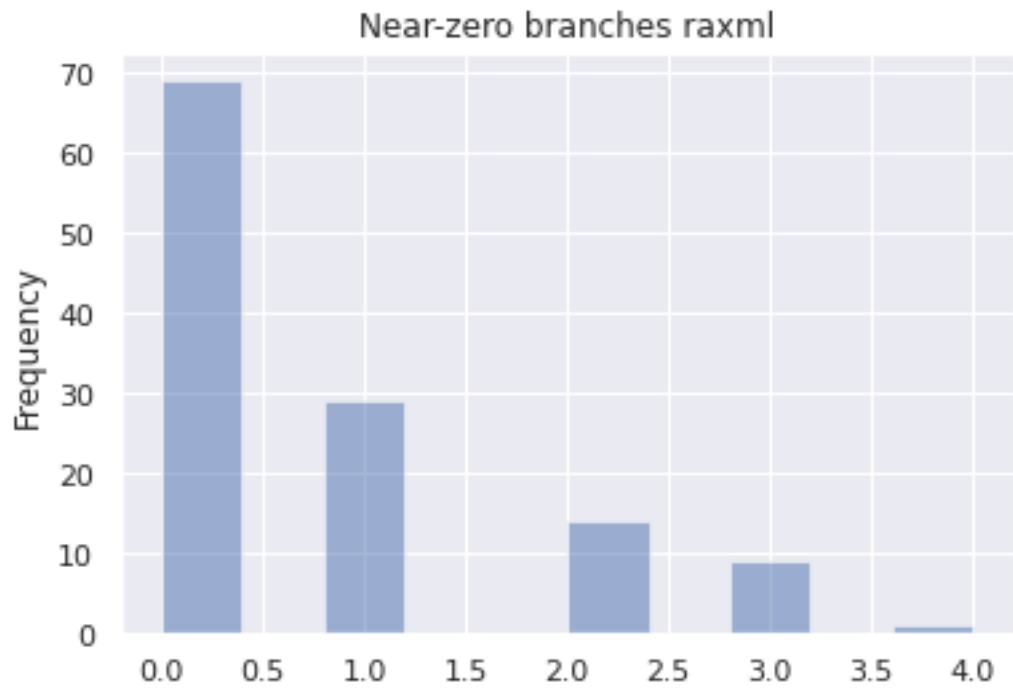
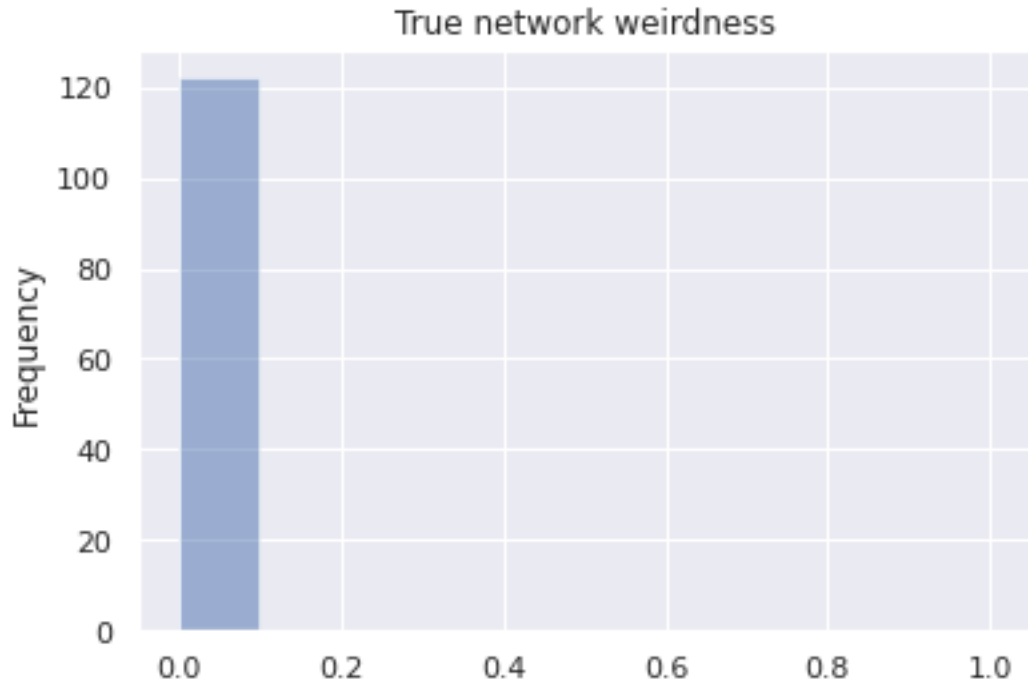
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



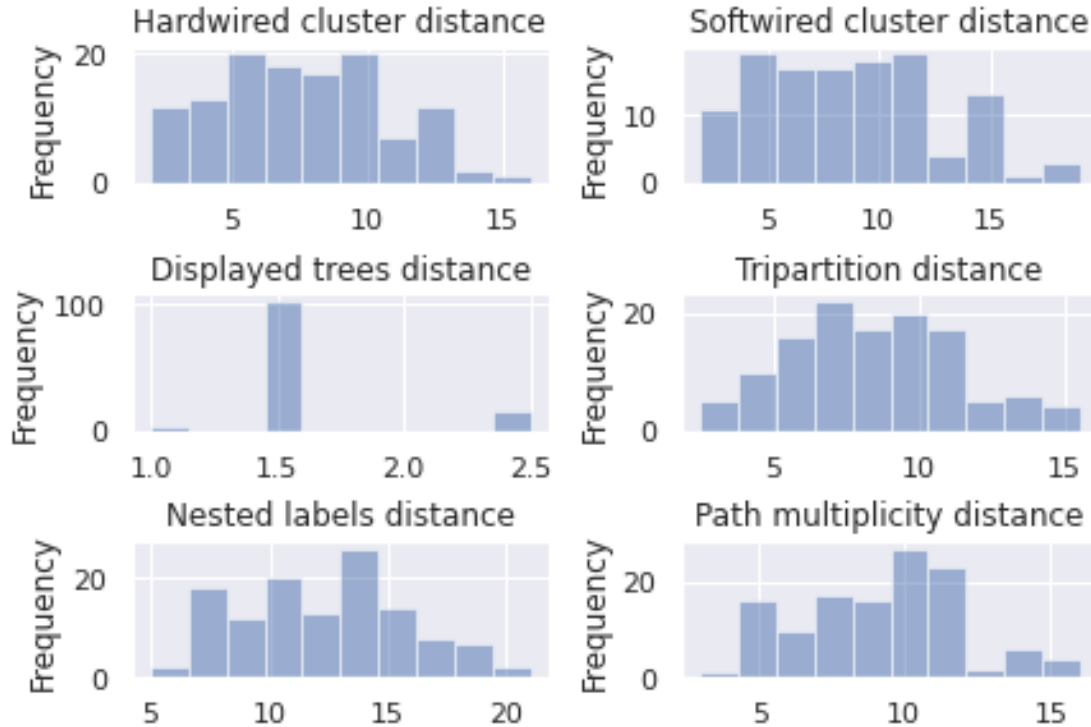
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



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1.2.2 Plots for LikelihoodType.BEST

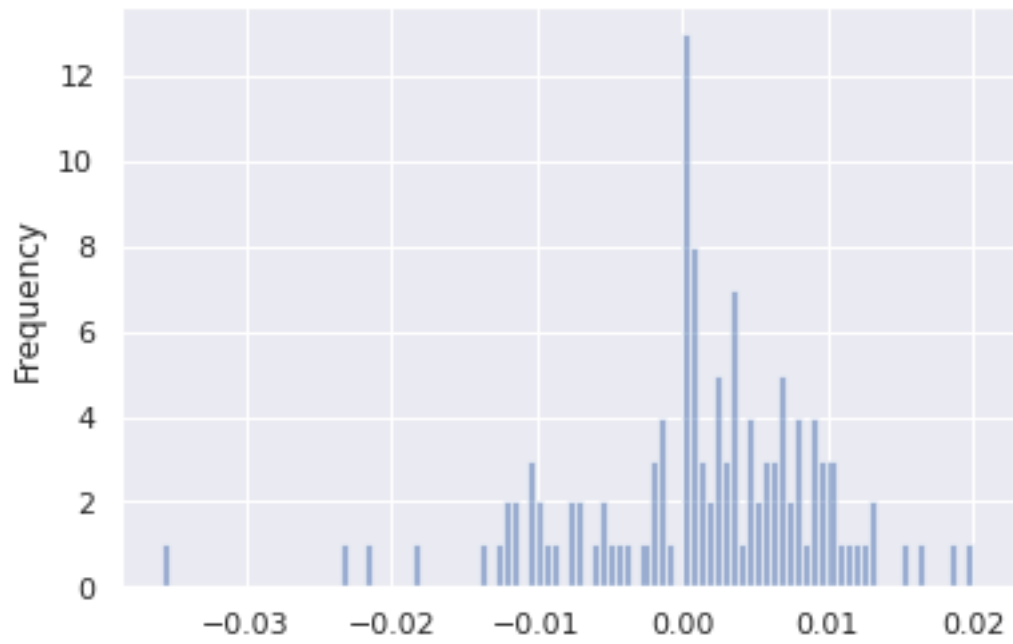
```
[13]: df_raxml_only_msasize_200_best = df_raxml_only_msasize_200.  
      ↪query('likelihood_type == "BEST"')  
      build_stats(df_raxml_only_msasize_200_best)
```

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

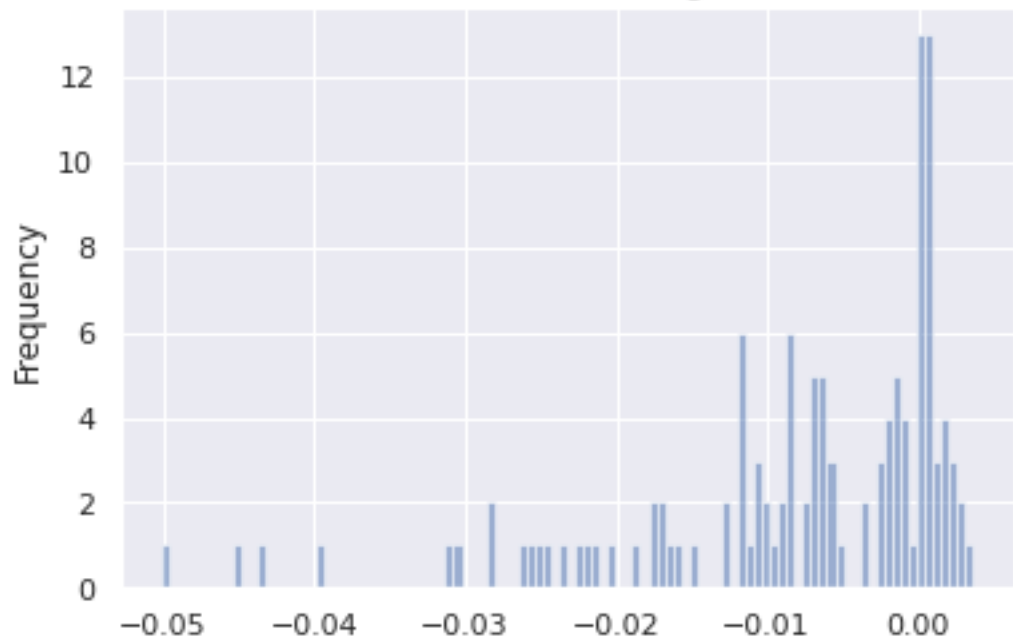
Inferred loglh better or equal: 38
Inferred loglh worse: 84

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

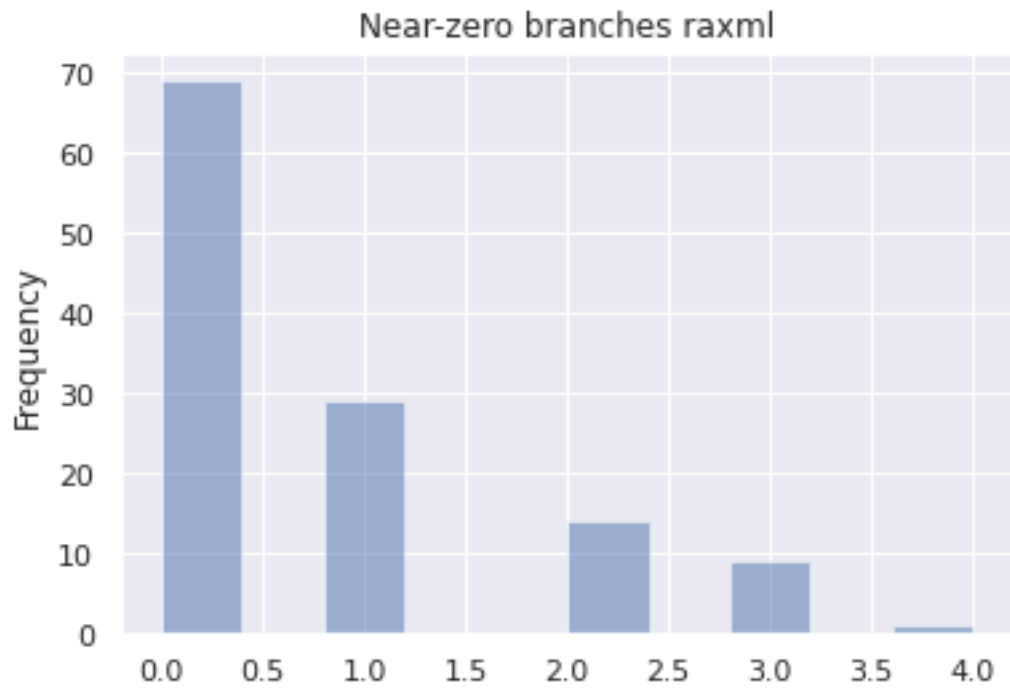
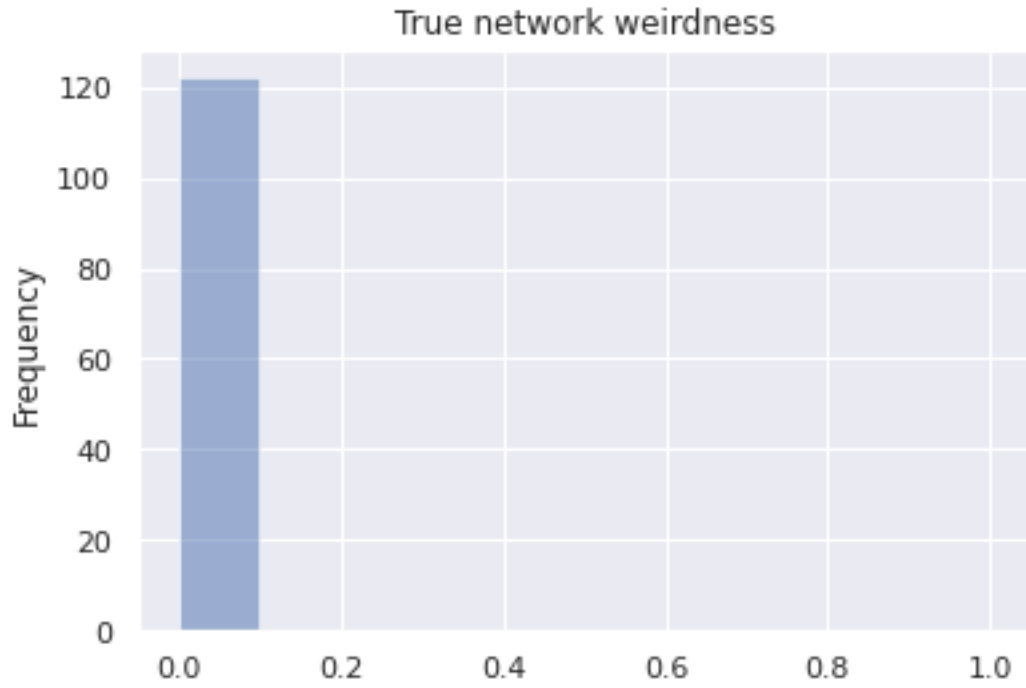
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



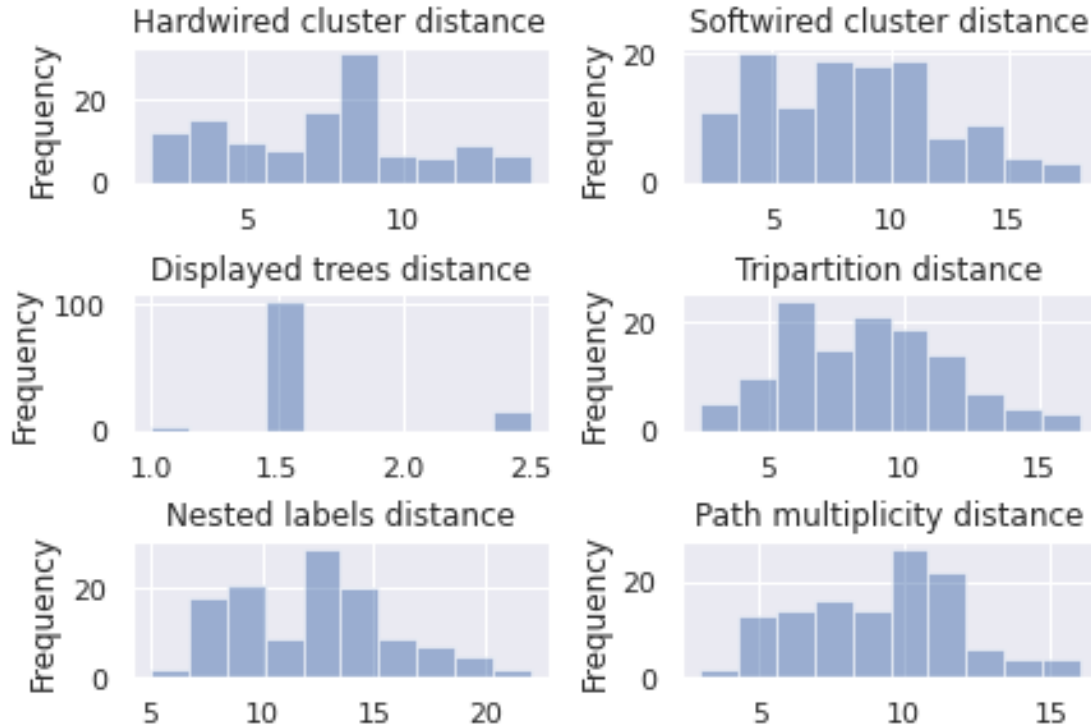
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<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 loglh better or equal: 0

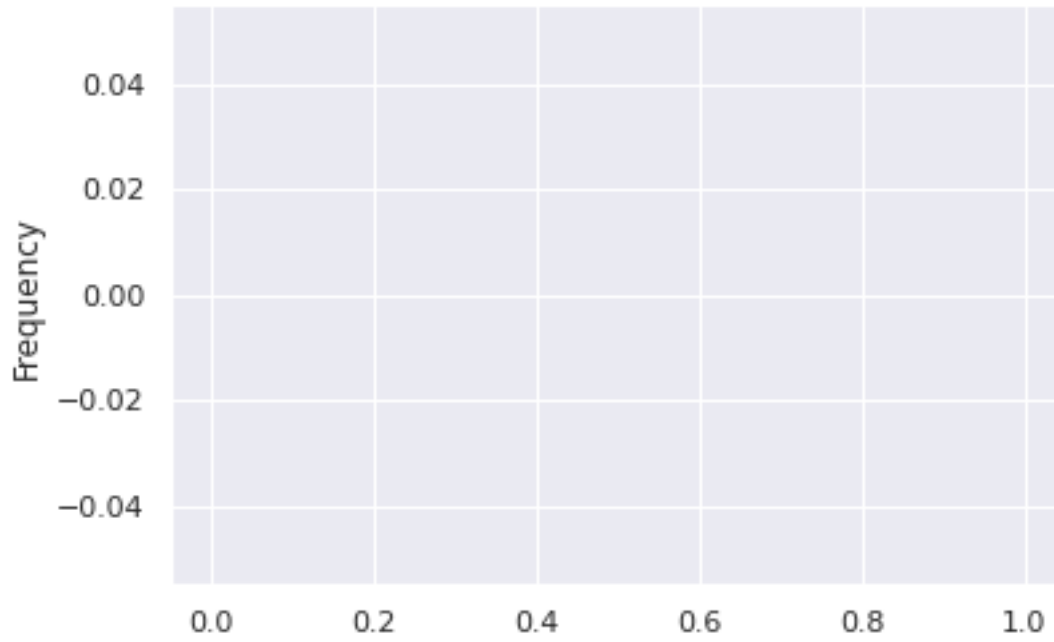
Inferred loglh worse: 0

Inferred n_reticulations less: 0

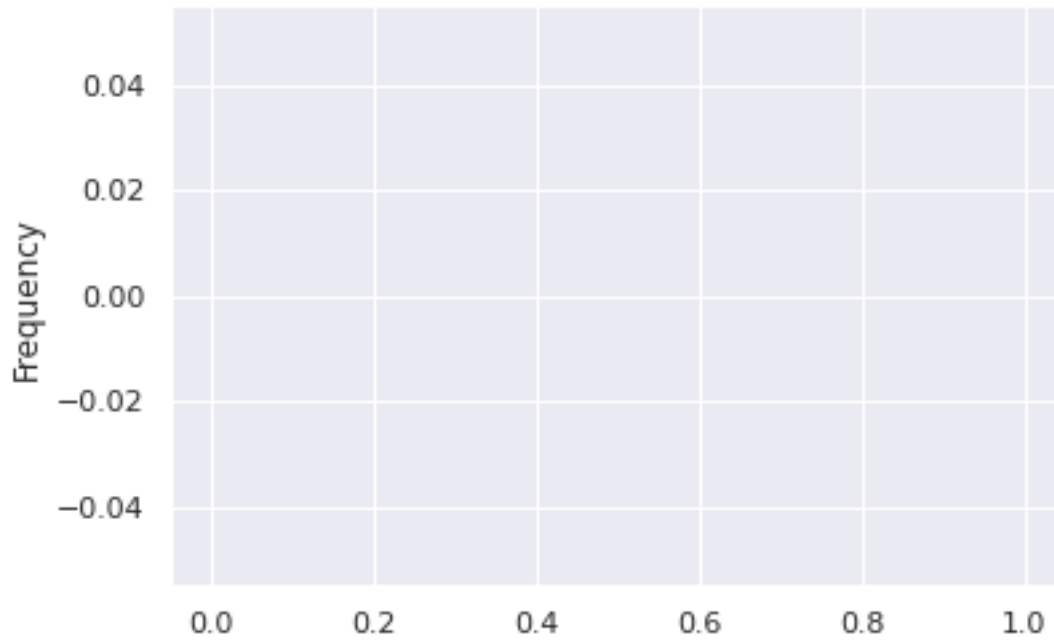
Inferred n_reticulations equal: 0

Inferred n_reticulations more: 0

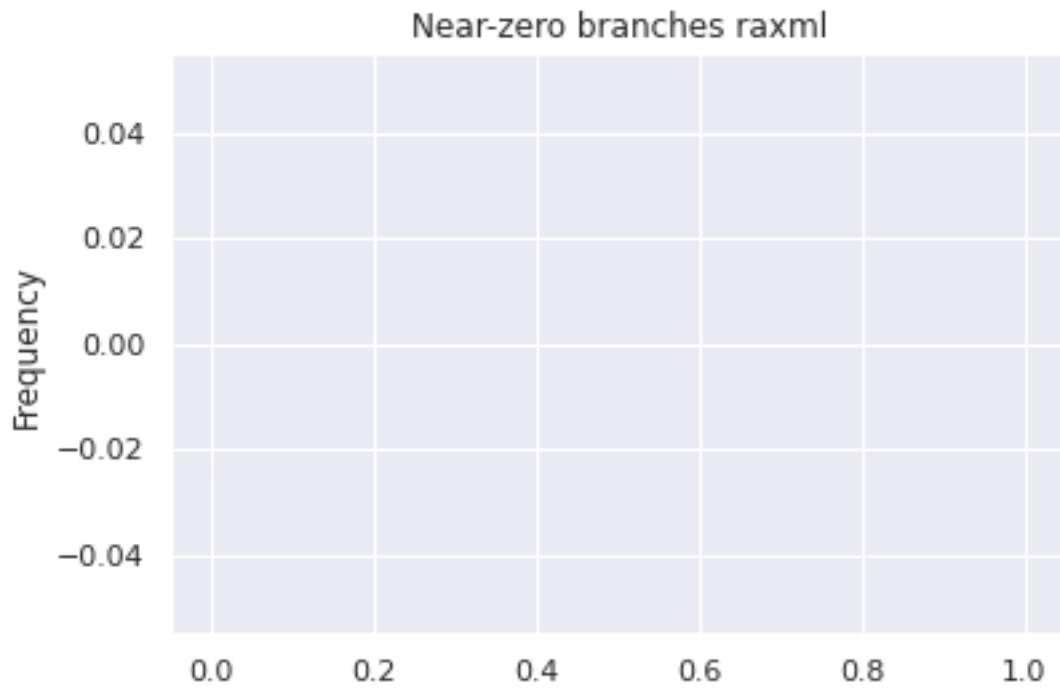
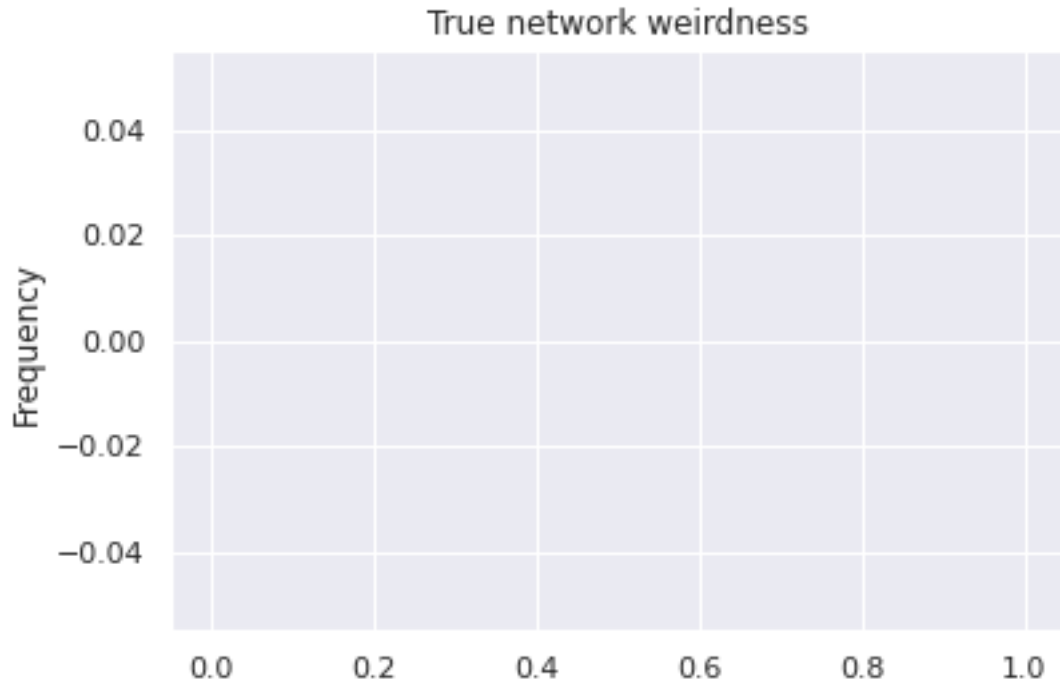
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



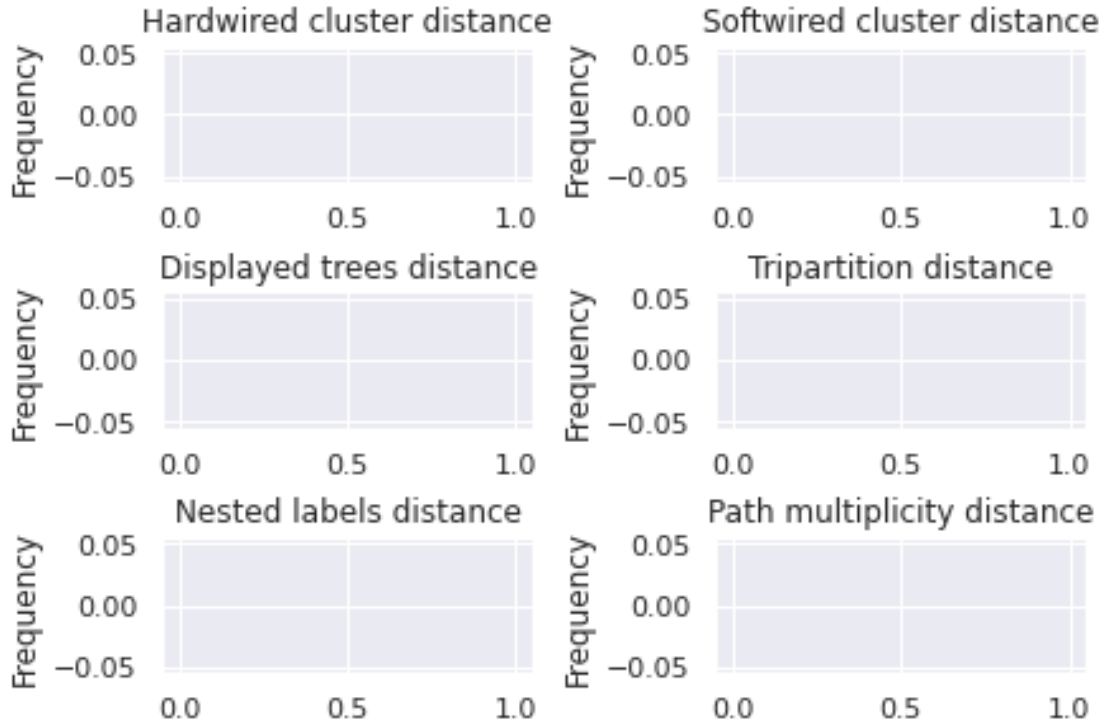
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>



2.1 Plots for $MSA_size \sim 100 * n_trees$

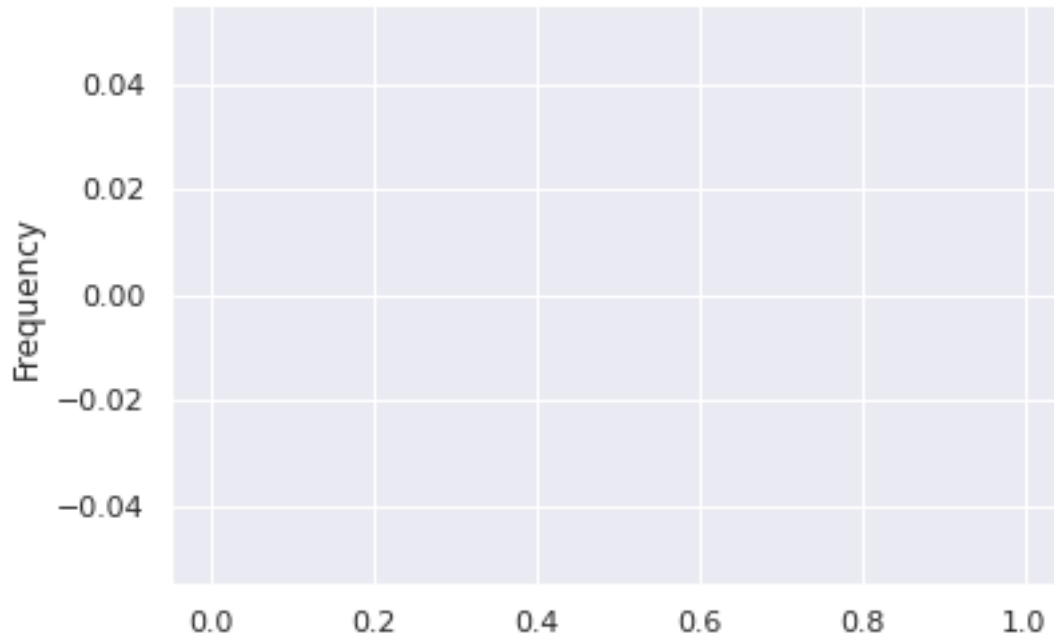
```
[15]: df_random_msasize_100 = df_random.query('msa_size == 100')
      build_stats(df_random_msasize_100)
```

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

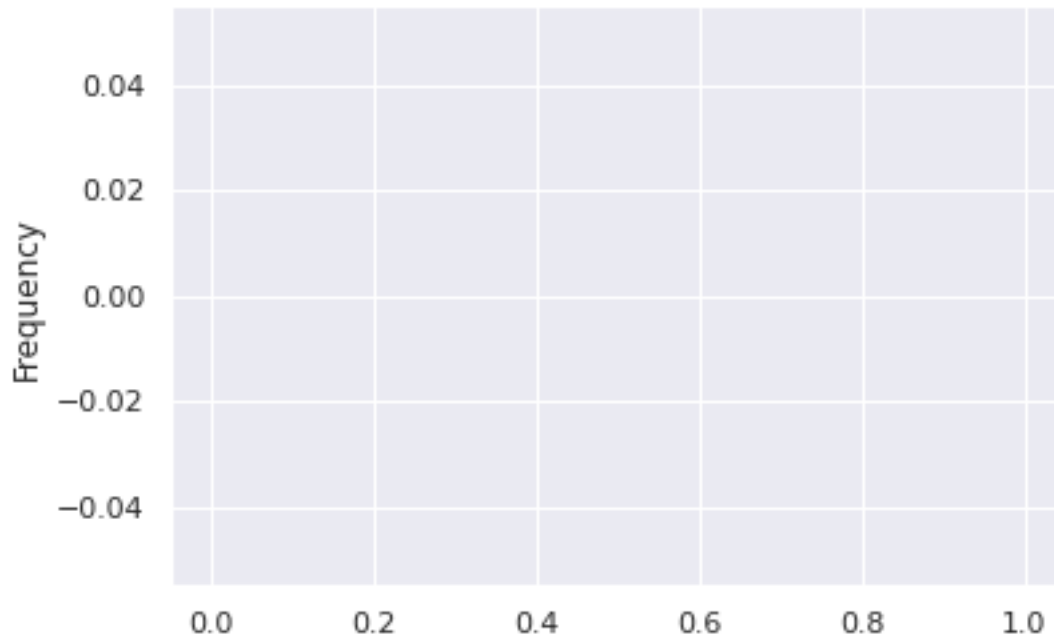
Inferred loglh better or equal: 0
Inferred loglh worse: 0

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

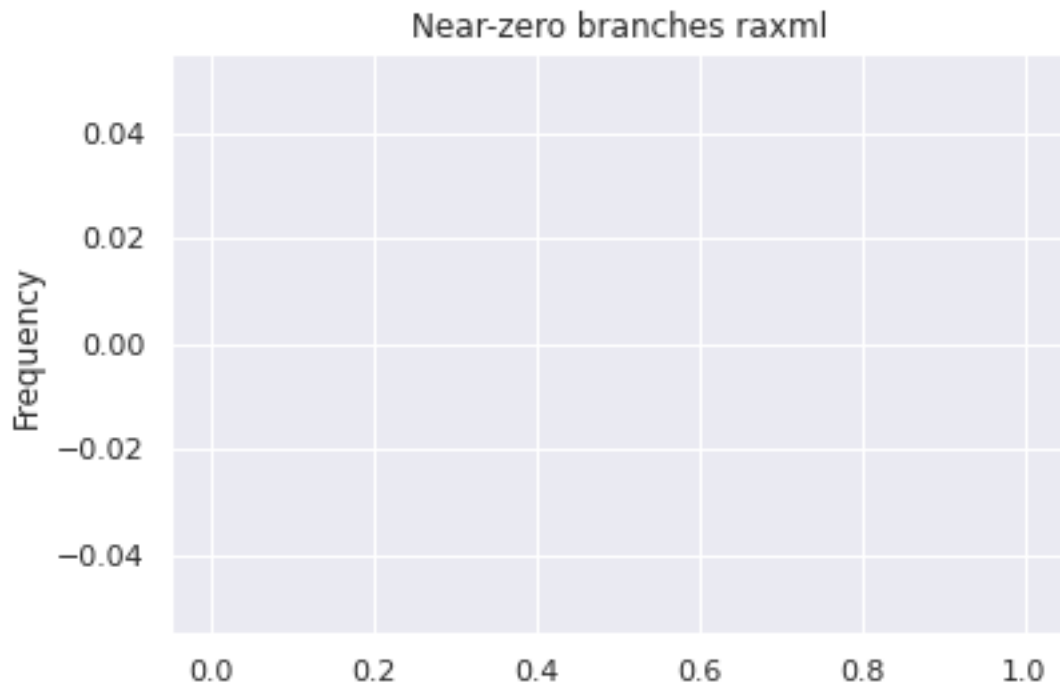
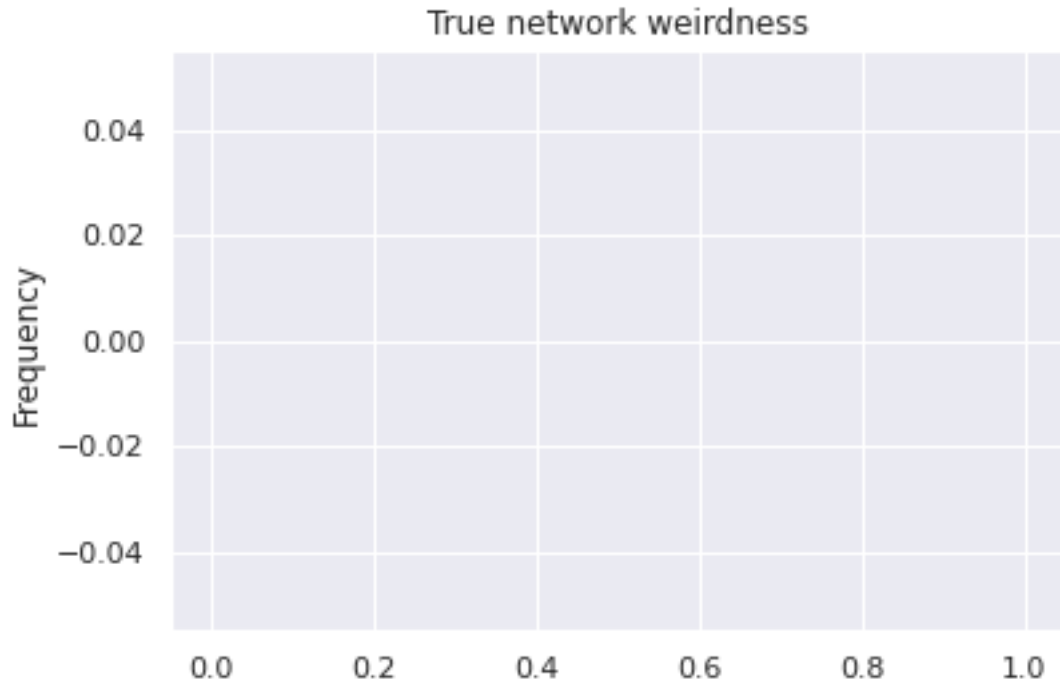
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



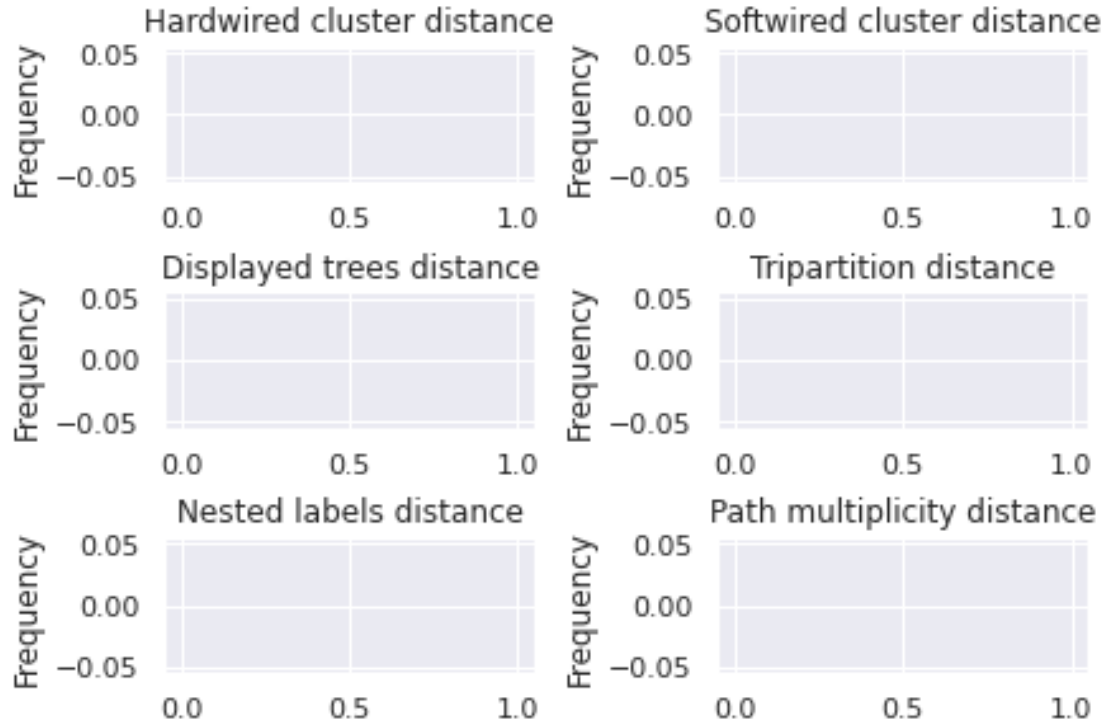
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>



2.1.1 Plots for LikelihoodType.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 loglh better or equal: 0

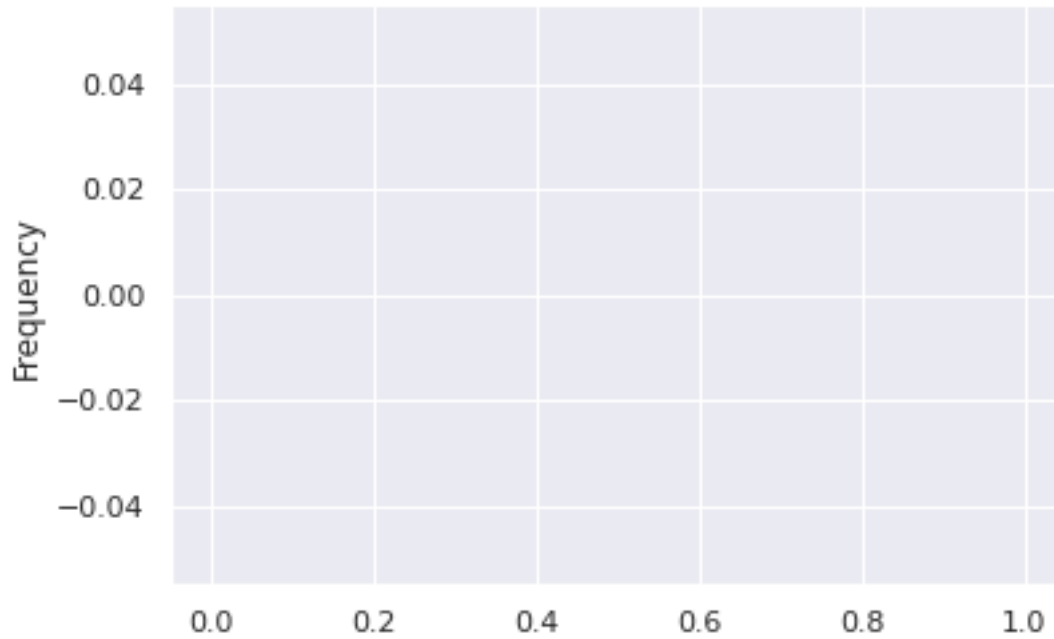
Inferred loglh worse: 0

Inferred n_reticulations less: 0

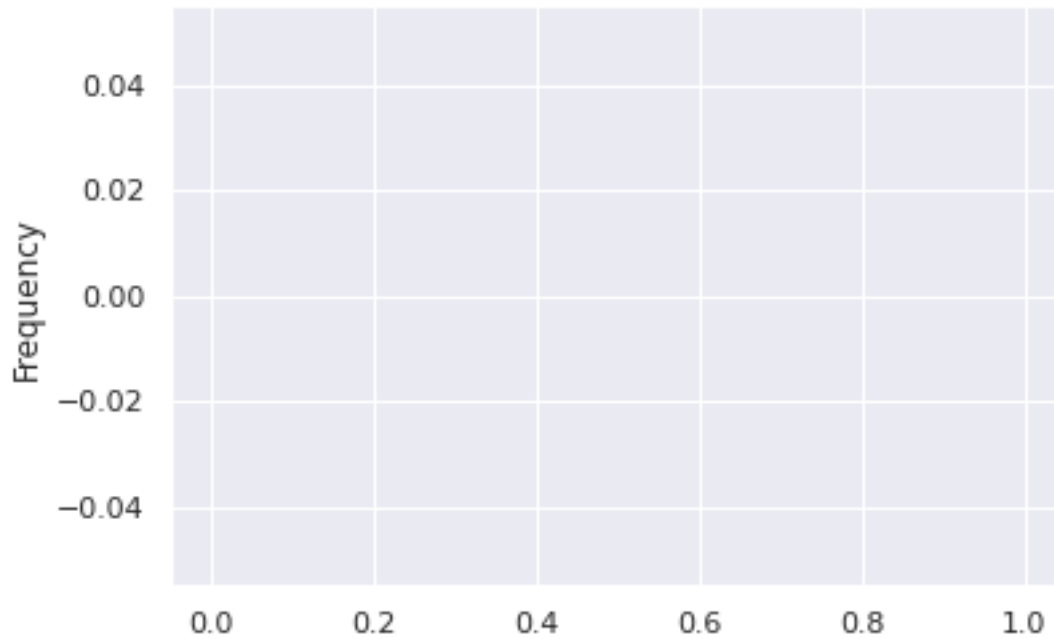
Inferred n_reticulations equal: 0

Inferred n_reticulations more: 0

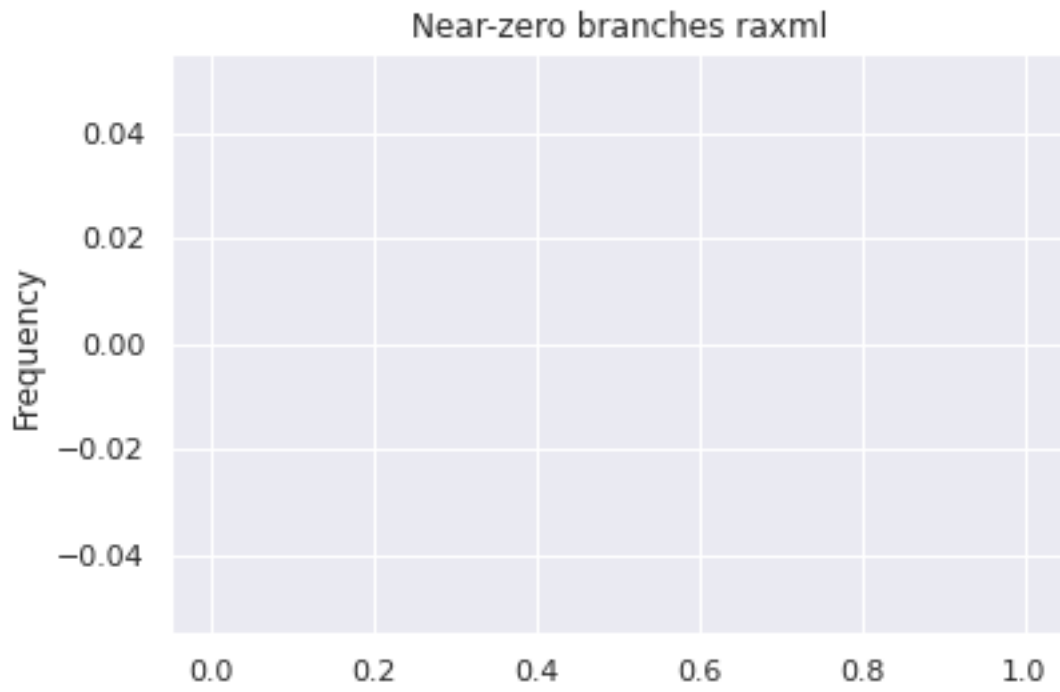
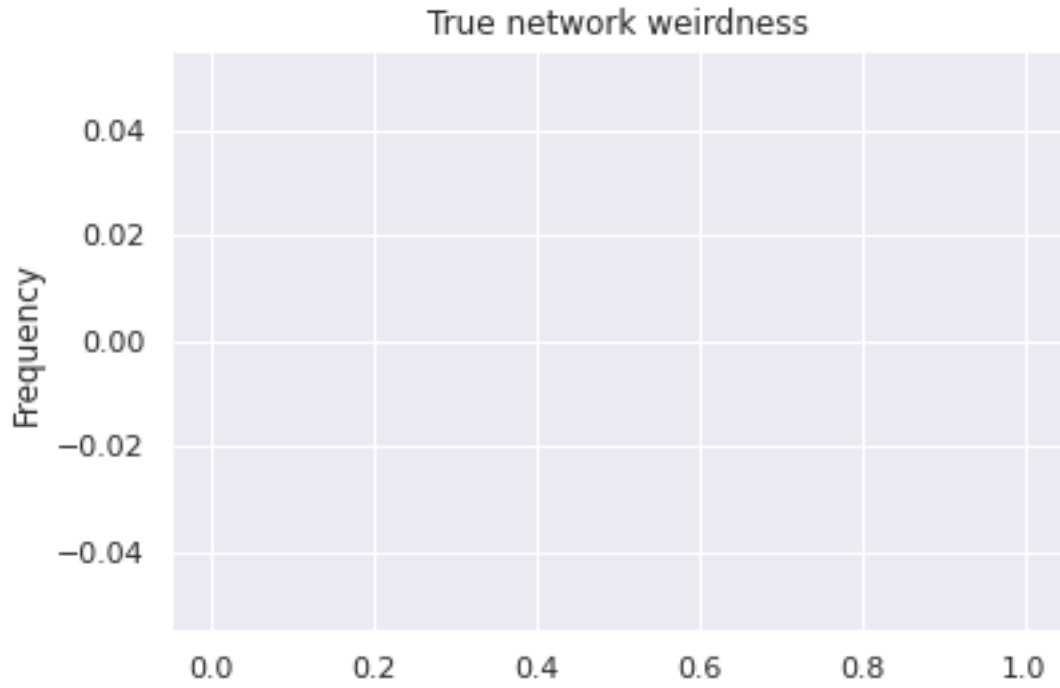
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



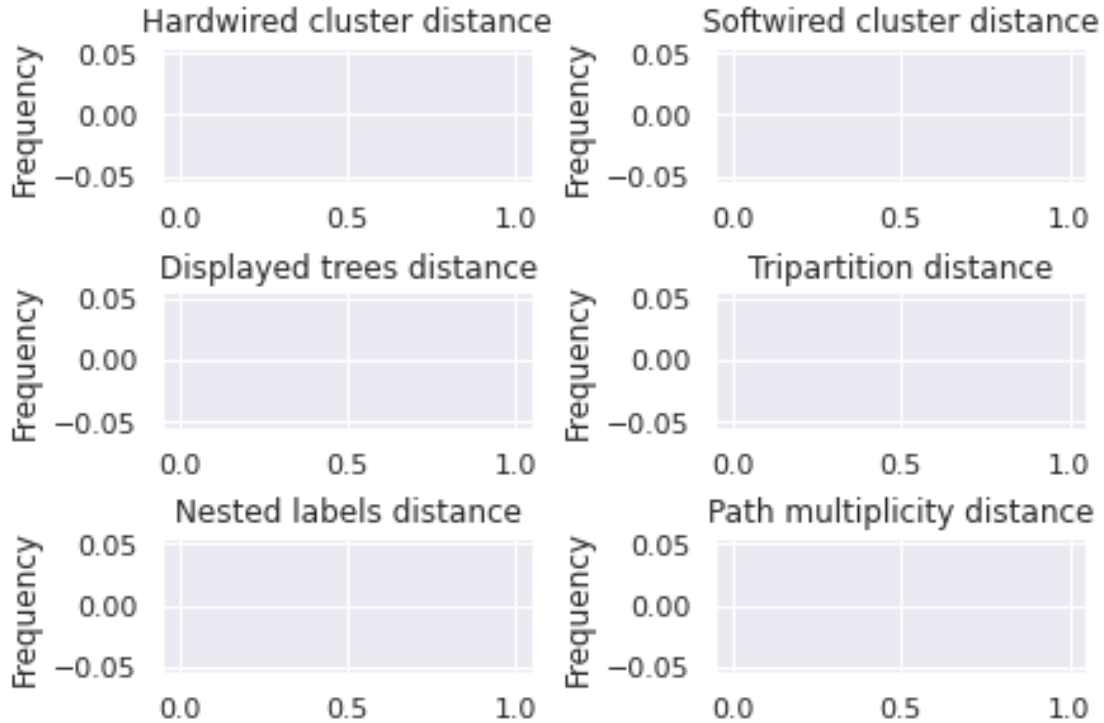
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<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 loglh better or equal: 0

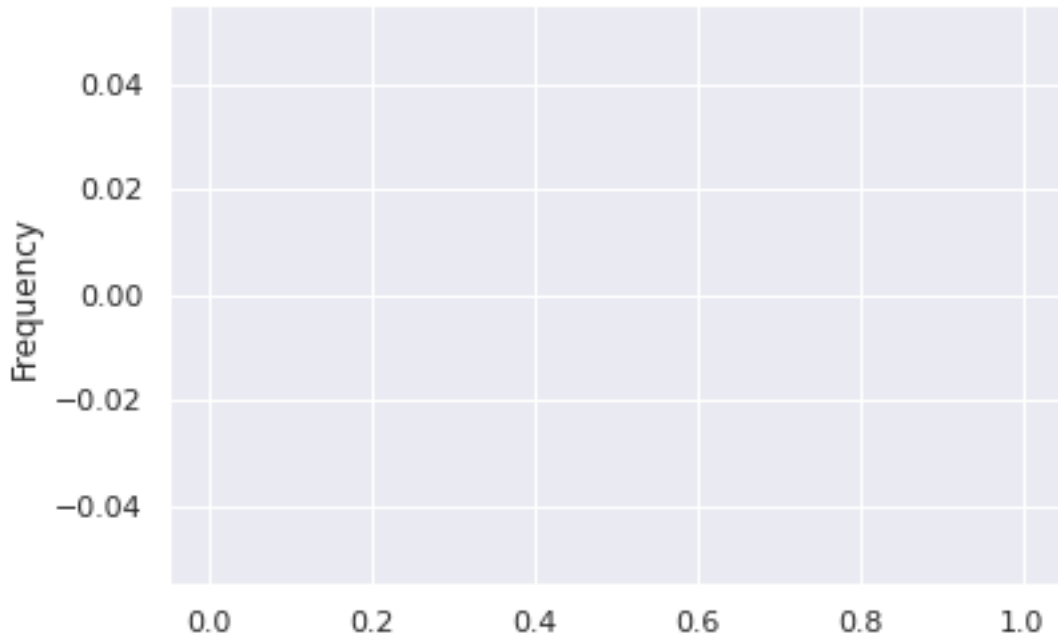
Inferred loglh worse: 0

Inferred n_reticulations less: 0

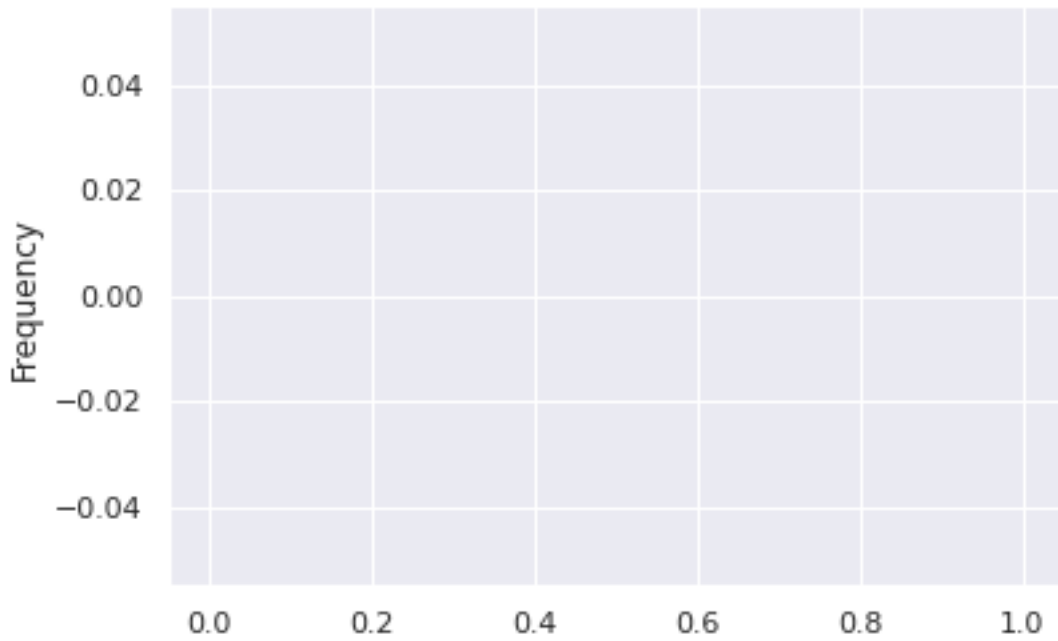
Inferred n_reticulations equal: 0

Inferred n_reticulations more: 0

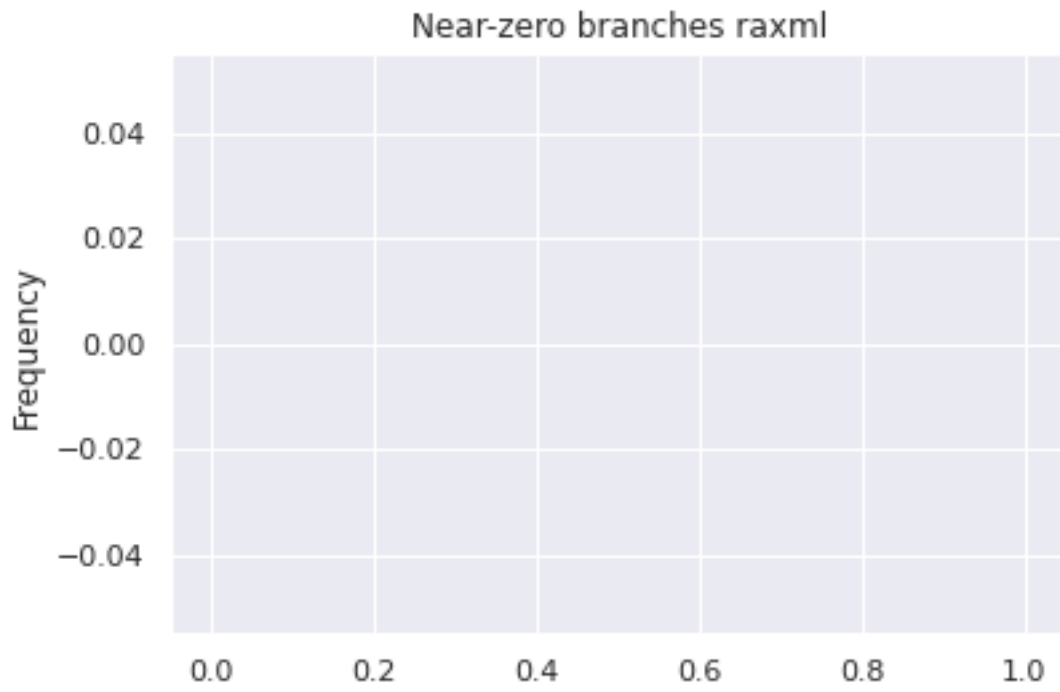
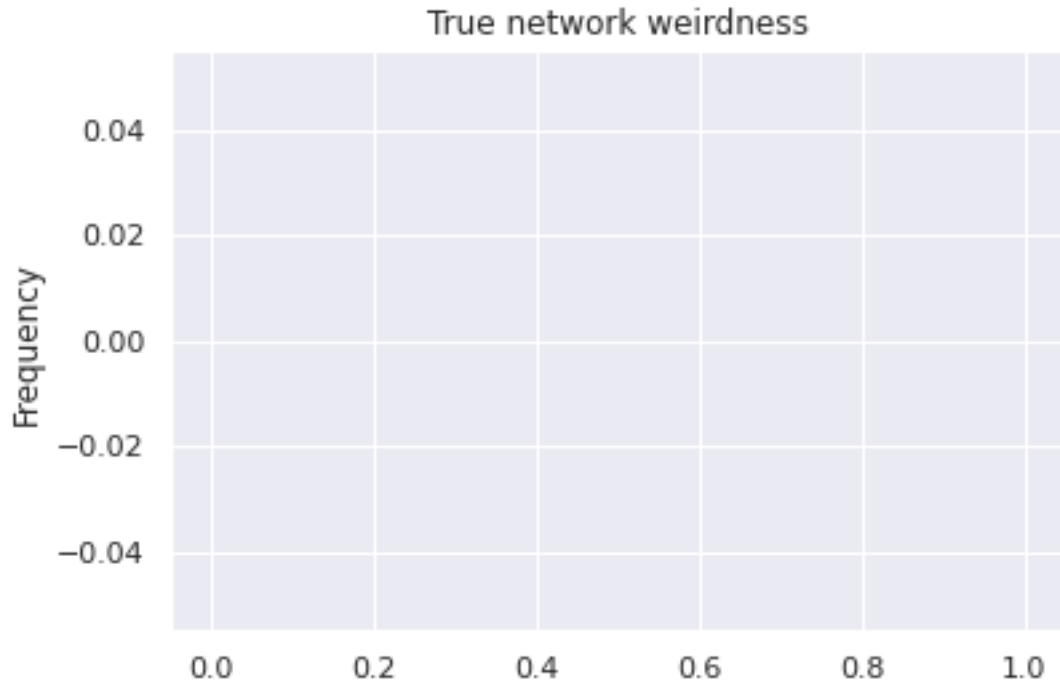
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



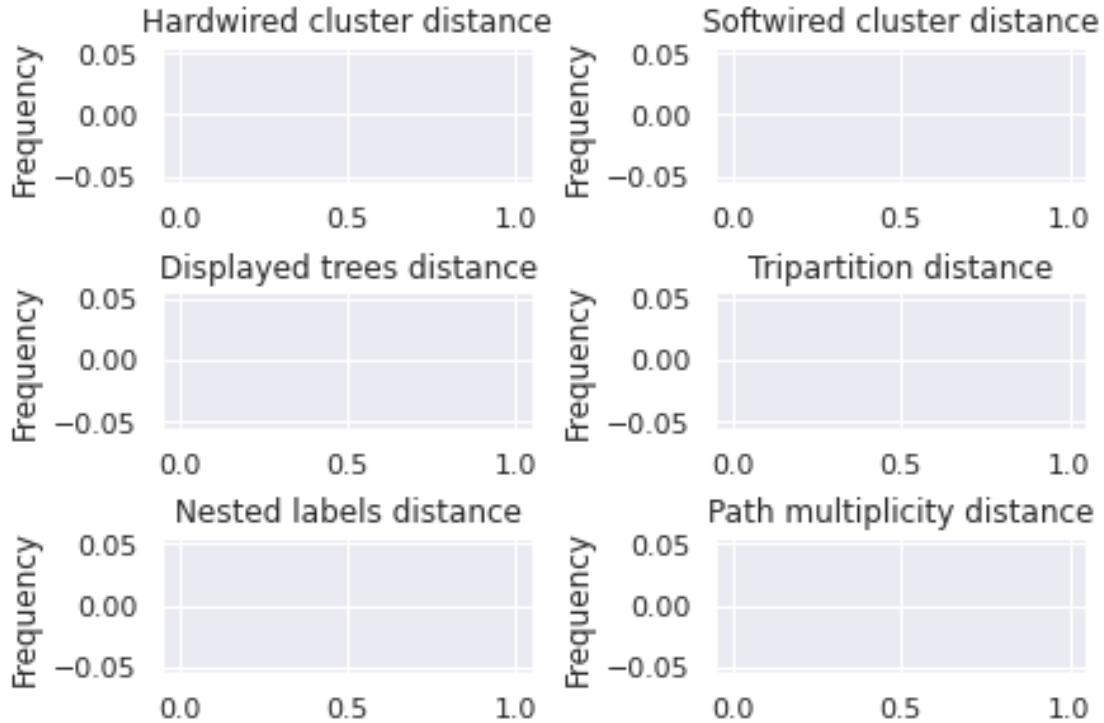
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>



2.2 Plots for $MSA_size \sim 200 * n_trees$

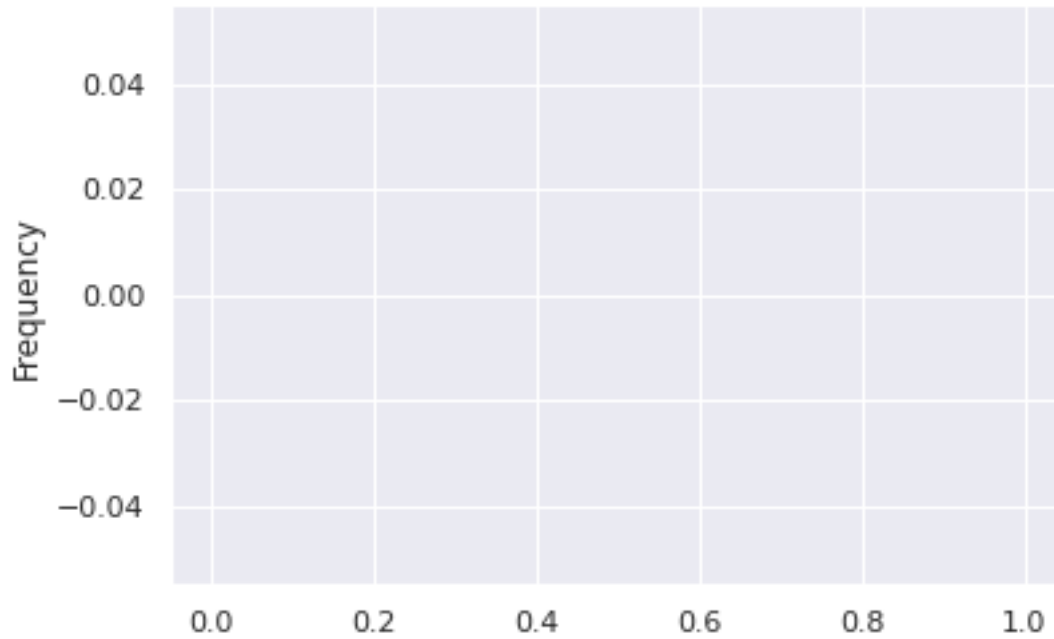
```
[18]: df_random_msasize_200 = df_random.query('msa_size == 200')
      build_stats(df_random_msasize_200)
```

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

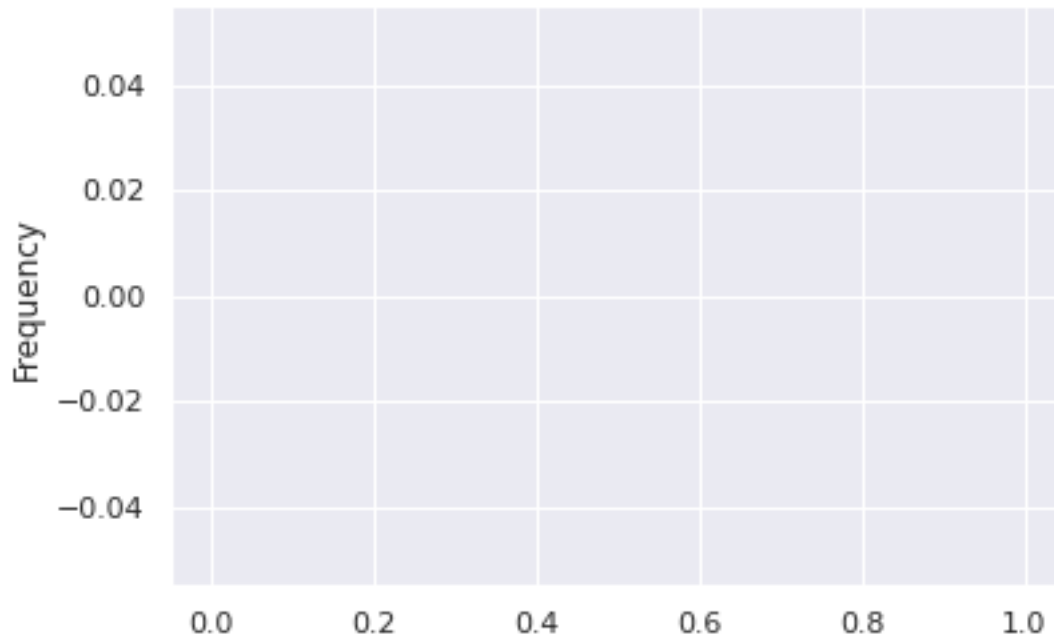
Inferred loglh better or equal: 0
Inferred loglh worse: 0

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

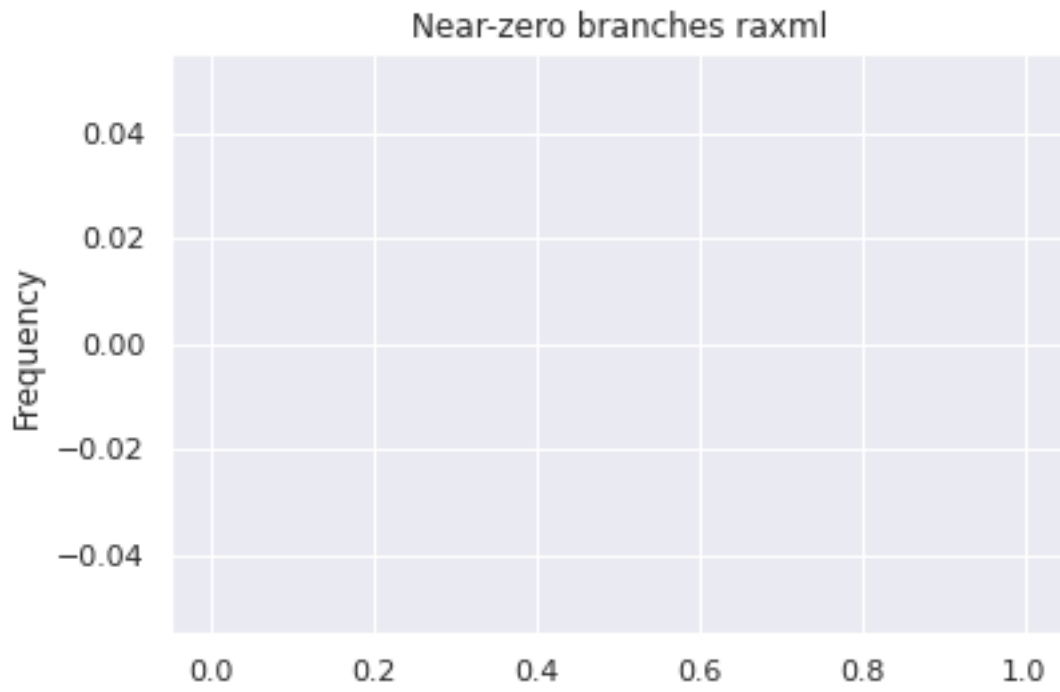
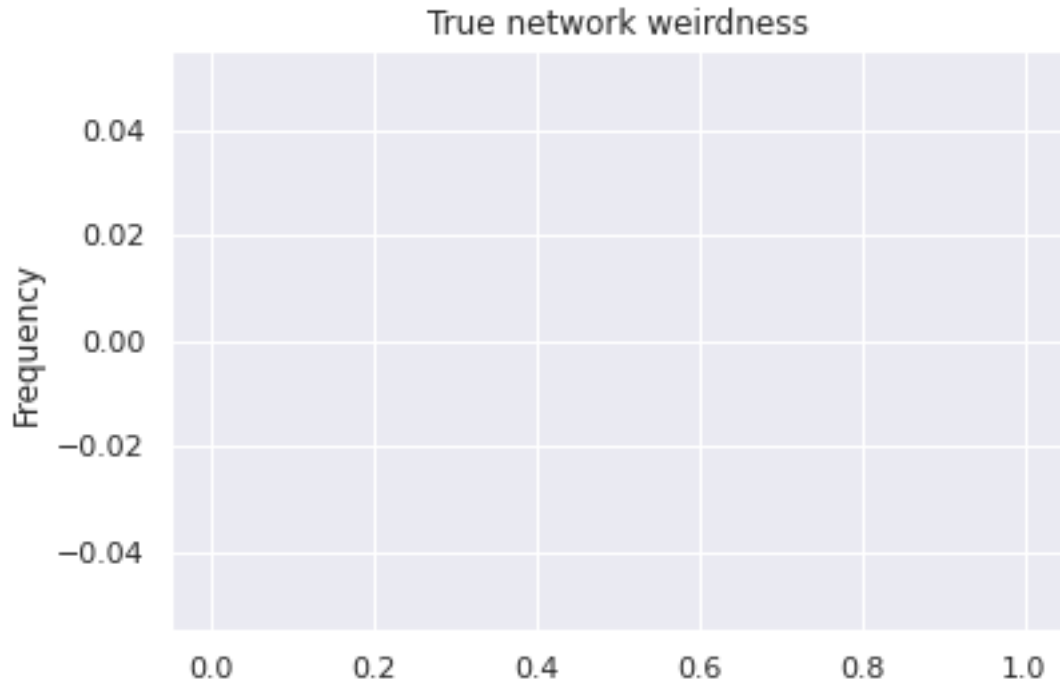
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



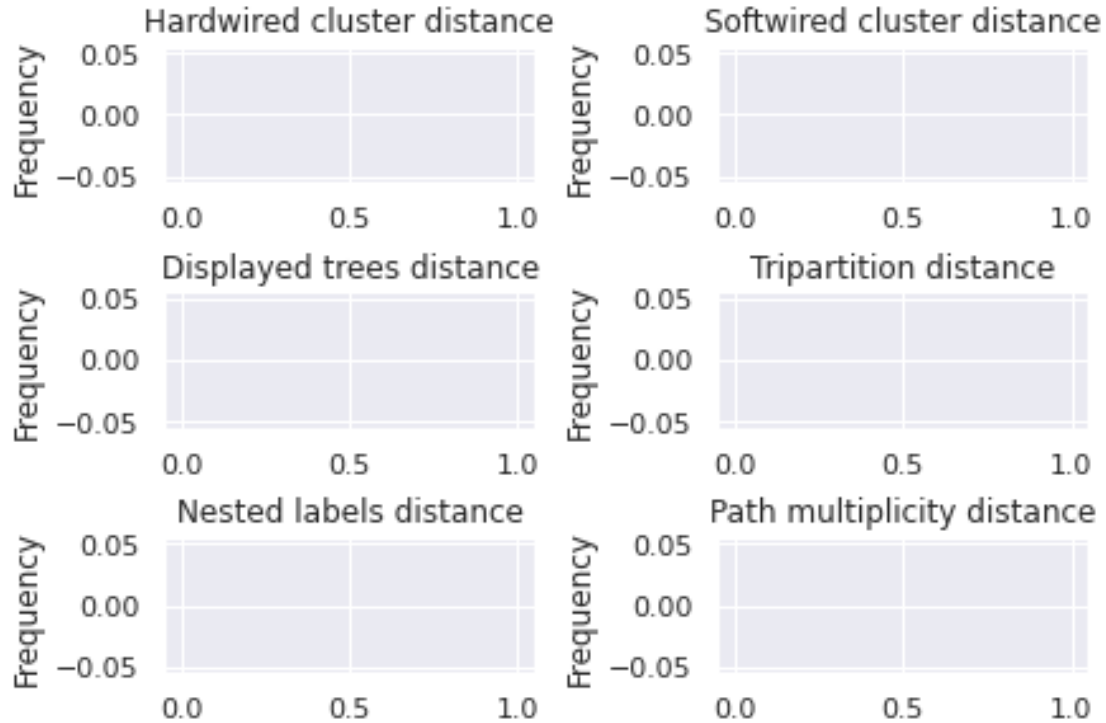
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>



2.2.1 Plots for LikelihoodType.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 loglh better or equal: 0

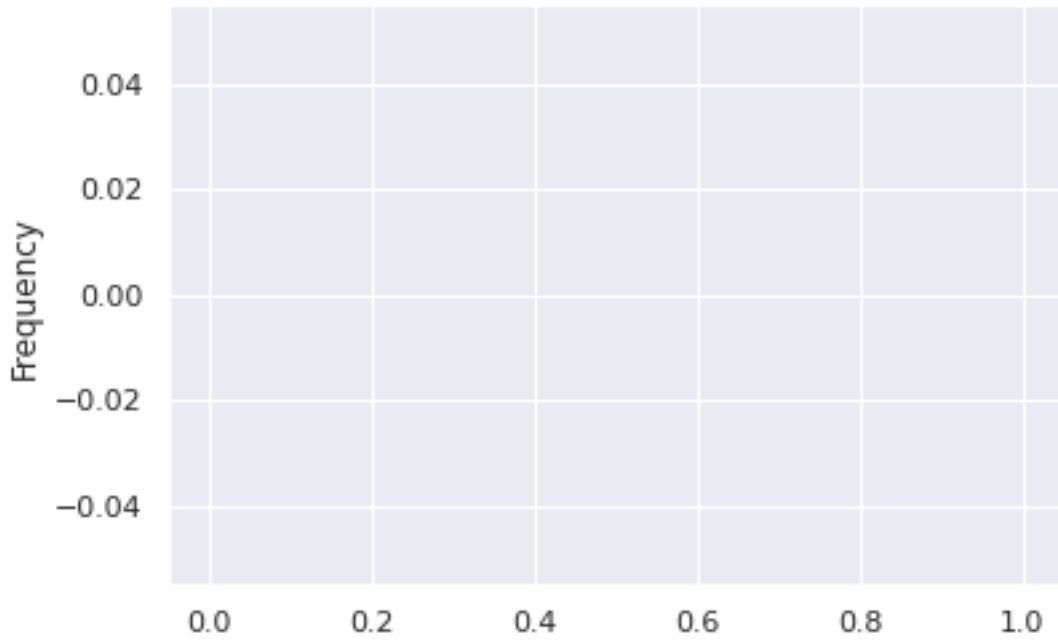
Inferred loglh worse: 0

Inferred n_reticulations less: 0

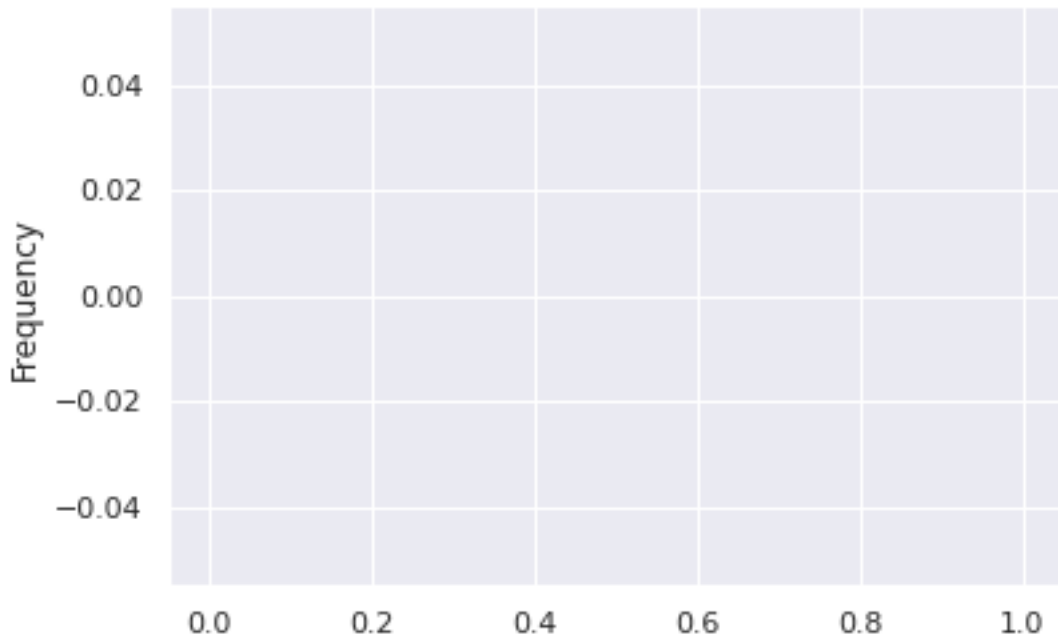
Inferred n_reticulations equal: 0

Inferred n_reticulations more: 0

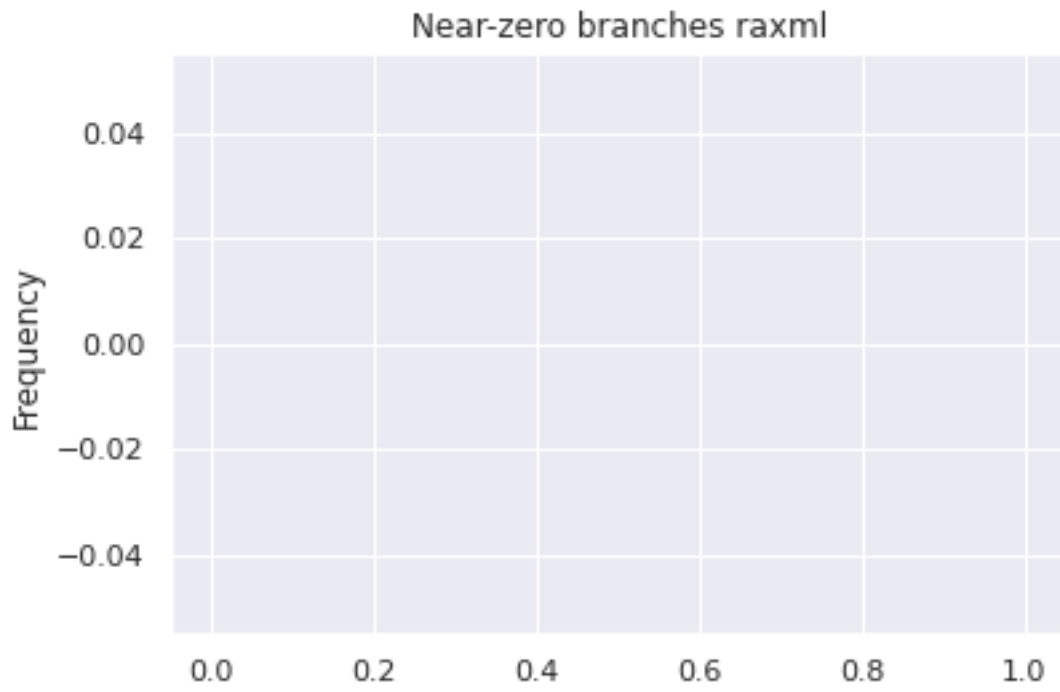
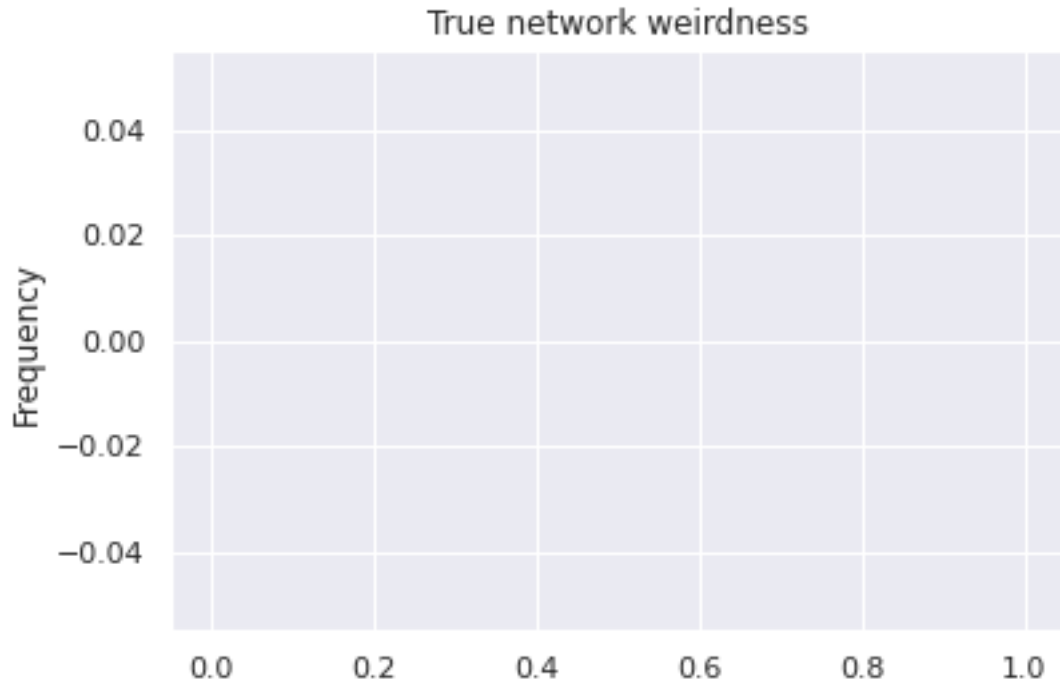
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



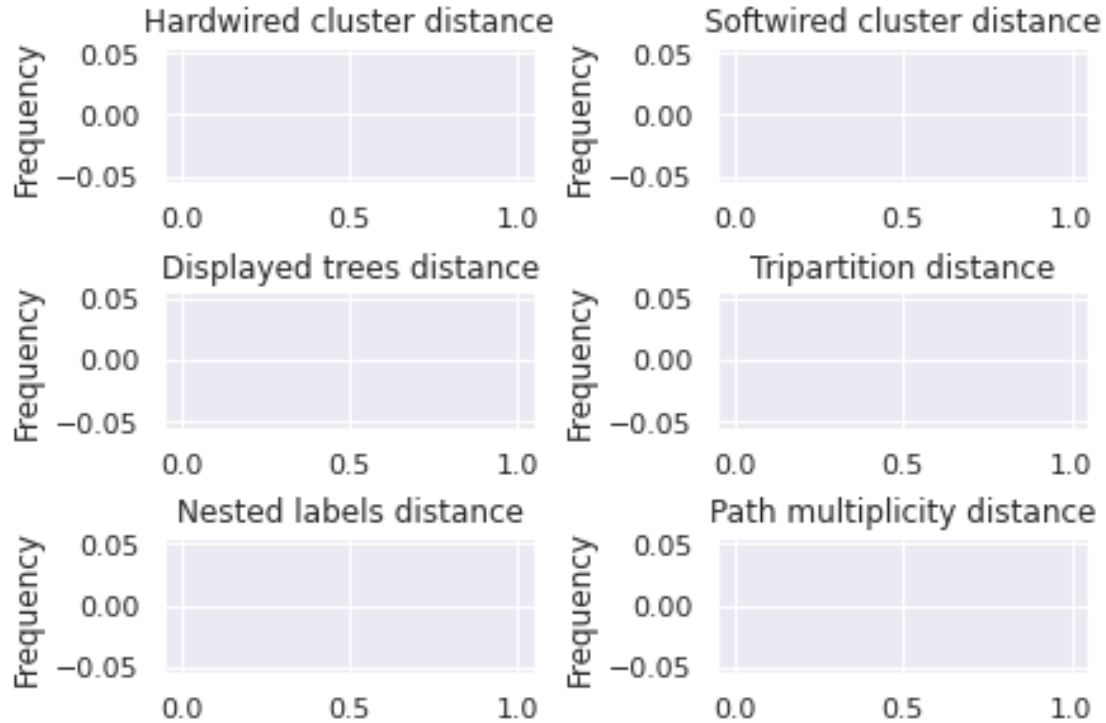
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<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 loglh better or equal: 0

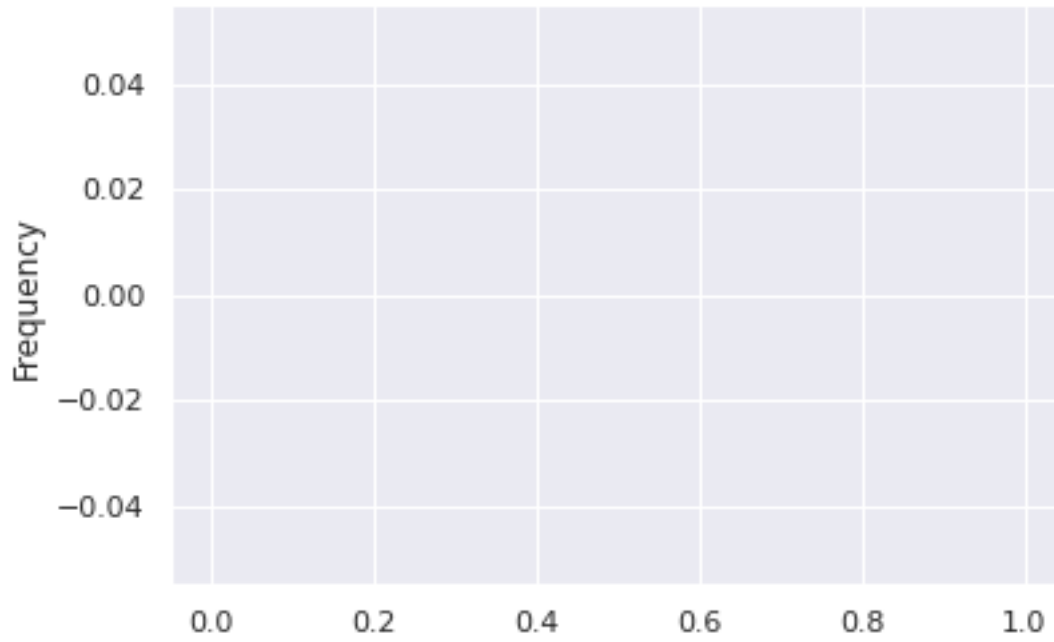
Inferred loglh worse: 0

Inferred n_reticulations less: 0

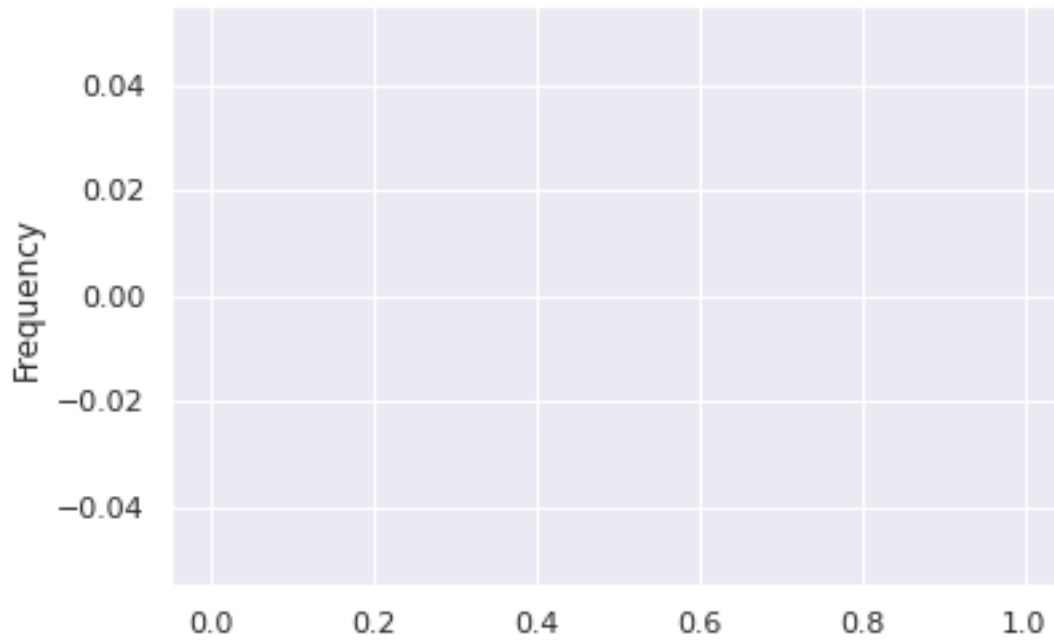
Inferred n_reticulations equal: 0

Inferred n_reticulations more: 0

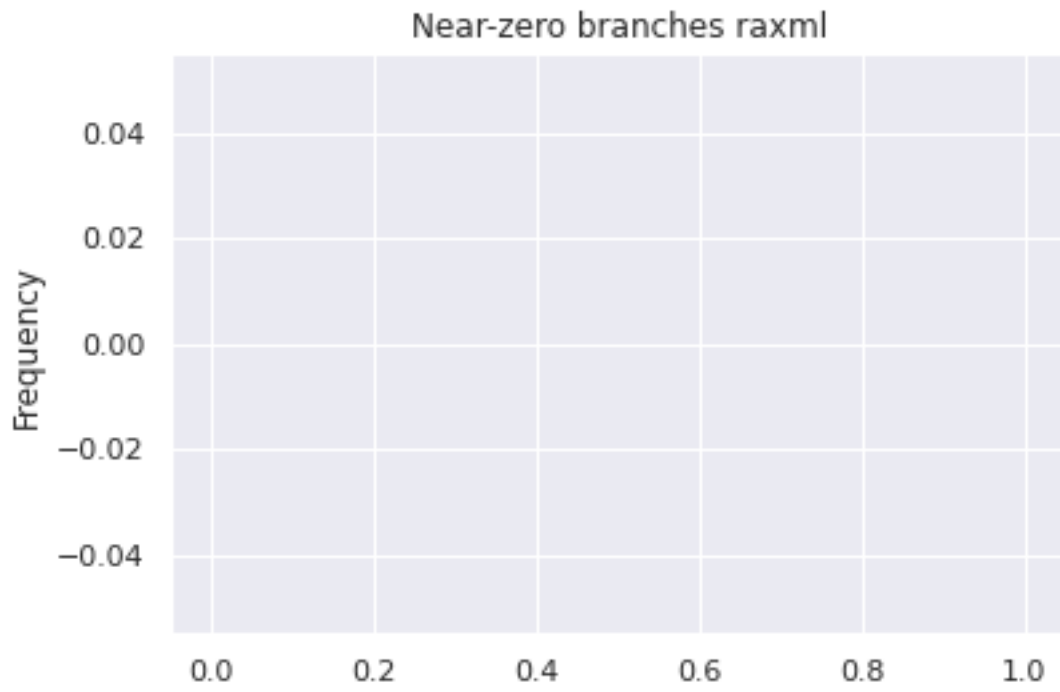
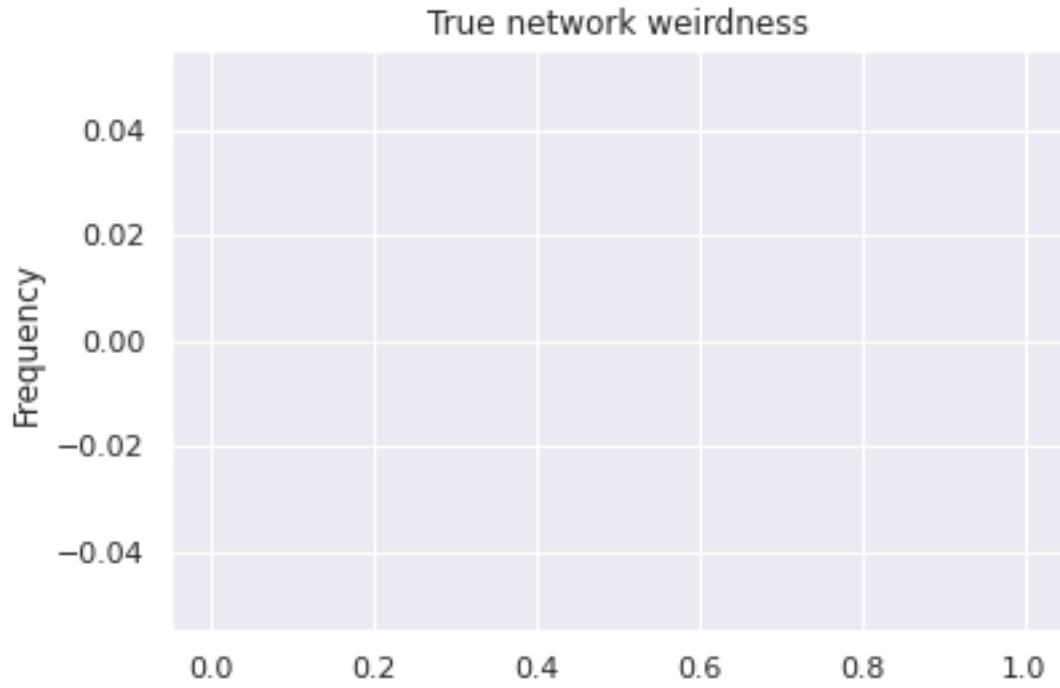
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



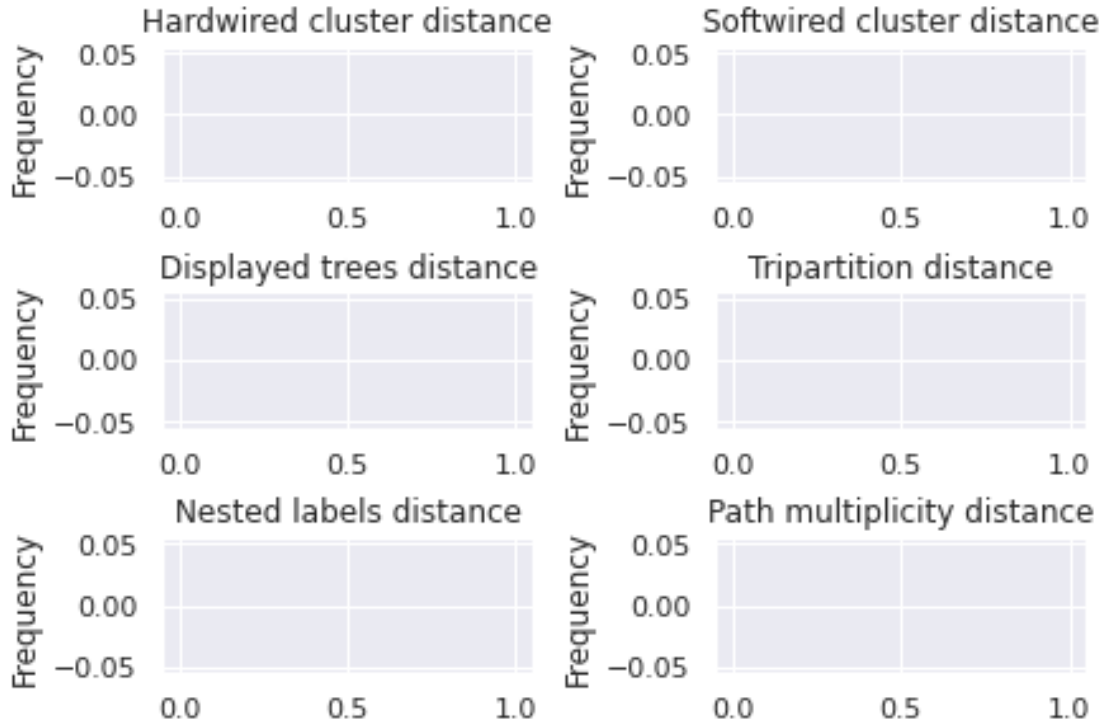
$(logl_true - logl_inferred) / logl_true$
value <0 means inferred logl was better



<Figure size 432x288 with 0 Axes>



<Figure size 432x288 with 0 Axes>



[]: