

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')
```

```

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_small_network_0_0/0_9_taxa_1_reticula...      9      2
1  datasets_small_network_0_0/0_9_taxa_1_reticula...      9      2
2  datasets_small_network_0_0/0_9_taxa_1_reticula...      9      2
3  datasets_small_network_0_0/0_9_taxa_1_reticula...      9      2
4  datasets_small_network_0_0/0_9_taxa_1_reticula...      9      2

n_reticulations  msa_size      sampling_type  simulation_type  \
0                1        101  PERFECT_SAMPLING      CELINE
1                1        101  PERFECT_SAMPLING      CELINE
2                1        101  PERFECT_SAMPLING      CELINE
3                1        101  PERFECT_SAMPLING      CELINE
4                1        201  PERFECT_SAMPLING      CELINE

                                celine_params  \
0  {'to': 0.29257489911596035| 'lambda': 13.92596...
1  {'to': 0.29257489911596035| 'lambda': 13.92596...
2  {'to': 0.29257489911596035| 'lambda': 13.92596...
3  {'to': 0.29257489911596035| 'lambda': 13.92596...
4  {'to': 0.29257489911596035| 'lambda': 13.92596...

                                seqgen_params  near_zero_branches_raxml  \
0  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                        1
1  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                        1
2  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                        1
3  -mHKY -t3.0 -f0.3|0.2|0.2|0.3                        1
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_small_network_0_0/0_9_taxa_1_reticula...
1  datasets_small_network_0_0/0_9_taxa_1_reticula...
2  datasets_small_network_0_0/0_9_taxa_1_reticula...
3  datasets_small_network_0_0/0_9_taxa_1_reticula...
4  datasets_small_network_0_0/0_9_taxa_1_reticula...

                                inferred_network_path  likelihood_type  \
0  datasets_small_network_0_0/0_9_taxa_1_reticula...      AVERAGE
1  datasets_small_network_0_0/0_9_taxa_1_reticula...      AVERAGE
2  datasets_small_network_0_0/0_9_taxa_1_reticula...      BEST
3  datasets_small_network_0_0/0_9_taxa_1_reticula...      BEST
```

```

4 datasets_small_network_0_0/0_9_taxa_1_reticula... AVERAGE

brlen_linkage_type start_type timeout n_random_start_networks \
0 LINKED FROM_RAXML 0 0
1 LINKED RANDOM 0 5
2 LINKED FROM_RAXML 0 0
3 LINKED RANDOM 0 5
4 LINKED FROM_RAXML 0 0

n_parsimony_start_networks runtime_inference n_reticulations_inferred \
0 0 403.473 0
1 5 4479.135 0
2 0 112.167 0
3 5 1381.504 0
4 0 191.855 0

bic_true logl_true bic_inferred logl_inferred bic_raxml \
0 1161.790768 -451.460827 1139.928369 -454.154318 1139.928108
1 1161.790768 -451.460827 1139.927152 -454.153709 1139.928108
2 1161.778885 -451.454886 1139.928369 -454.154318 1139.928108
3 1161.778885 -451.454886 1139.941146 -454.160706 1139.928108
4 2046.490494 -880.735187 2035.762447 -890.372222 2035.762098

logl_raxml rf_absolute_raxml rf_relative_raxml rf_absolute_inferred \
0 -454.154187 -1 -1 -1
1 -454.154187 -1 -1 -1
2 -454.154187 -1 -1 -1
3 -454.154187 -1 -1 -1
4 -890.372048 -1 -1 -1

rf_relative_inferred hardwired_cluster_distance \
0 -1 4.0
1 -1 4.0
2 -1 4.0
3 -1 4.0
4 -1 4.0

softwired_cluster_distance displayed_trees_distance \
0 5.5 1.5
1 5.5 1.5
2 5.5 1.5
3 4.5 1.5
4 6.5 1.5

tripartition_distance nested_labels_distance path_multiplicity_distance \
0 5.5 7.0 6.0
1 5.5 7.0 6.0

```

2	5.5	7.0	6.0
3	5.5	7.0	6.0
4	5.5	7.0	6.0

	bic_diff	logl_diff
0	0.018818	-0.005966
1	0.018819	-0.005965
2	0.018808	-0.005979
3	0.018797	-0.005994
4	0.005242	-0.010942

```
[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: 977

Inferred BIC worse: 39

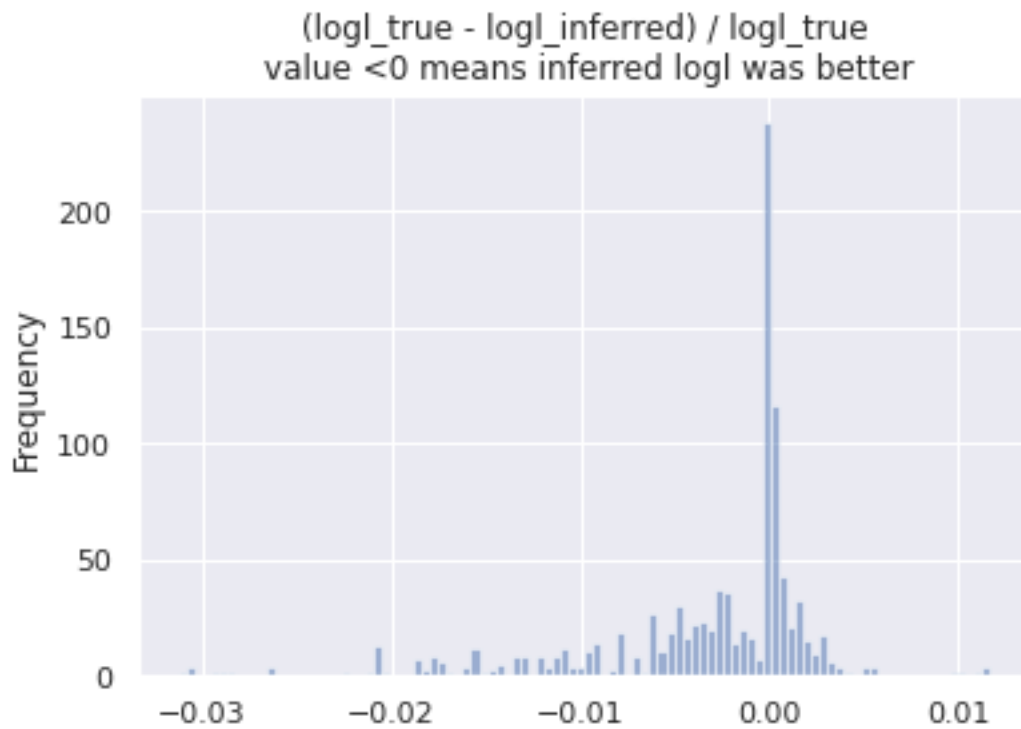
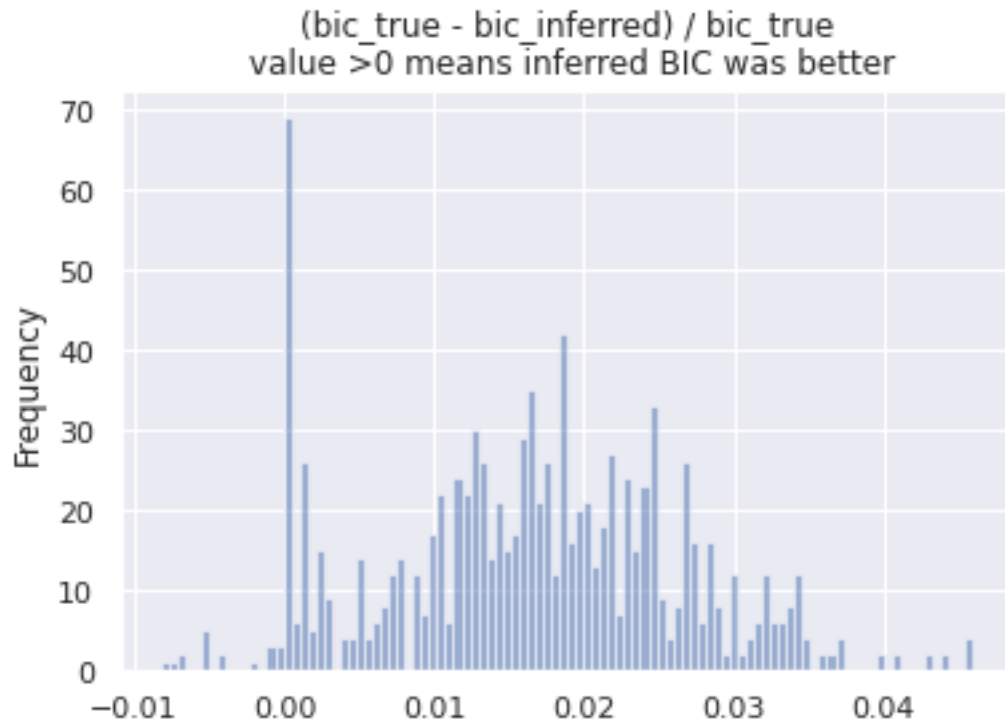
Inferred loglh better or equal: 452

Inferred loglh worse: 564

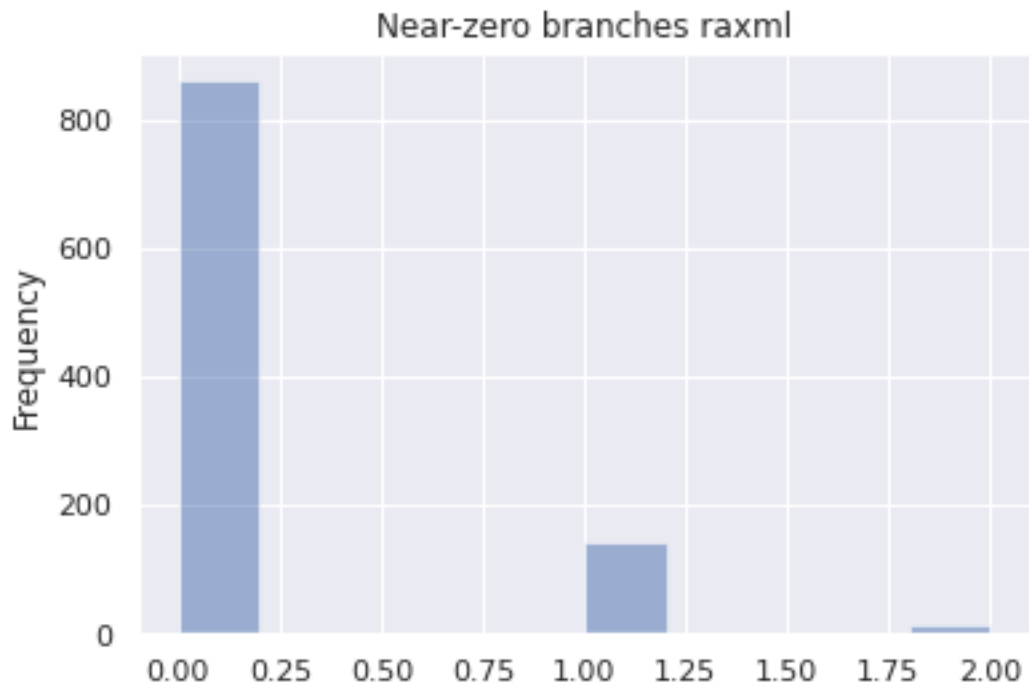
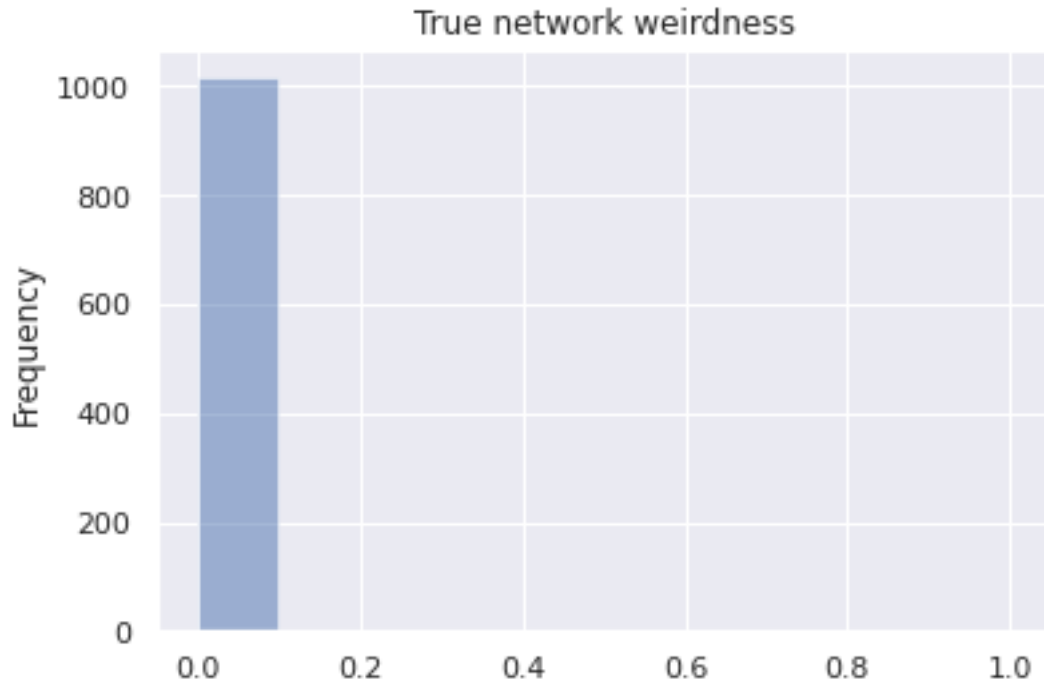
Inferred n_reticulations less: 912

Inferred n_reticulations equal: 104

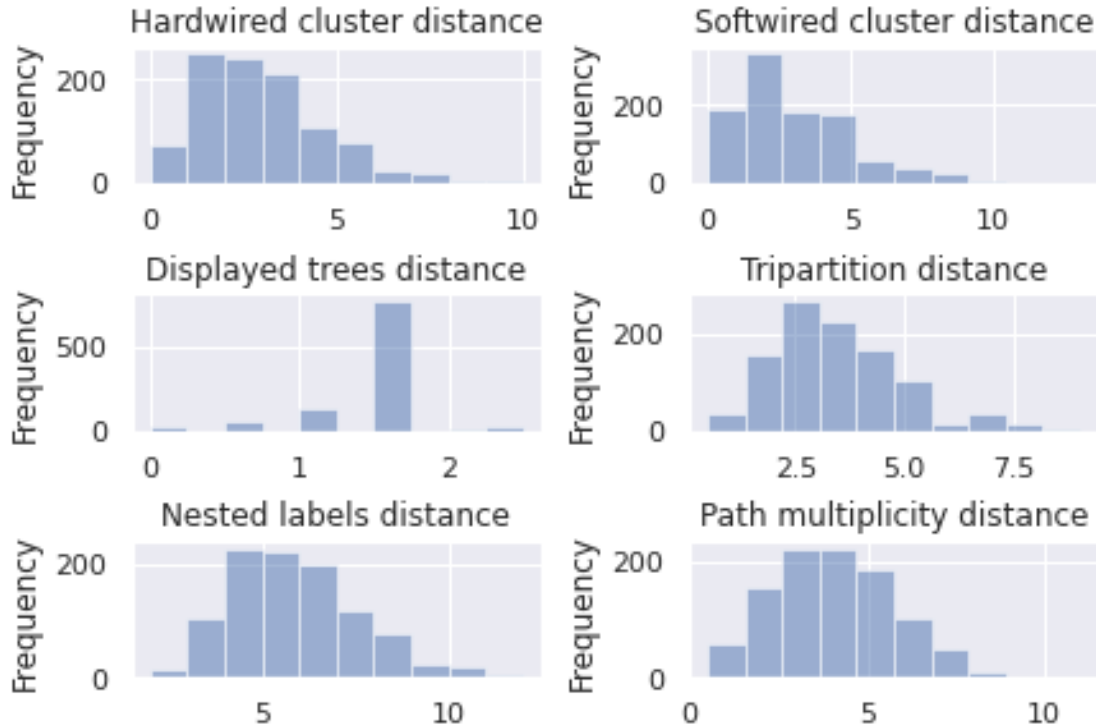
Inferred n_reticulations more: 0



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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: 474

Inferred BIC worse: 34

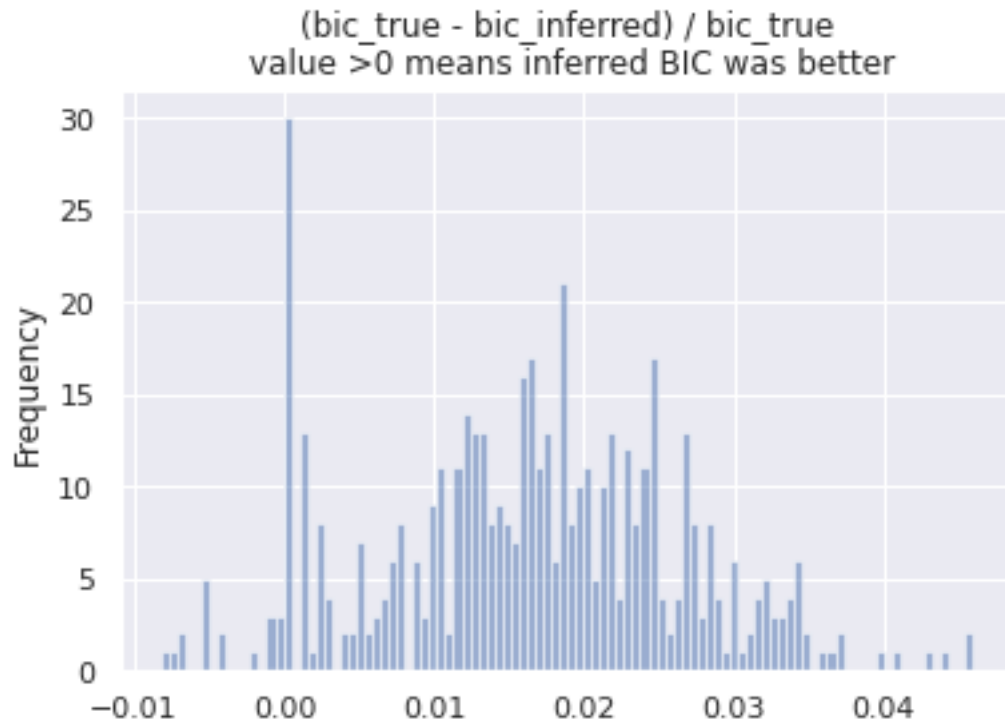
Inferred loglh better or equal: 212

Inferred loglh worse: 296

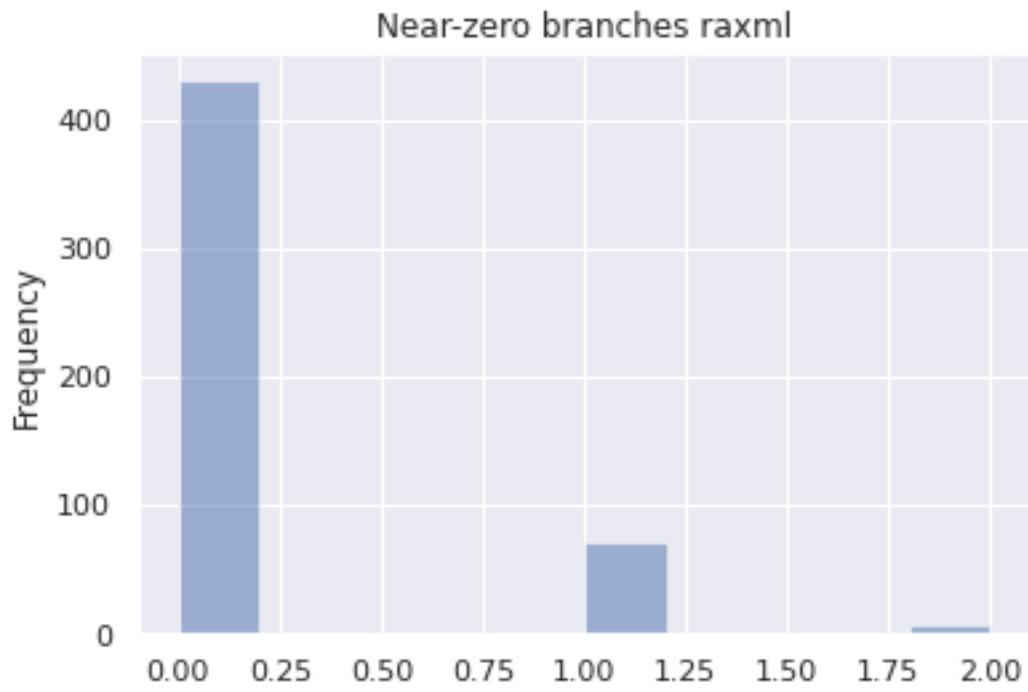
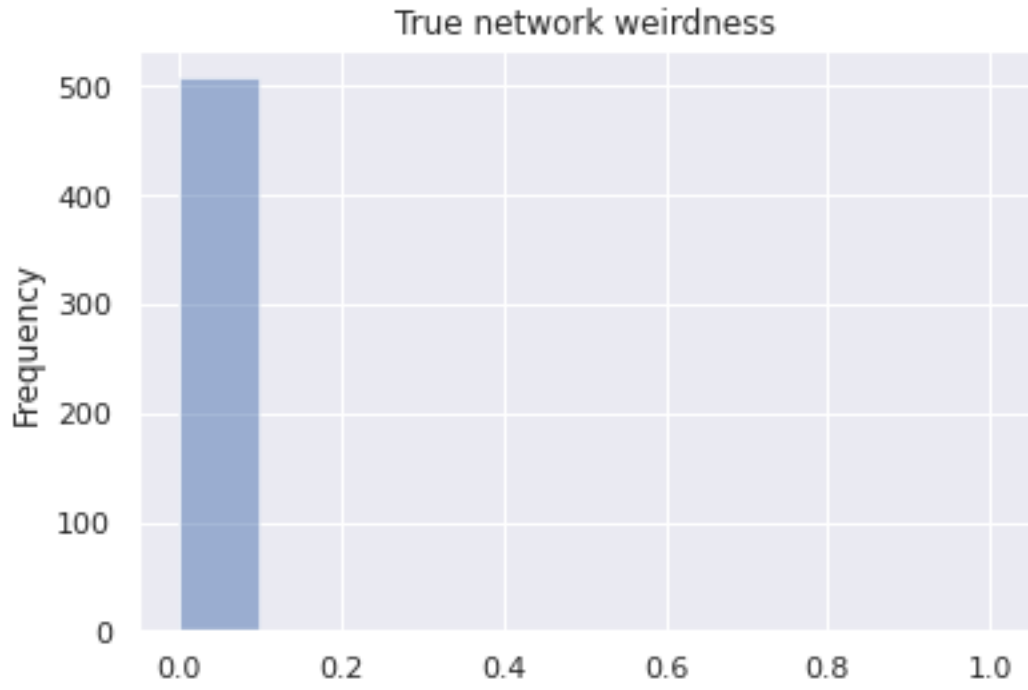
Inferred n_reticulations less: 462

Inferred n_reticulations equal: 46

Inferred n_reticulations more: 0



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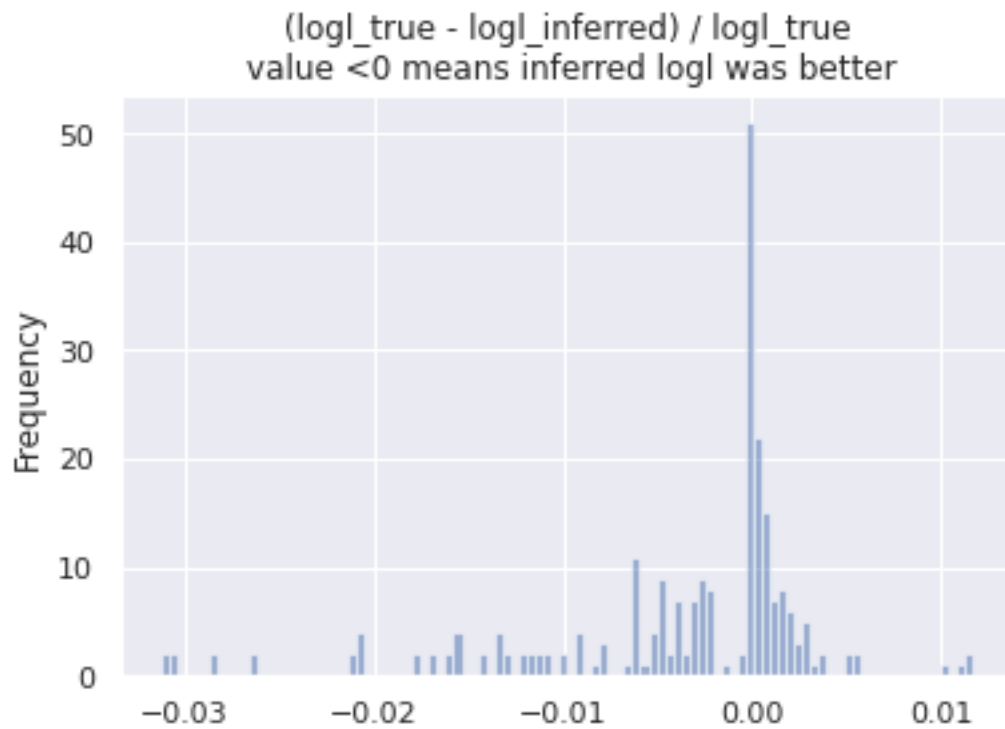
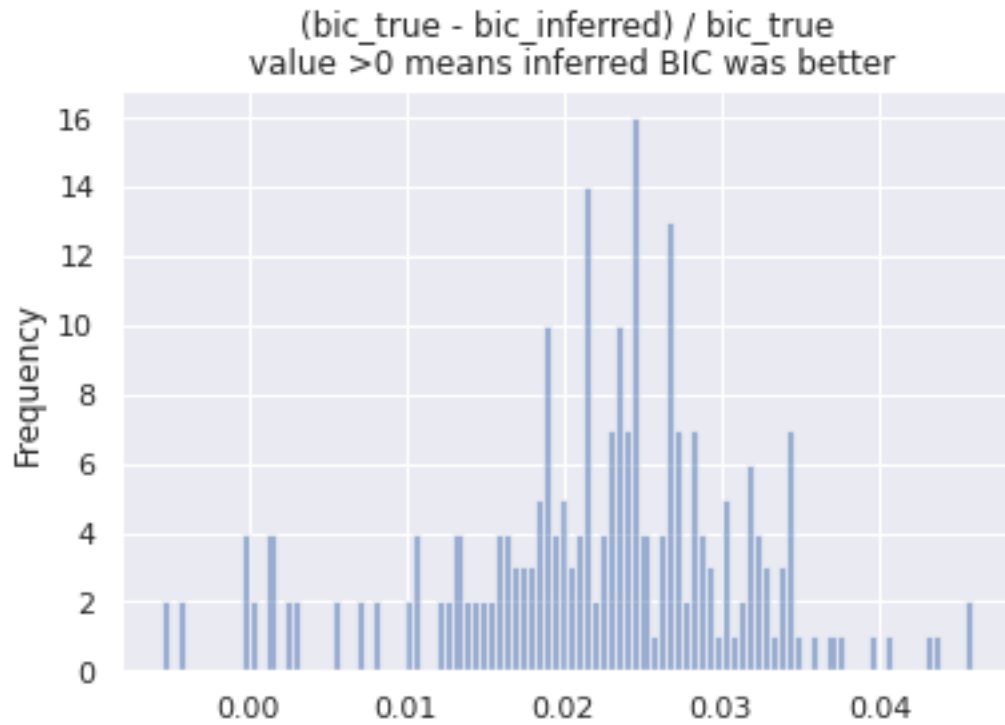
1.1 Plots for MSA_size ~ 100*n_trees

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

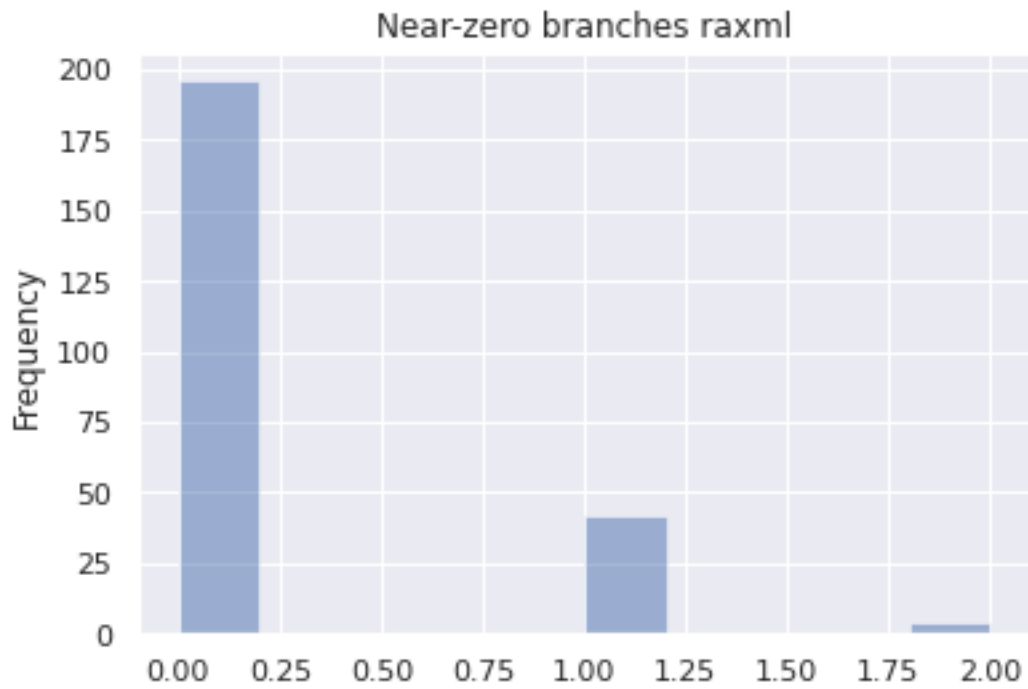
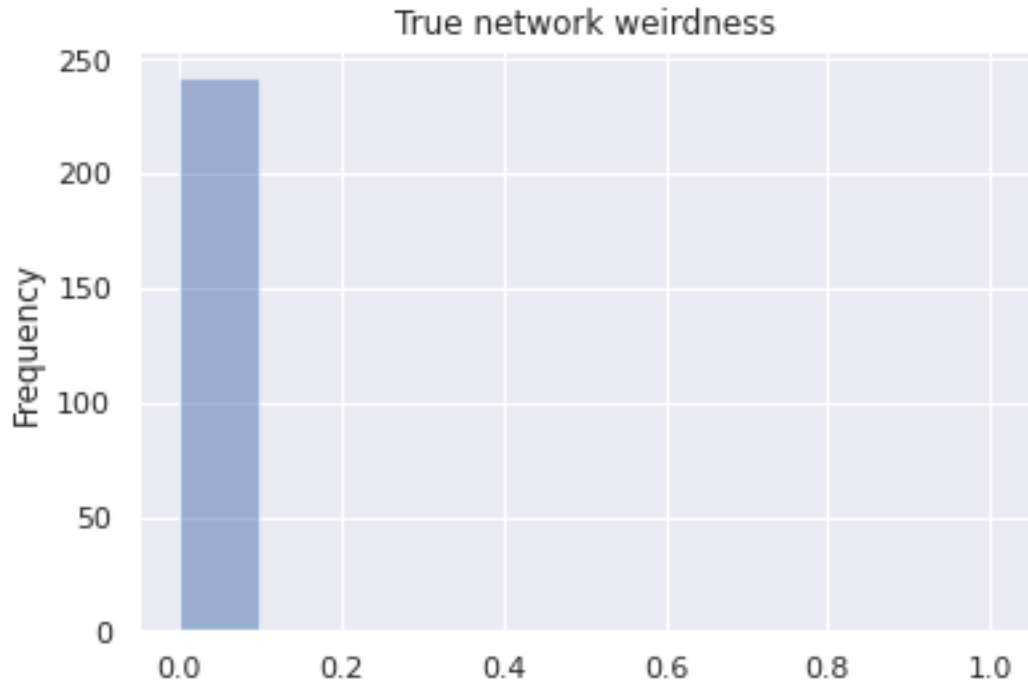
Inferred BIC better or equal: 234
Inferred BIC worse: 8

Inferred loglh better or equal: 114
Inferred loglh worse: 128

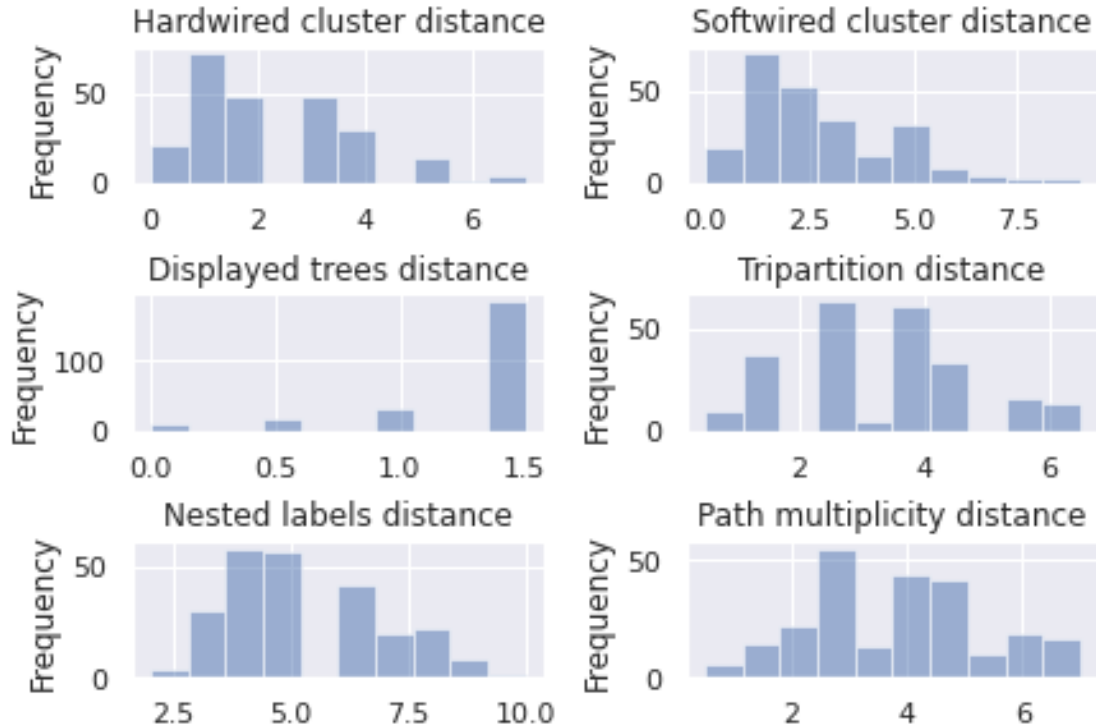
Inferred n_reticulations less: 230
Inferred n_reticulations equal: 12
Inferred n_reticulations more: 0



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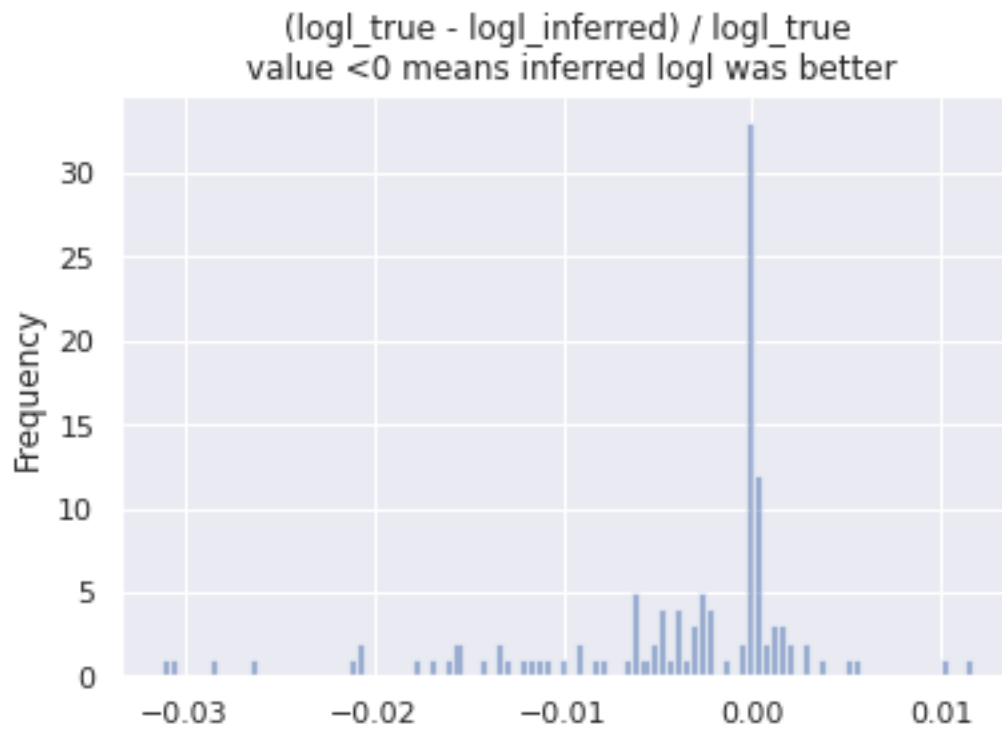
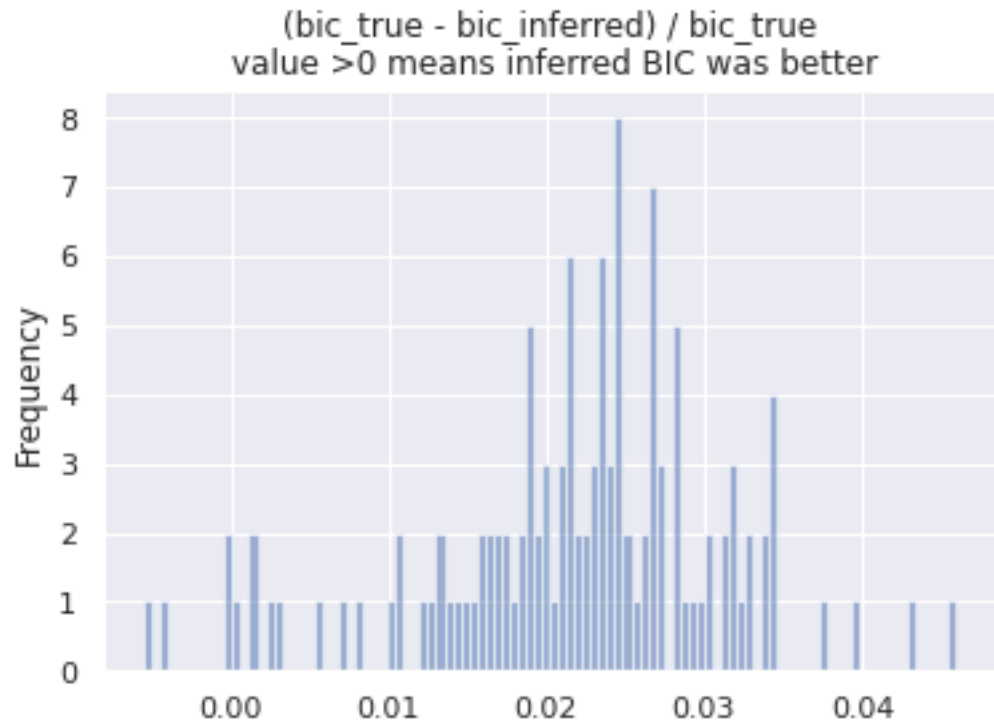
1.1.1 Plots for LikelihoodType.AVERAGE

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

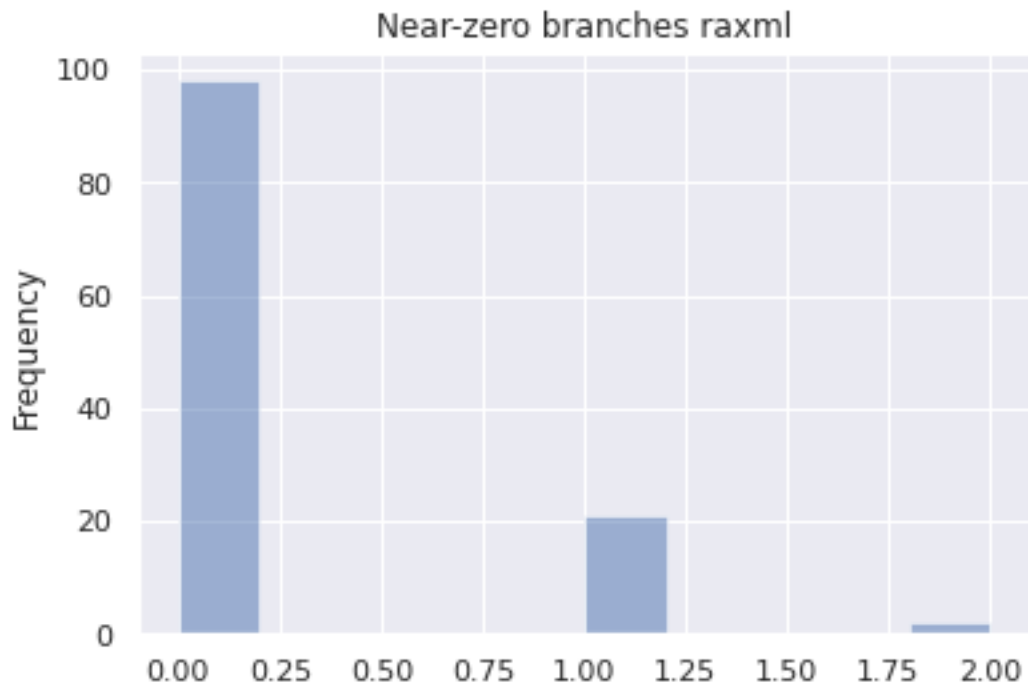
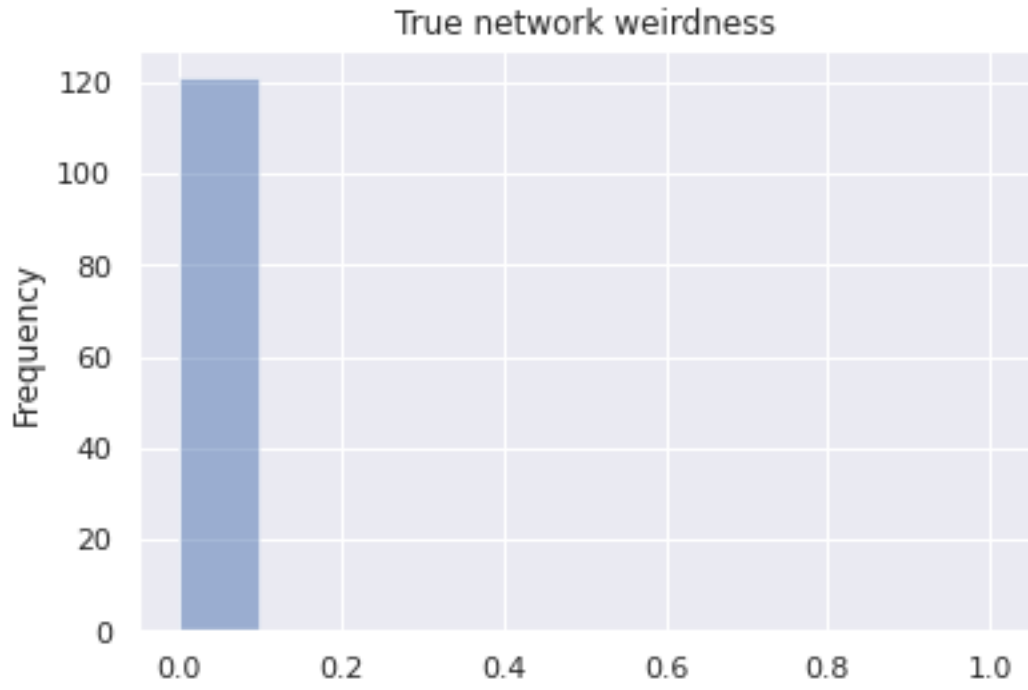
Inferred BIC better or equal: 117
Inferred BIC worse: 4

Inferred loglh better or equal: 53
Inferred loglh worse: 68

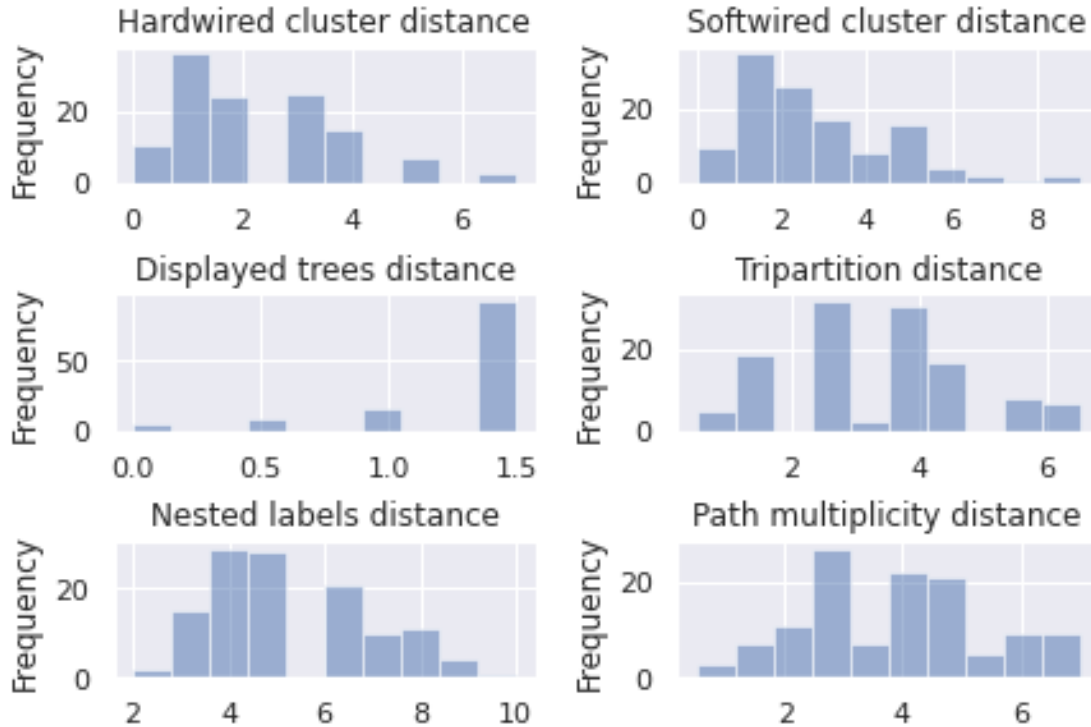
Inferred n_reticulations less: 115
Inferred n_reticulations equal: 6
Inferred n_reticulations more: 0



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1.1.2 Plots for LikelihoodType.BEST

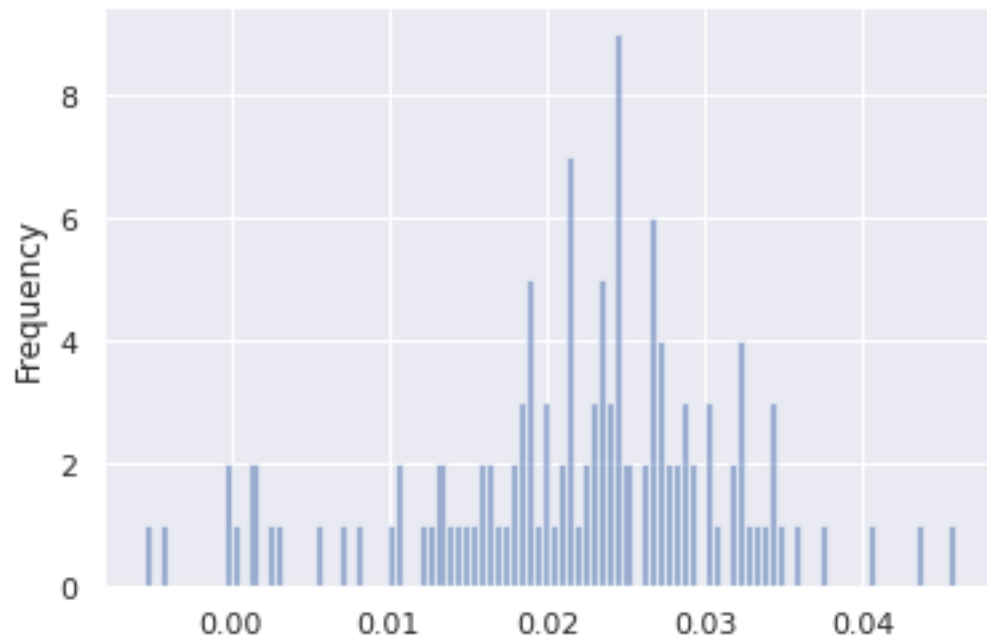
```
[10]: df_raxml_only_msasize_100_best = df_raxml_only_msasize_100.  
      ↪query('likelihood_type == "BEST"')  
      build_stats(df_raxml_only_msasize_100_best)
```

Inferred BIC better or equal: 117
Inferred BIC worse: 4

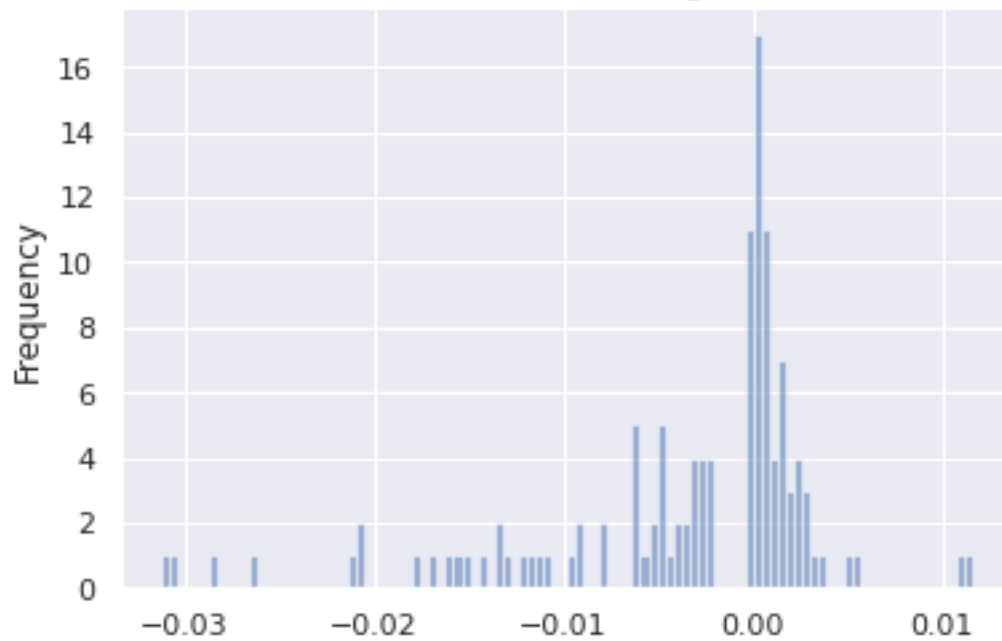
Inferred loglh better or equal: 61
Inferred loglh worse: 60

Inferred n_reticulations less: 115
Inferred n_reticulations equal: 6
Inferred n_reticulations more: 0

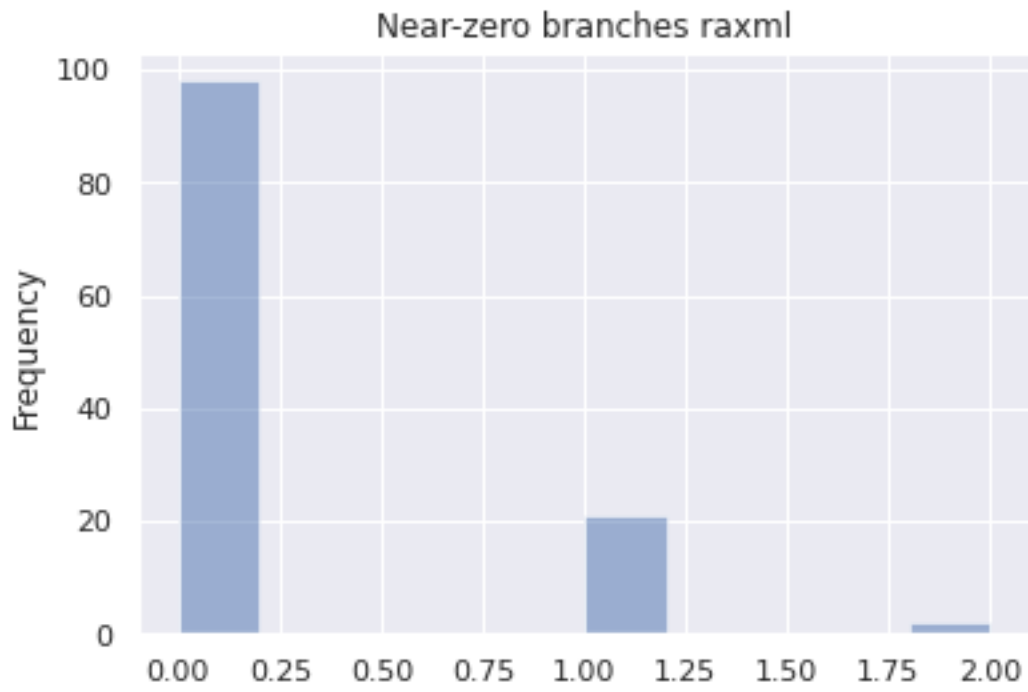
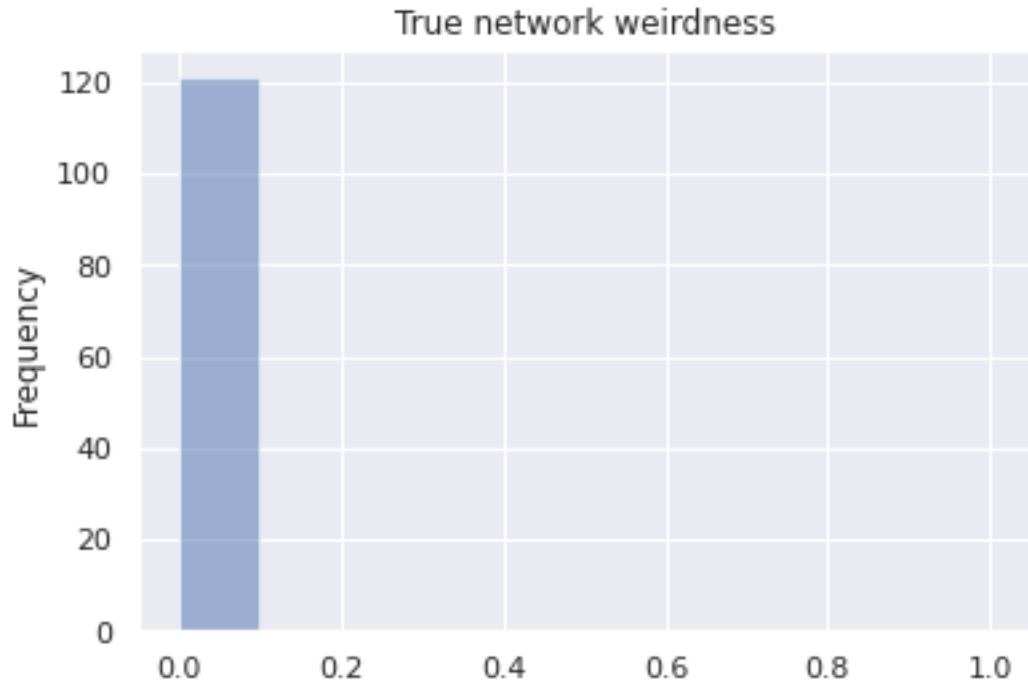
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



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



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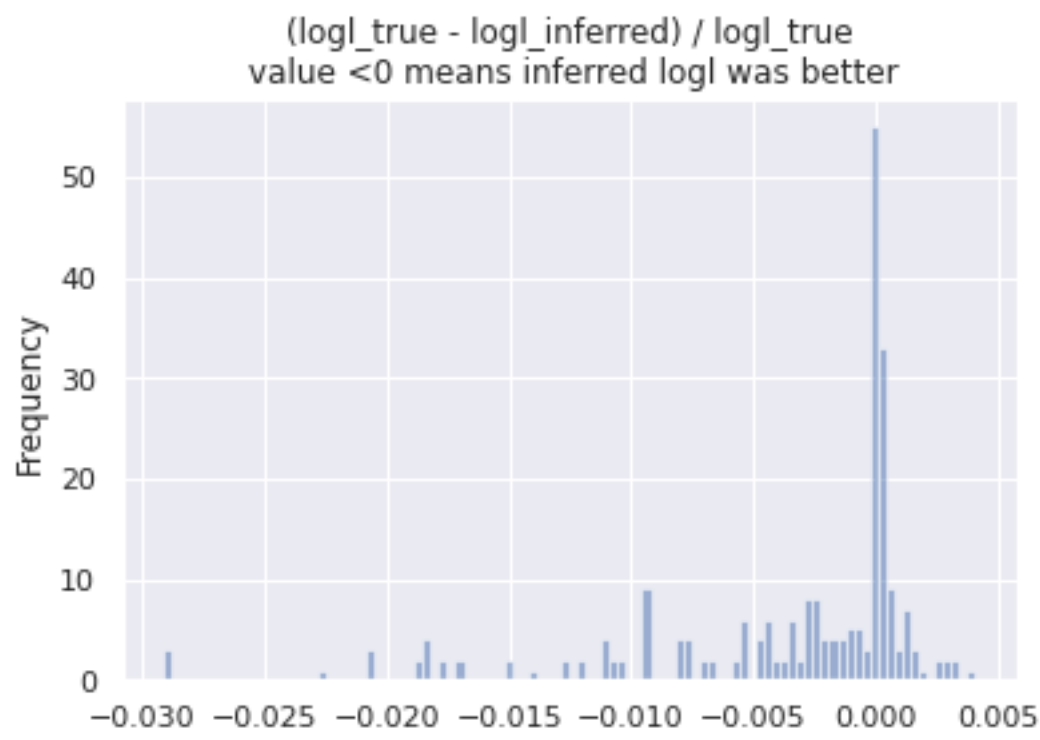
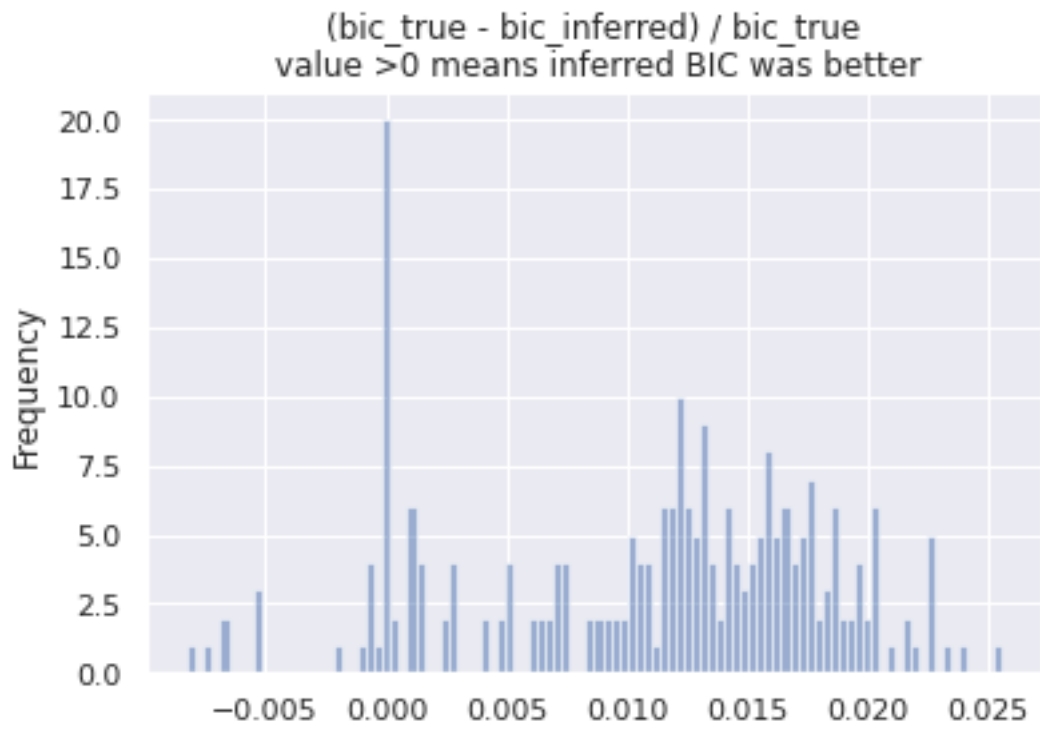
1.2 Plots for MSA_size ~ 200*n_trees

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

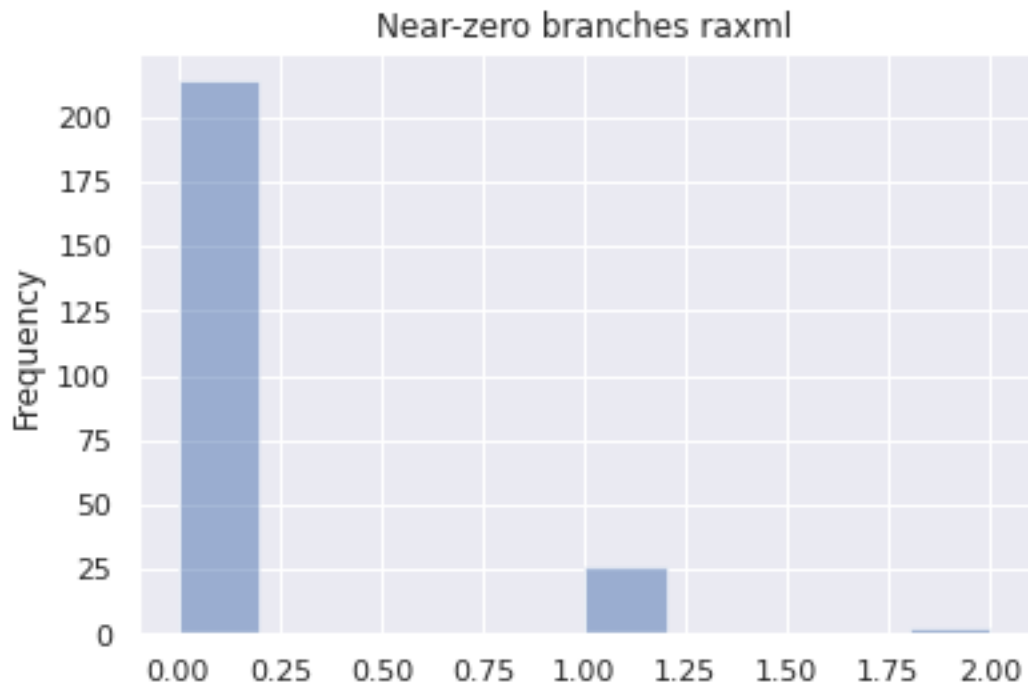
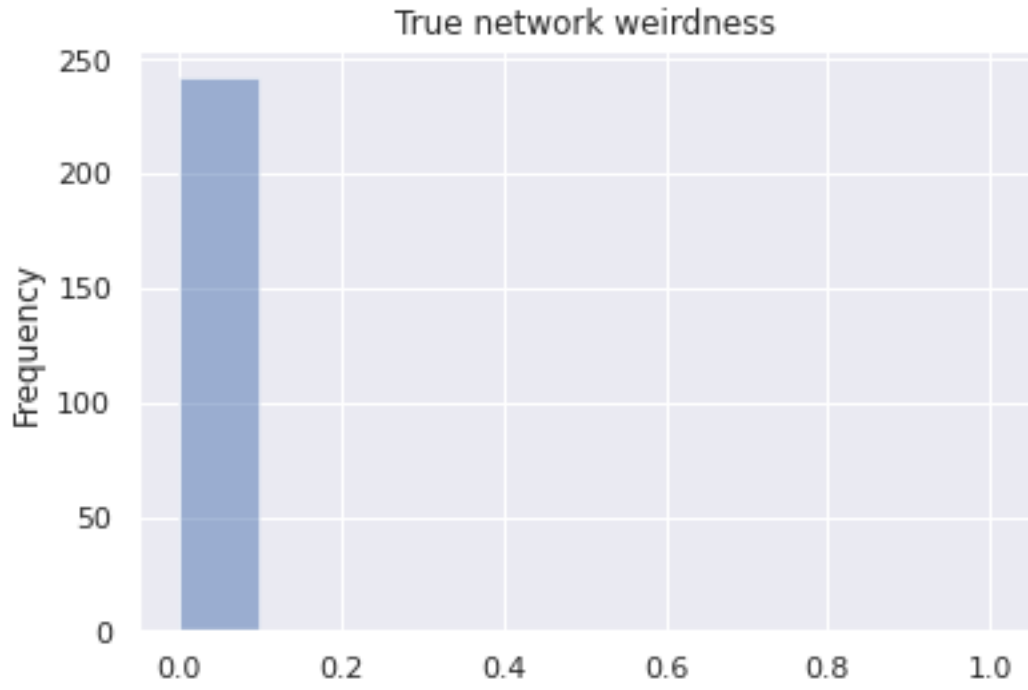
Inferred BIC better or equal: 216
Inferred BIC worse: 26

Inferred loglh better or equal: 96
Inferred loglh worse: 146

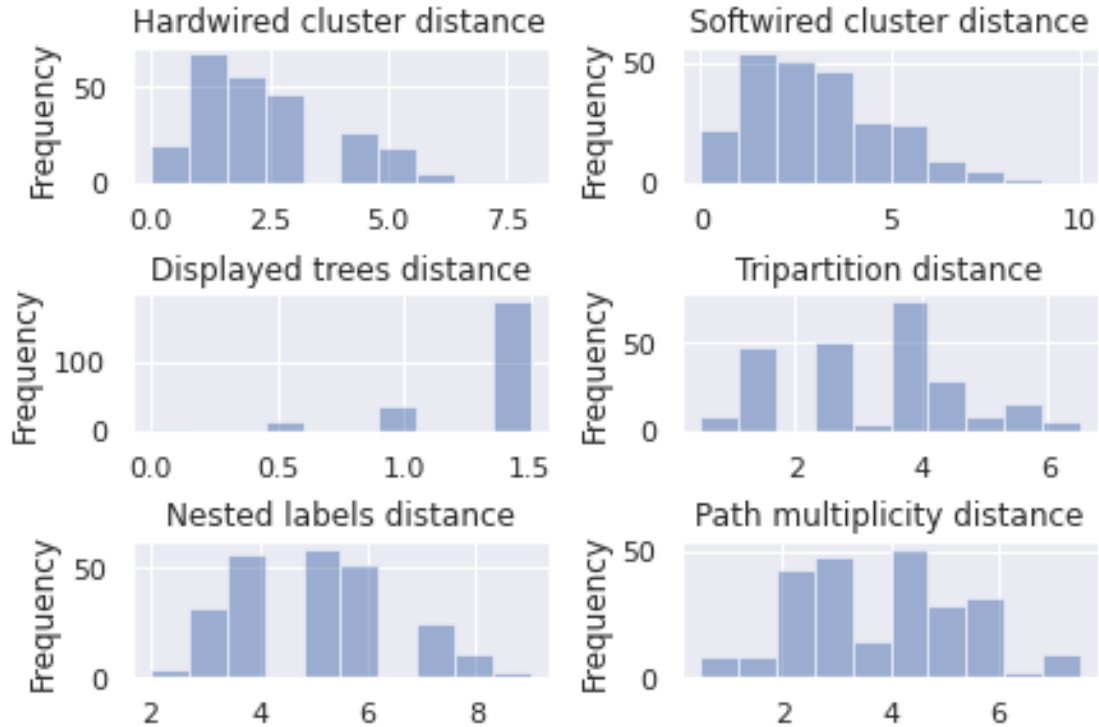
Inferred n_reticulations less: 208
Inferred n_reticulations equal: 34
Inferred n_reticulations more: 0



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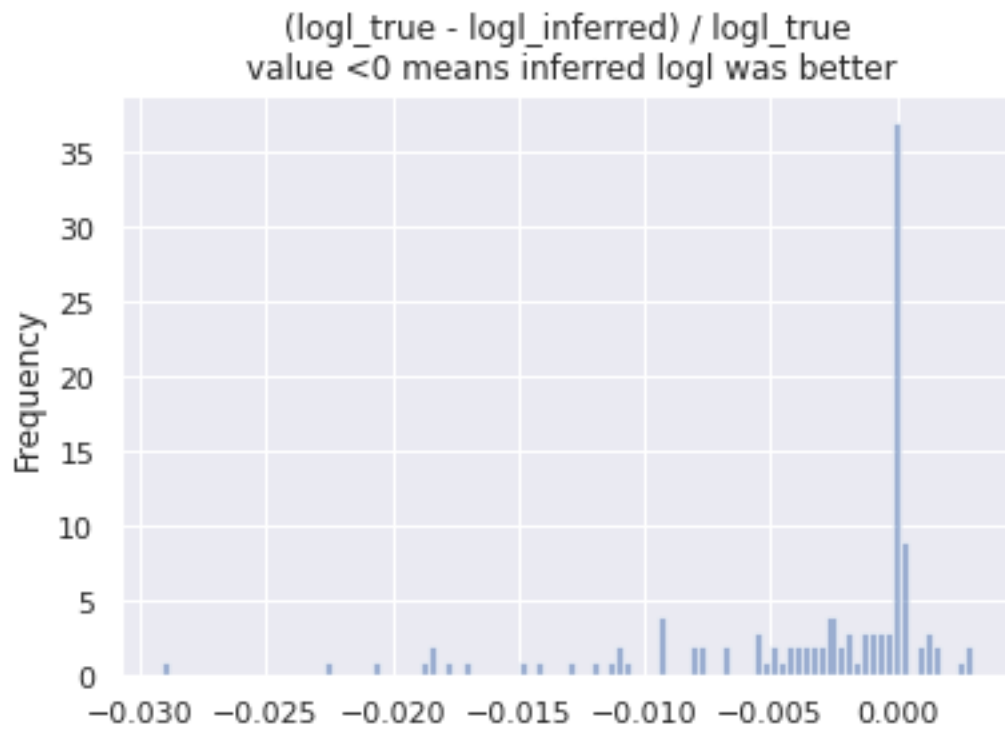
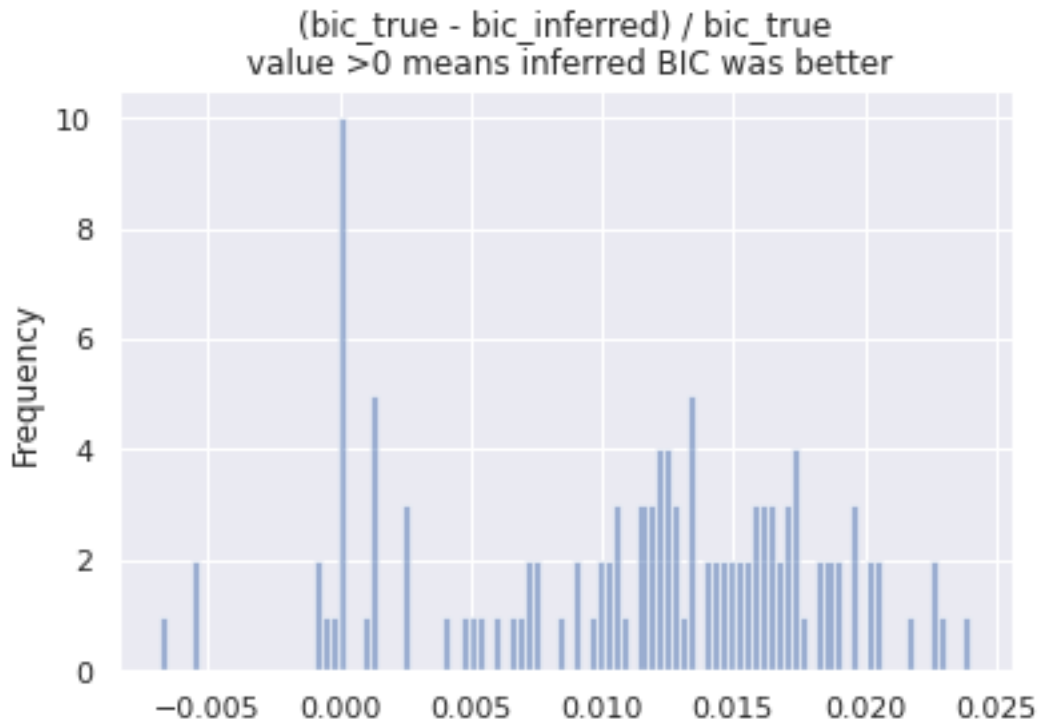
1.2.1 Plots for LikelihoodType.AVERAGE

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

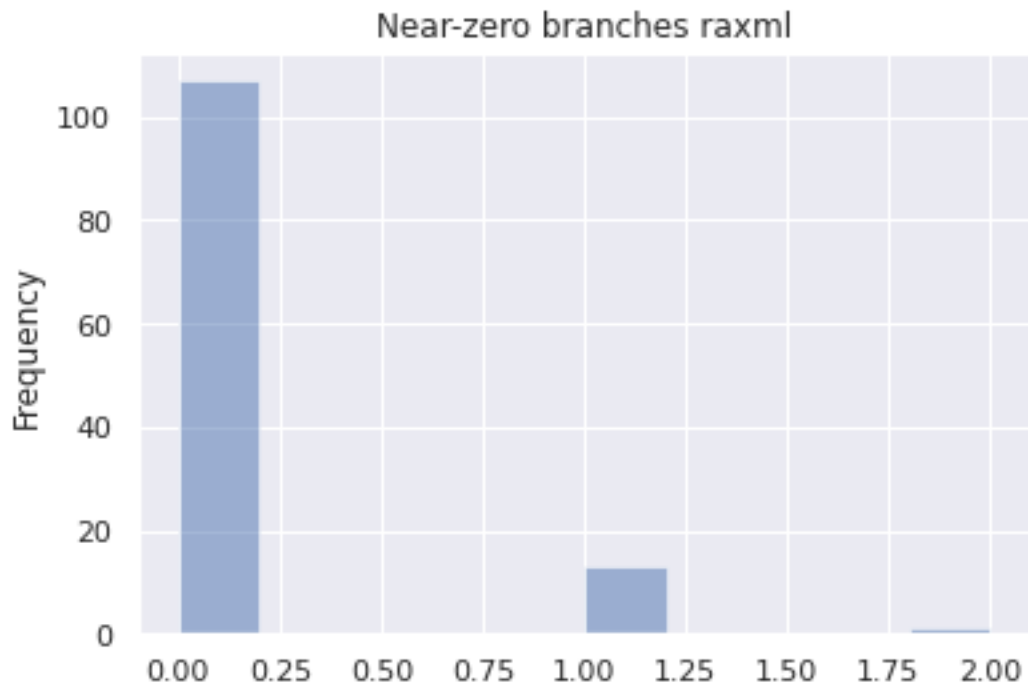
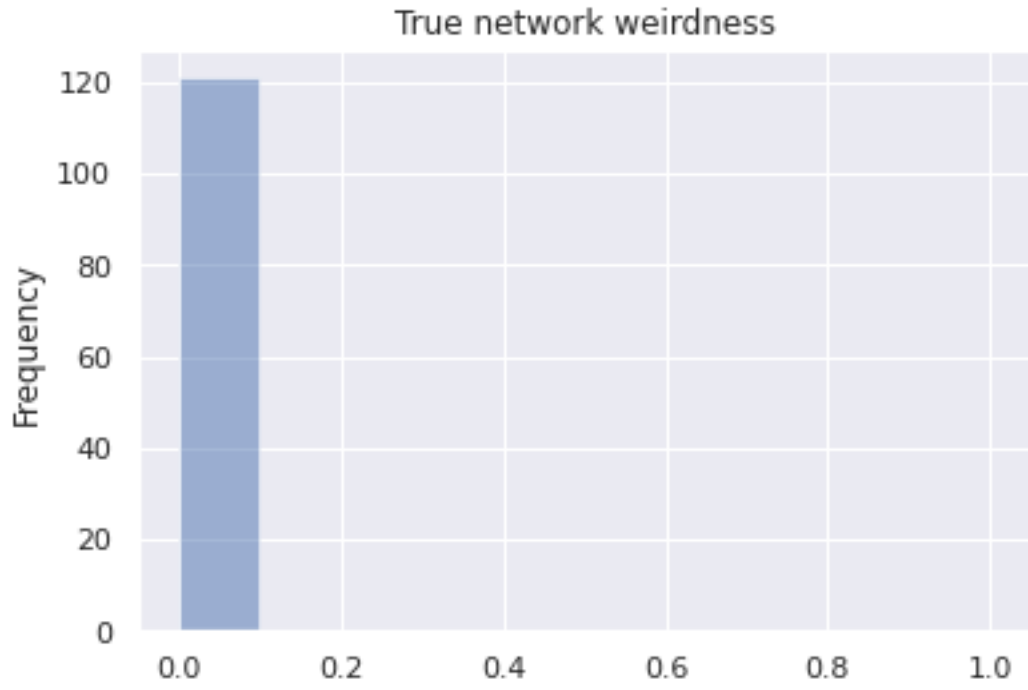
Inferred BIC better or equal: 109
Inferred BIC worse: 12

Inferred loglh better or equal: 45
Inferred loglh worse: 76

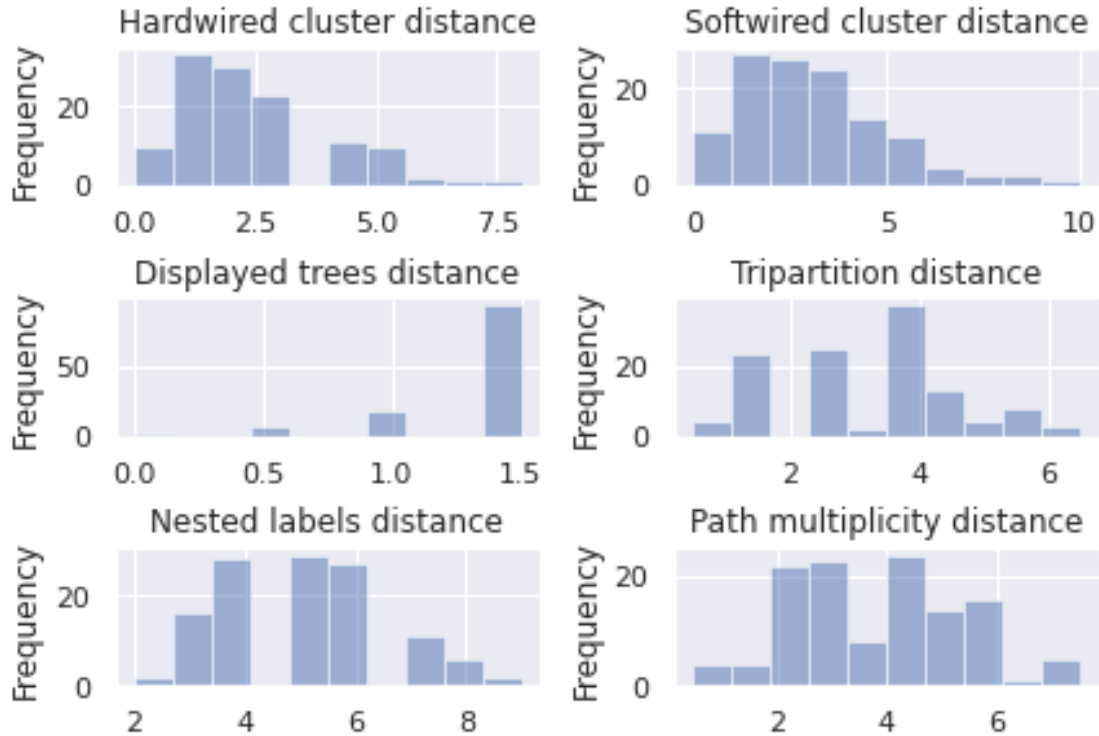
Inferred n_reticulations less: 104
Inferred n_reticulations equal: 17
Inferred n_reticulations more: 0



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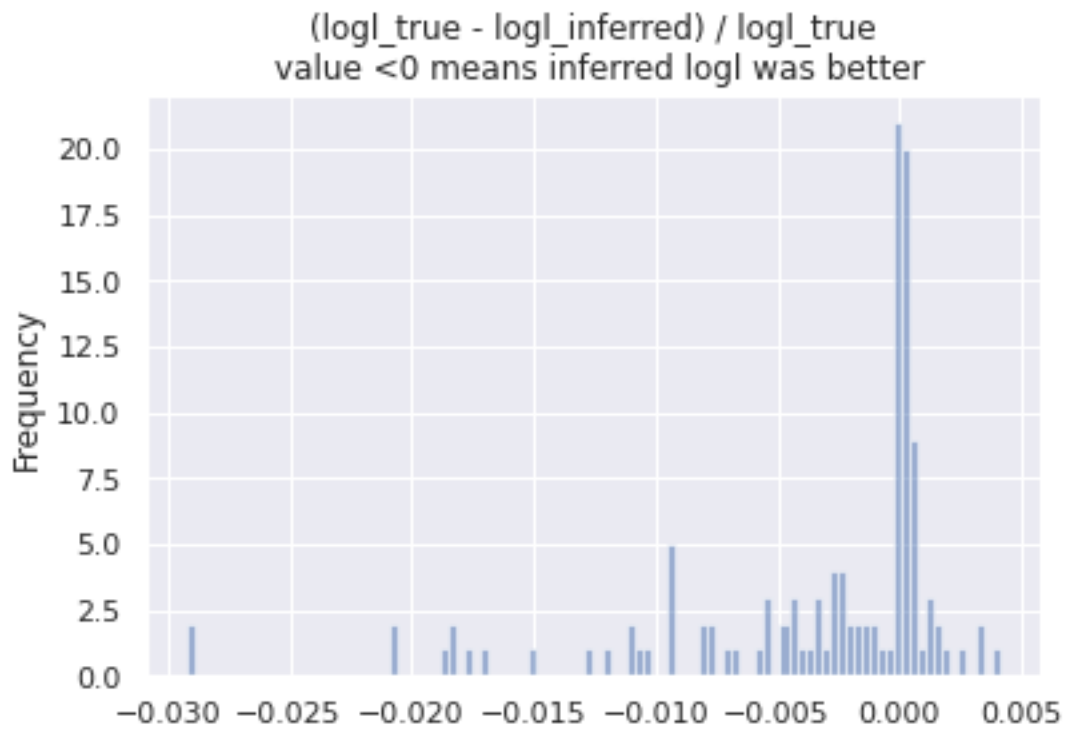
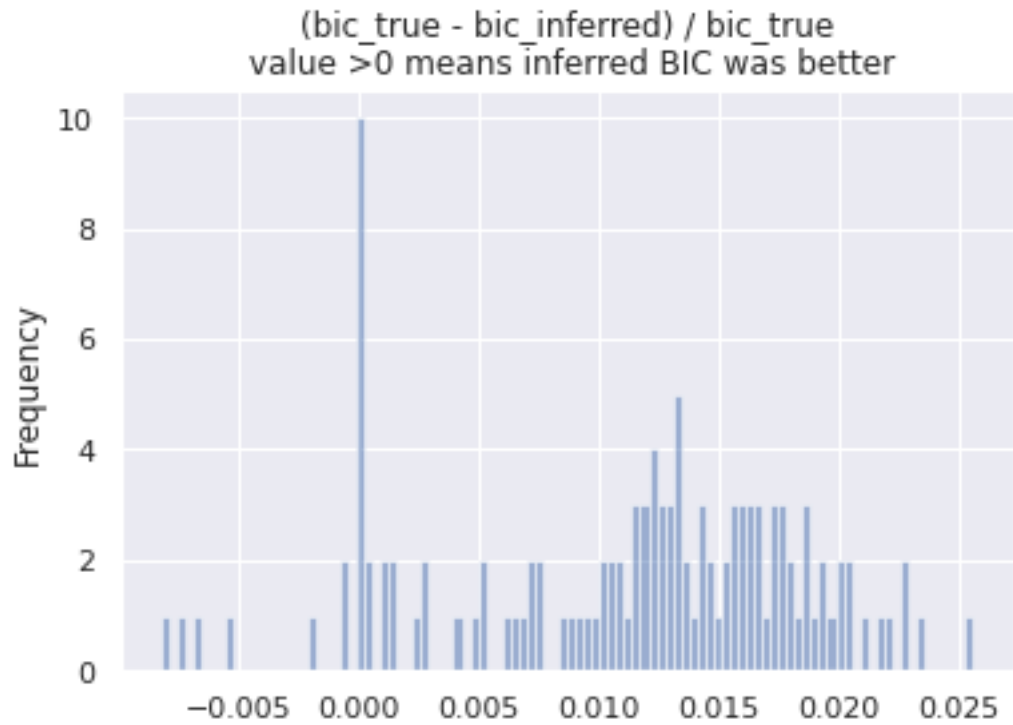
1.2.2 Plots for LikelihoodType.BEST

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

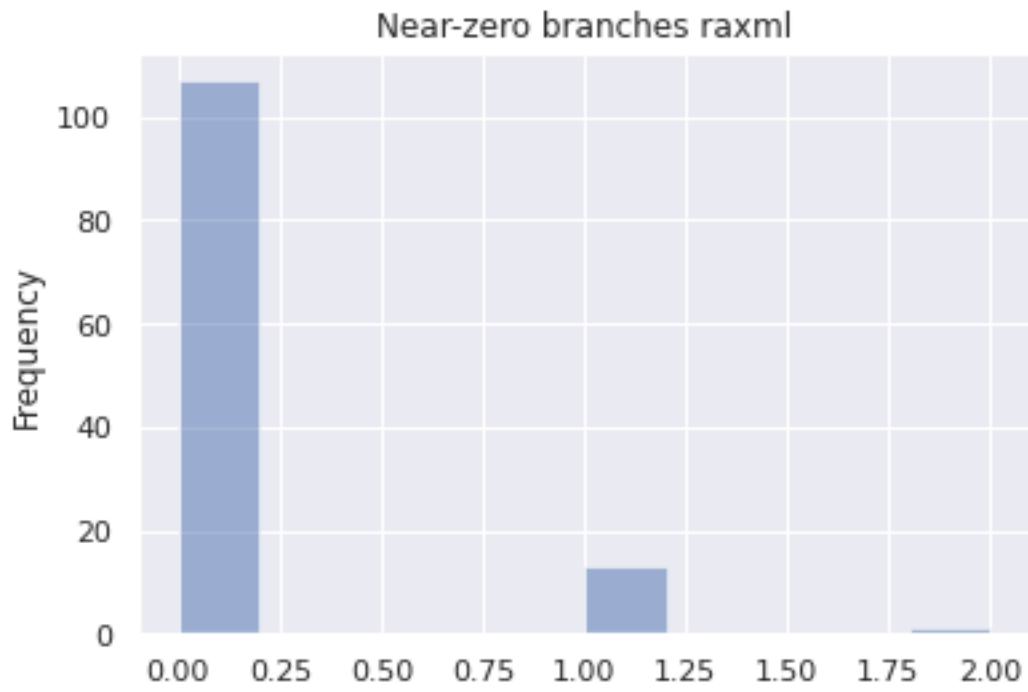
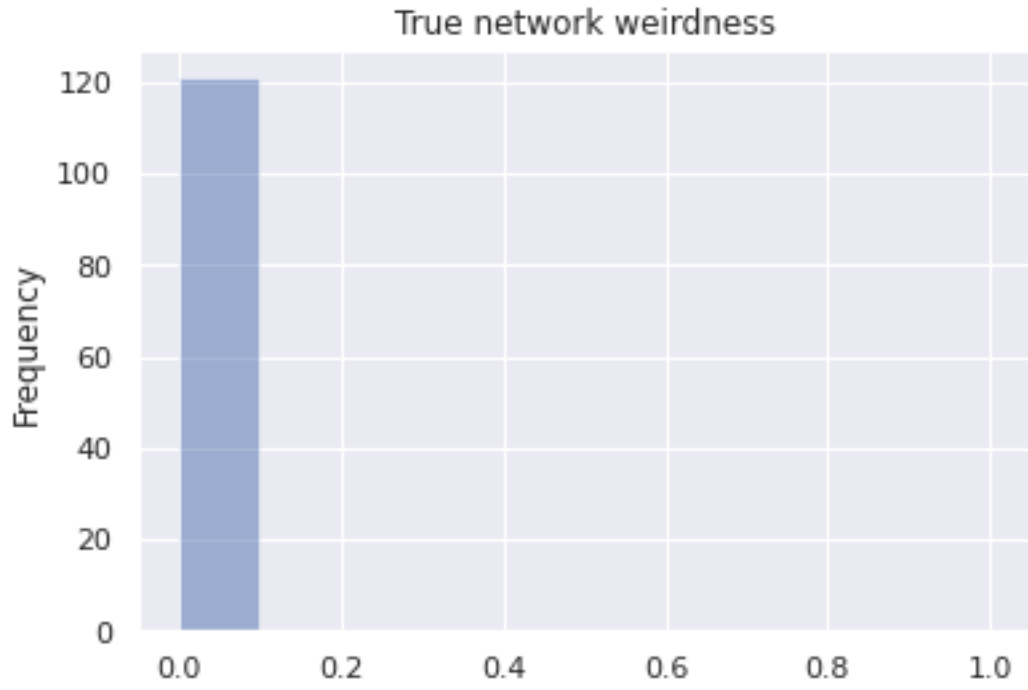
Inferred BIC better or equal: 107
Inferred BIC worse: 14

Inferred loglh better or equal: 51
Inferred loglh worse: 70

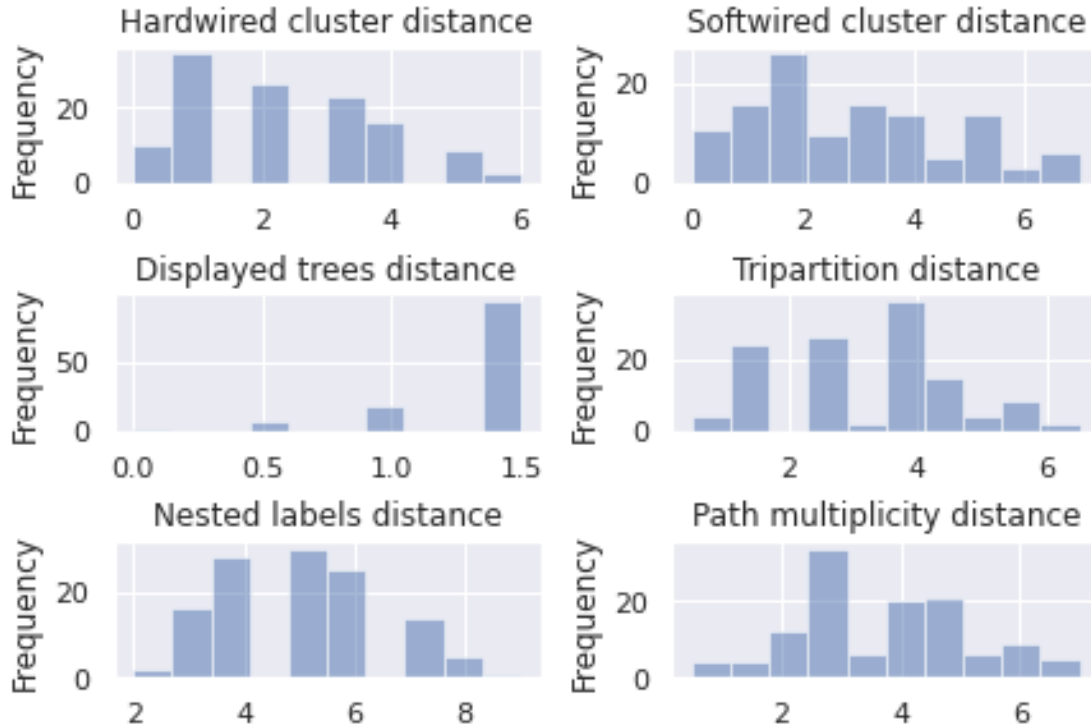
Inferred n_reticulations less: 104
Inferred n_reticulations equal: 17
Inferred n_reticulations more: 0



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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: 503

Inferred BIC worse: 5

Inferred loglh better or equal: 240

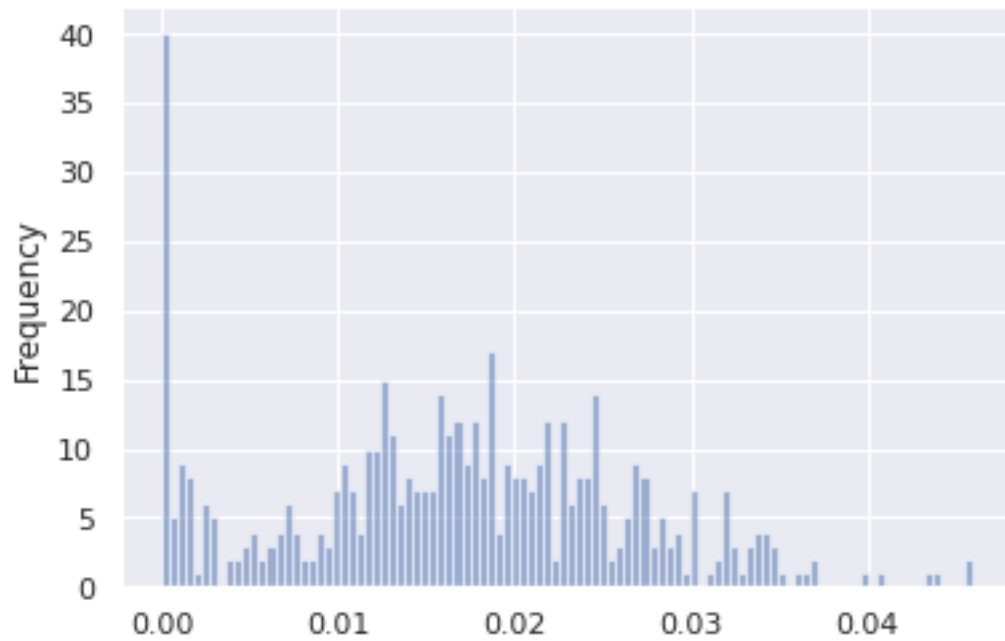
Inferred loglh worse: 268

Inferred n_reticulations less: 450

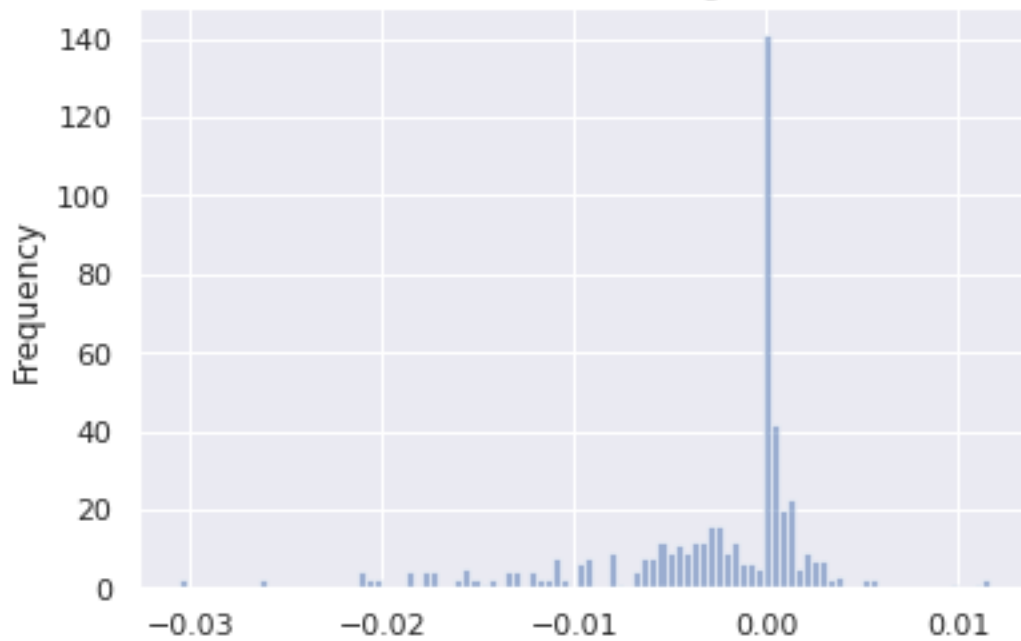
Inferred n_reticulations equal: 58

Inferred n_reticulations more: 0

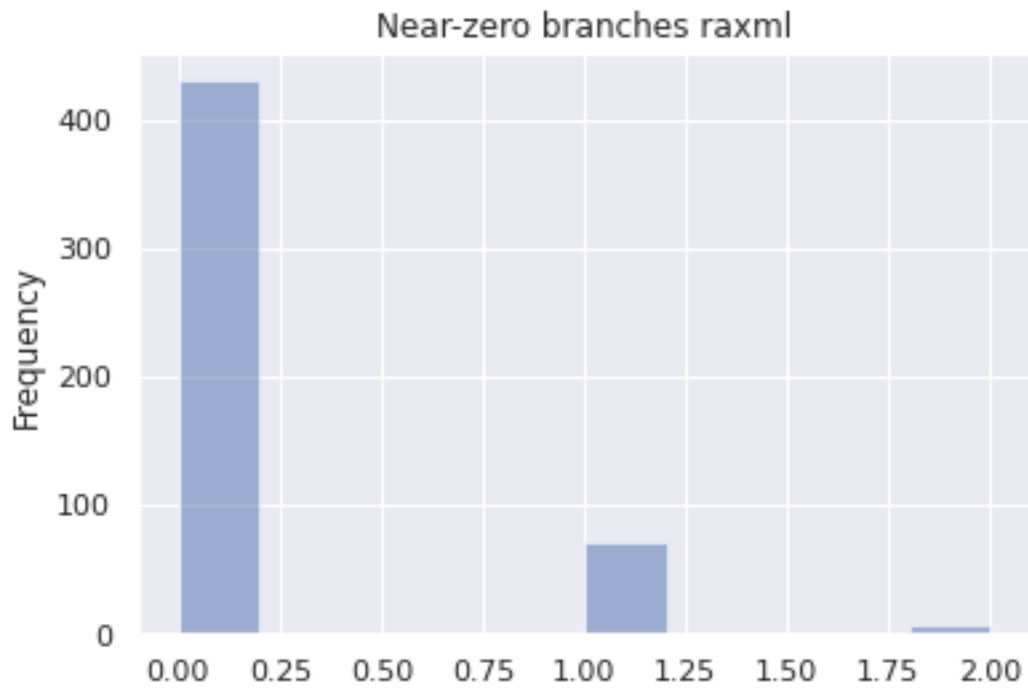
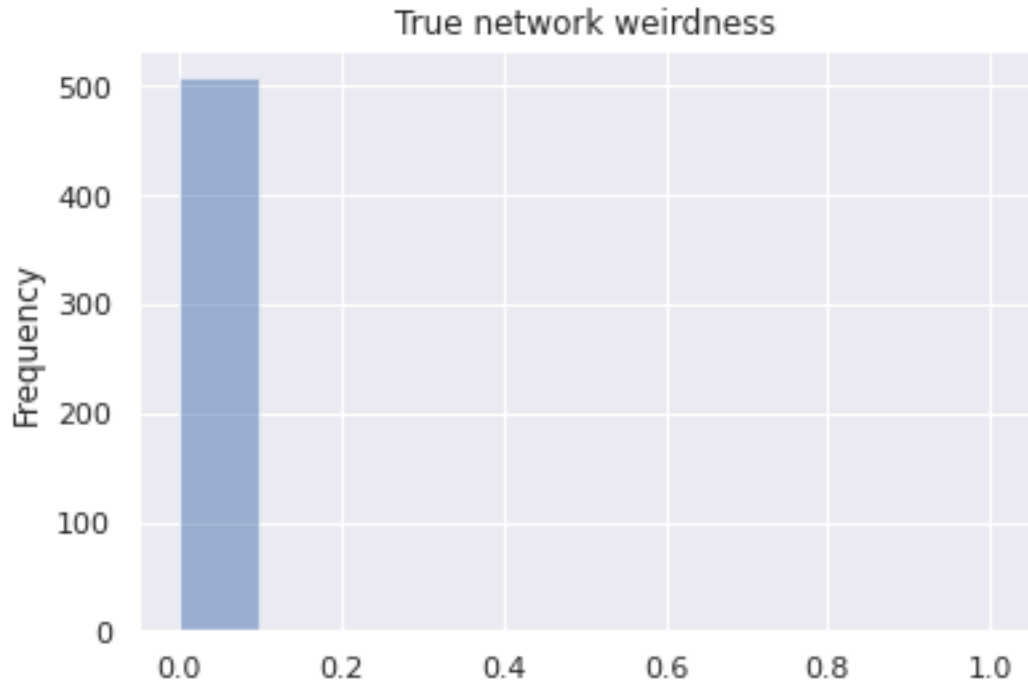
$(bic_true - bic_inferred) / bic_true$
value >0 means inferred BIC was better



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



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<Figure size 432x288 with 0 Axes>



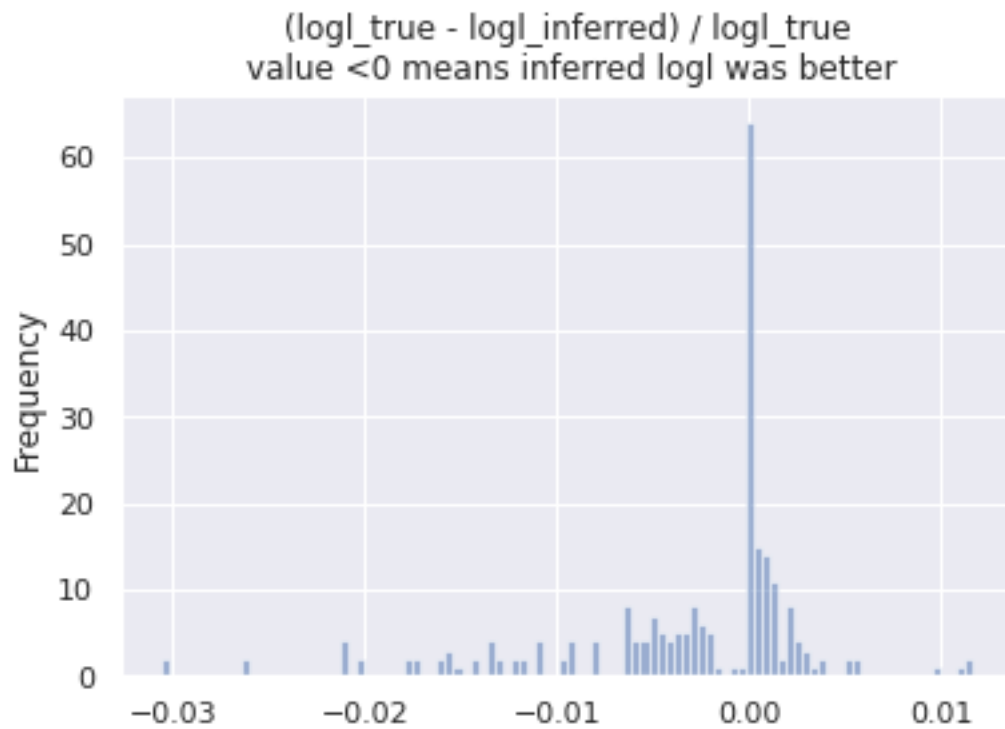
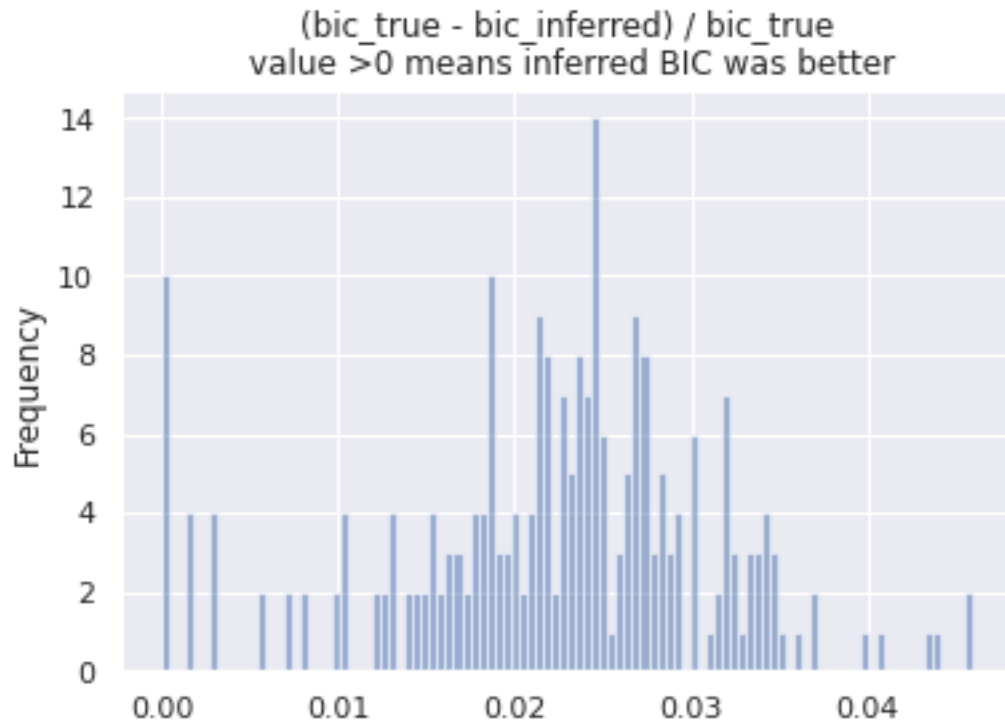
2.1 Plots for $MSA_size \sim 100 * n_trees$

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

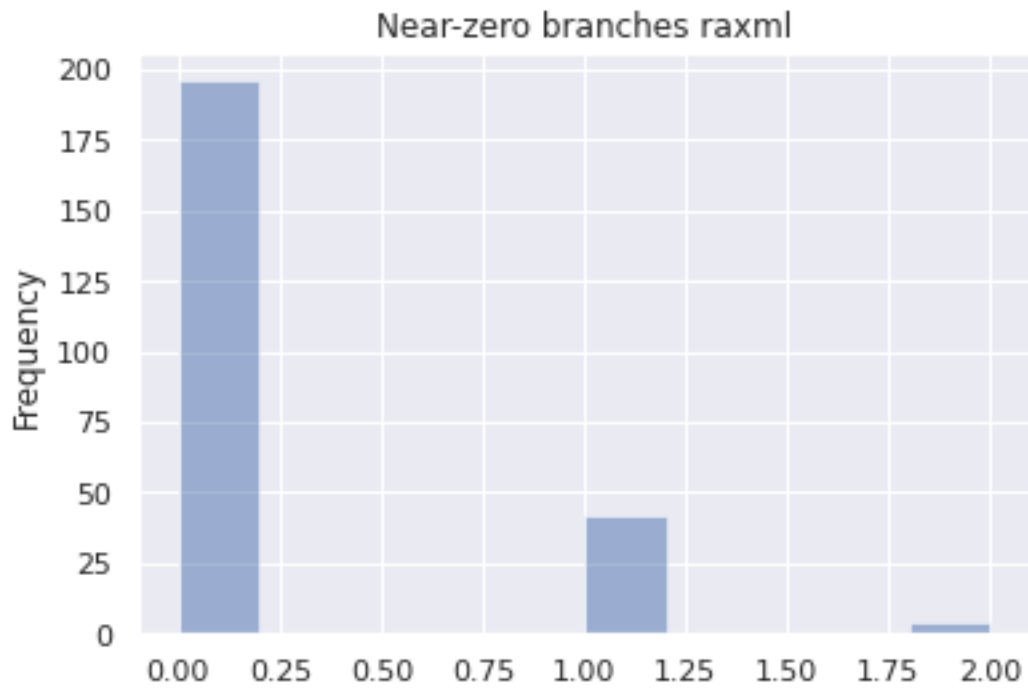
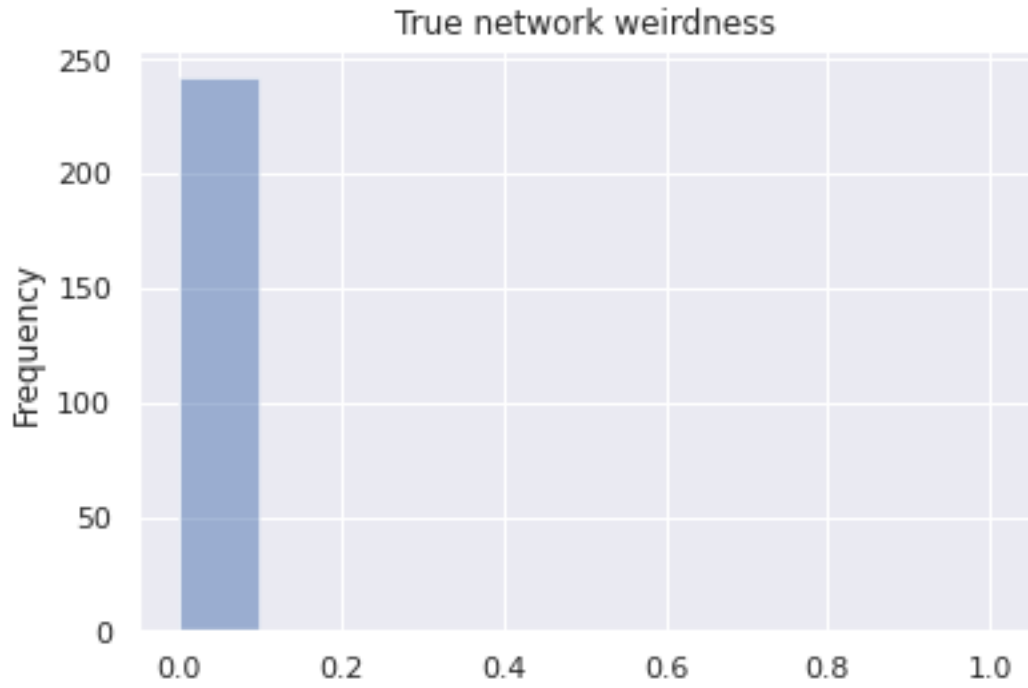
Inferred BIC better or equal: 240
Inferred BIC worse: 2

Inferred loglh better or equal: 115
Inferred loglh worse: 127

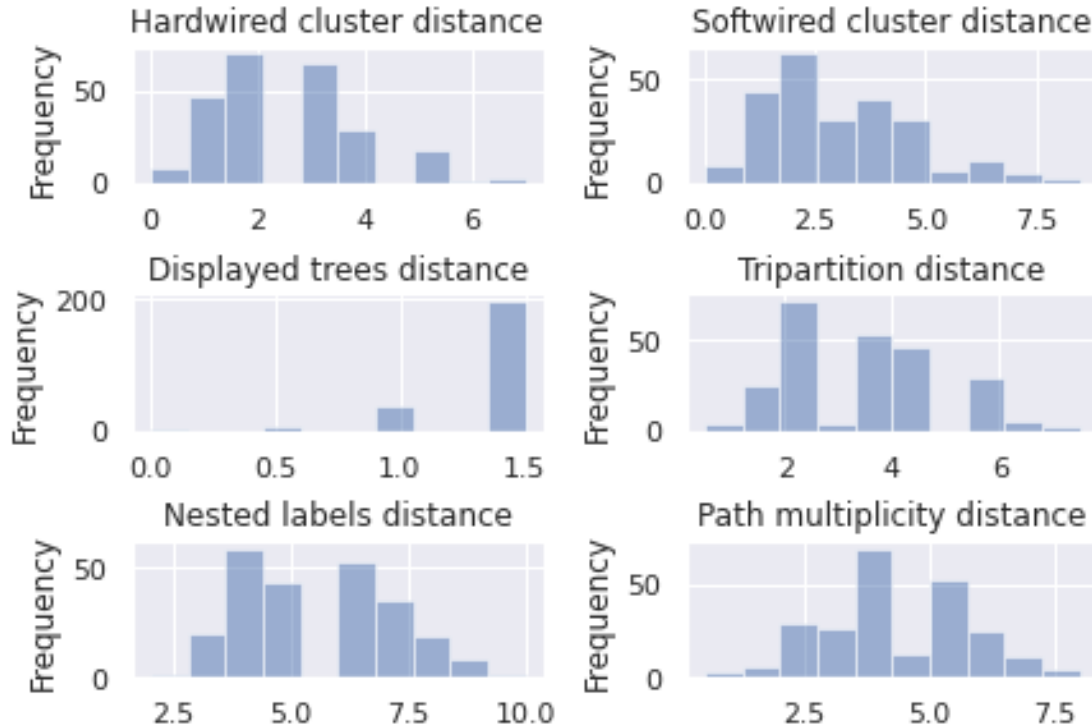
Inferred n_reticulations less: 226
Inferred n_reticulations equal: 16
Inferred n_reticulations more: 0



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<Figure size 432x288 with 0 Axes>



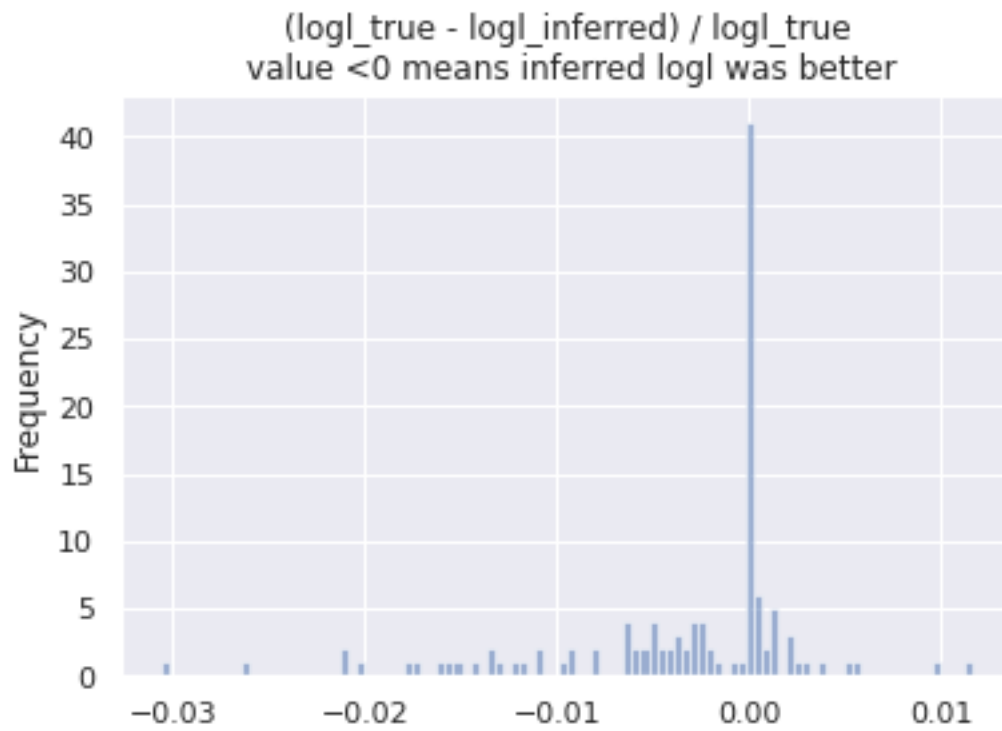
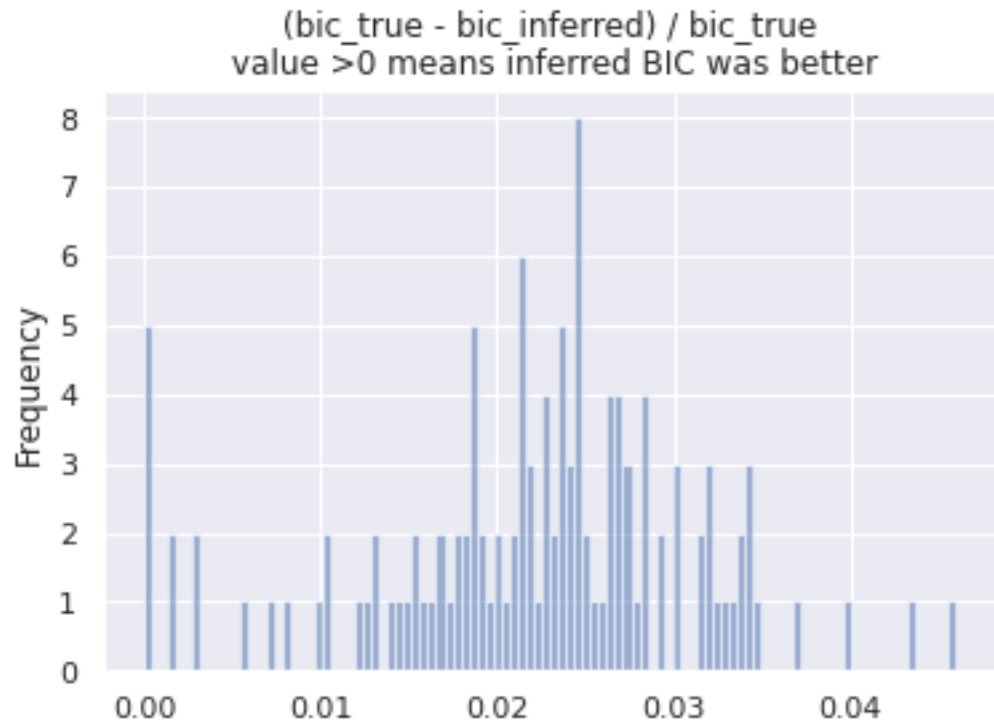
2.1.1 Plots for LikelihoodType.AVERAGE

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

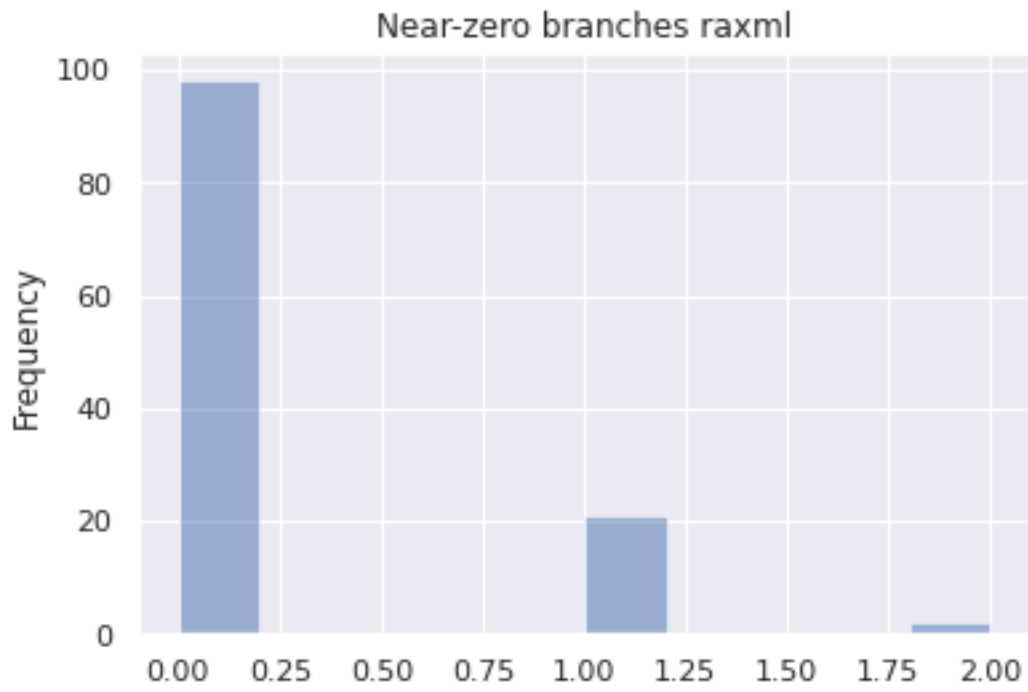
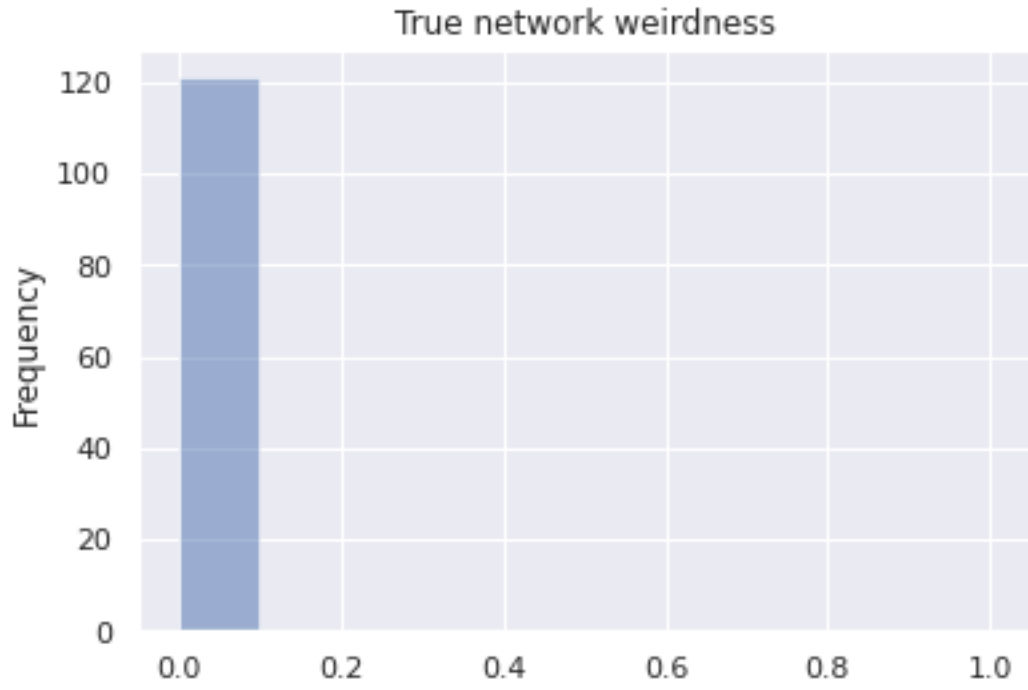
Inferred BIC better or equal: 120
Inferred BIC worse: 1

Inferred loglh better or equal: 51
Inferred loglh worse: 70

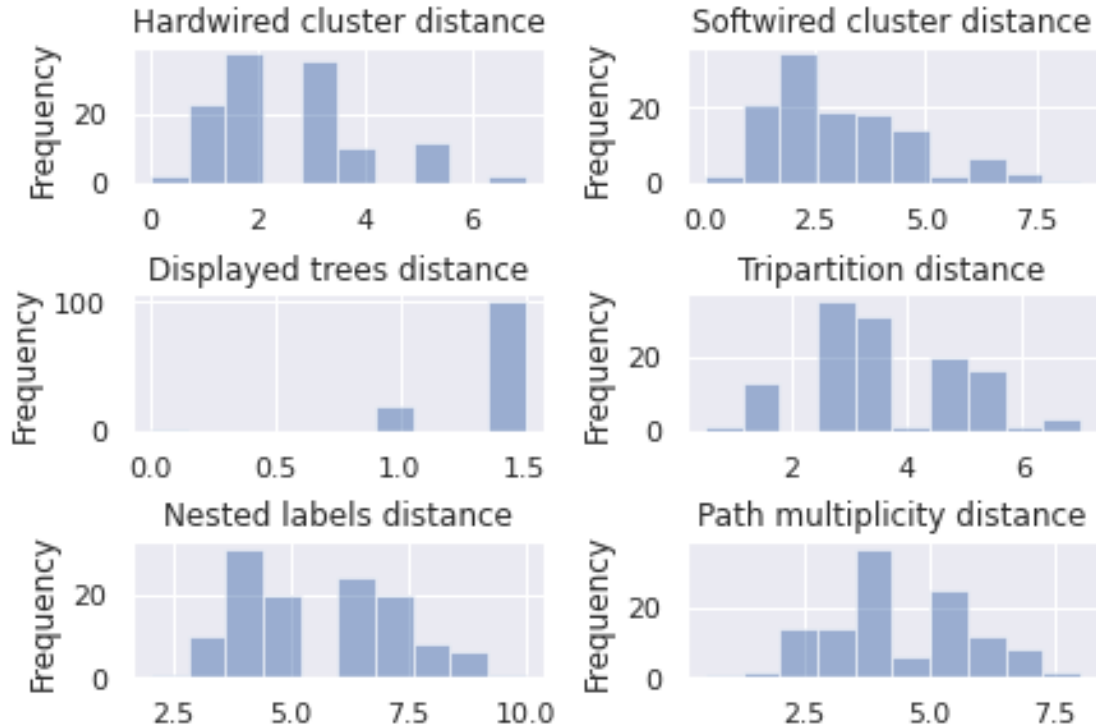
Inferred n_reticulations less: 113
Inferred n_reticulations equal: 8
Inferred n_reticulations more: 0



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<Figure size 432x288 with 0 Axes>



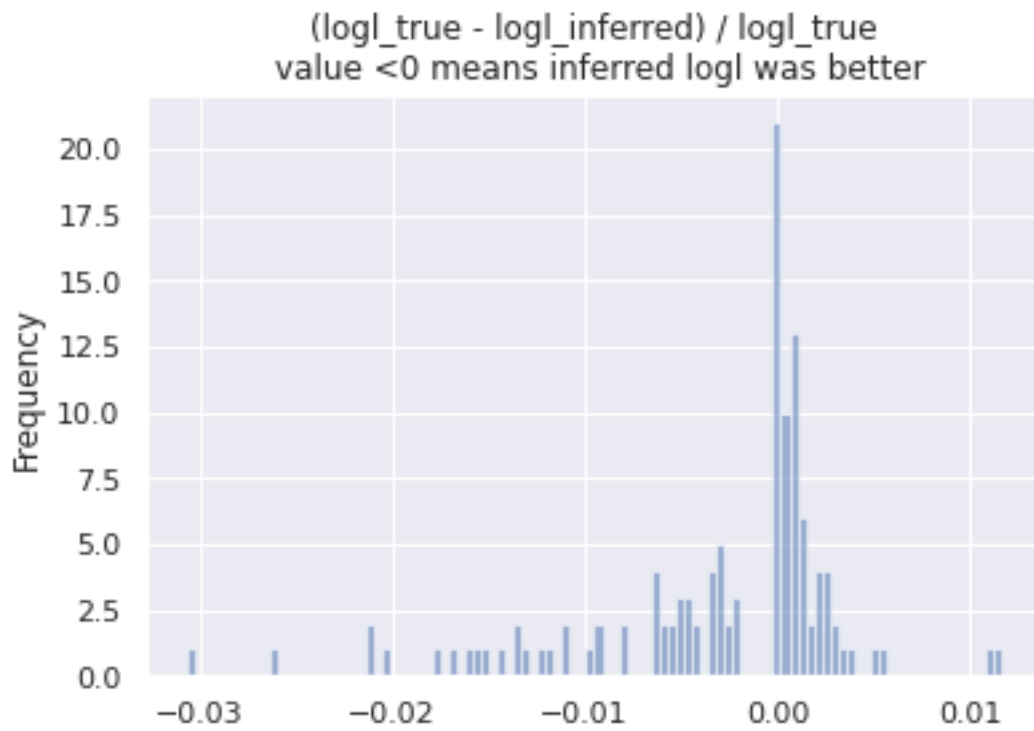
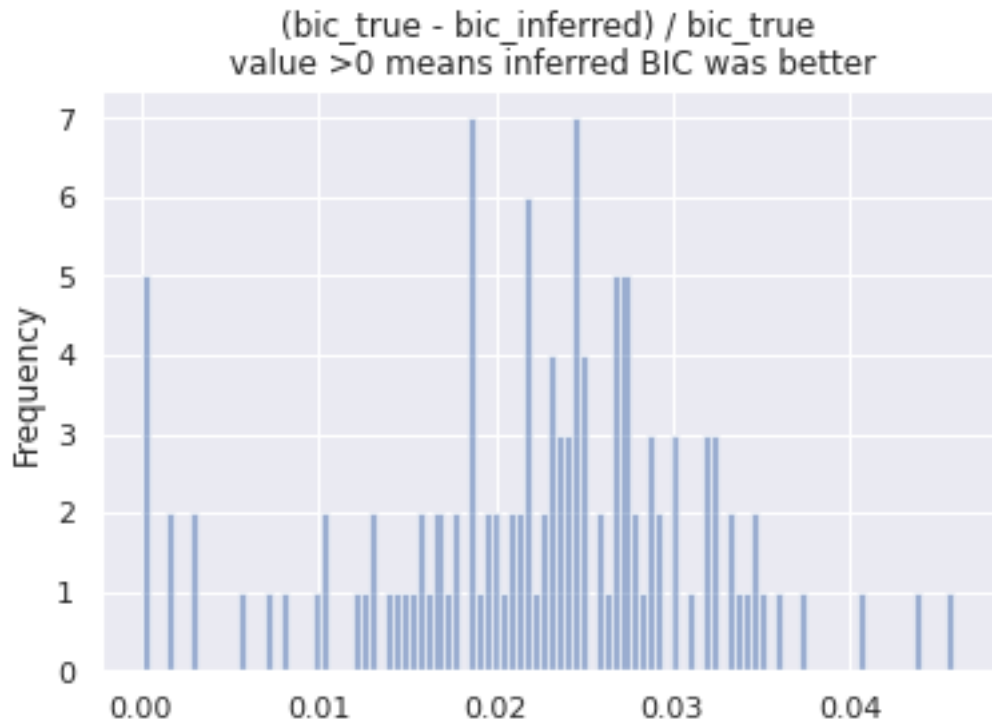
2.1.2 Plots for LikelihoodType.BEST

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

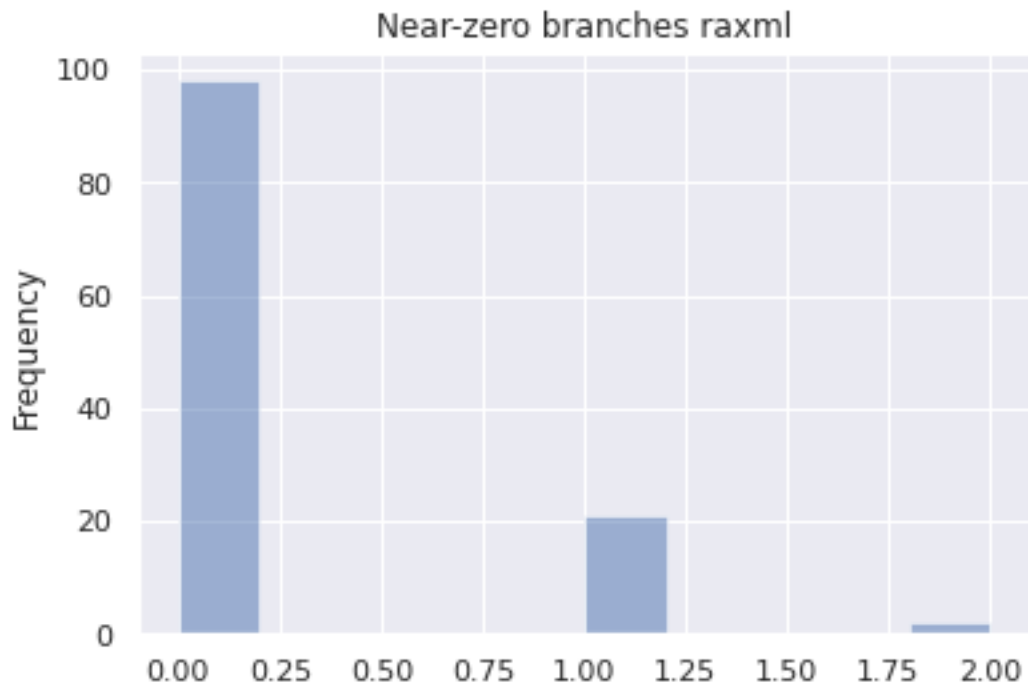
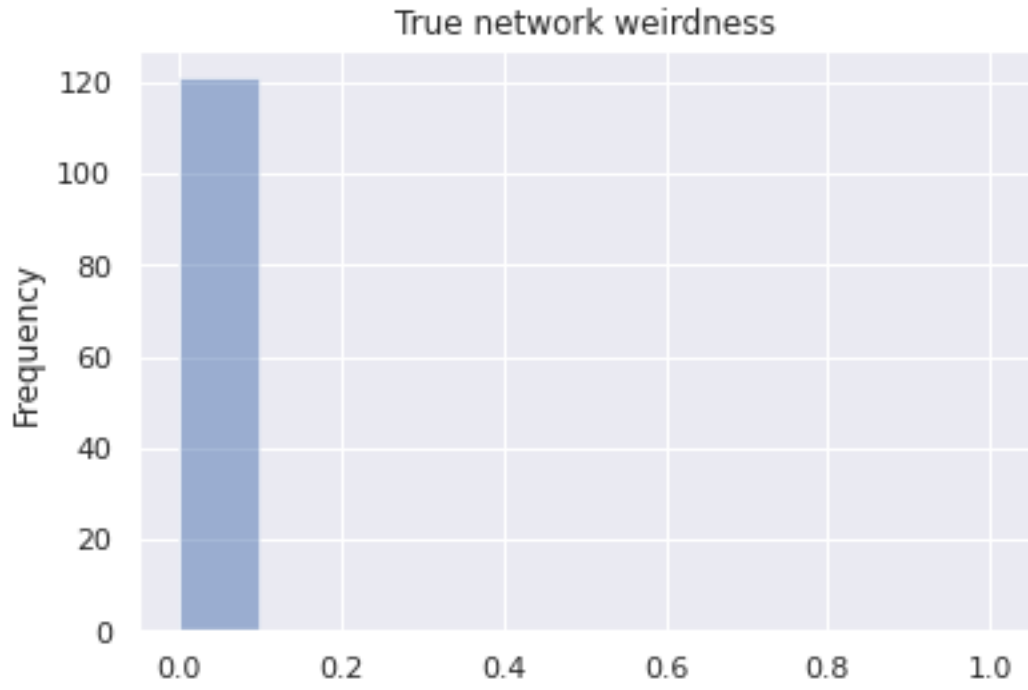
Inferred BIC better or equal: 120
Inferred BIC worse: 1

Inferred loglh better or equal: 64
Inferred loglh worse: 57

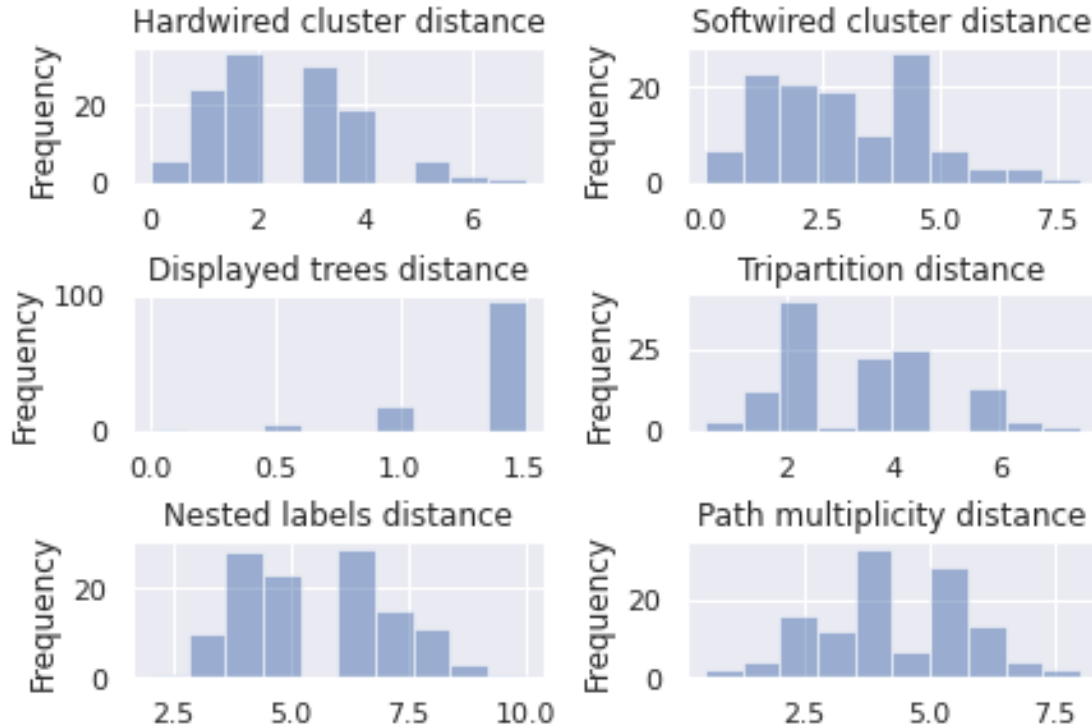
Inferred n_reticulations less: 113
Inferred n_reticulations equal: 8
Inferred n_reticulations more: 0



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<Figure size 432x288 with 0 Axes>



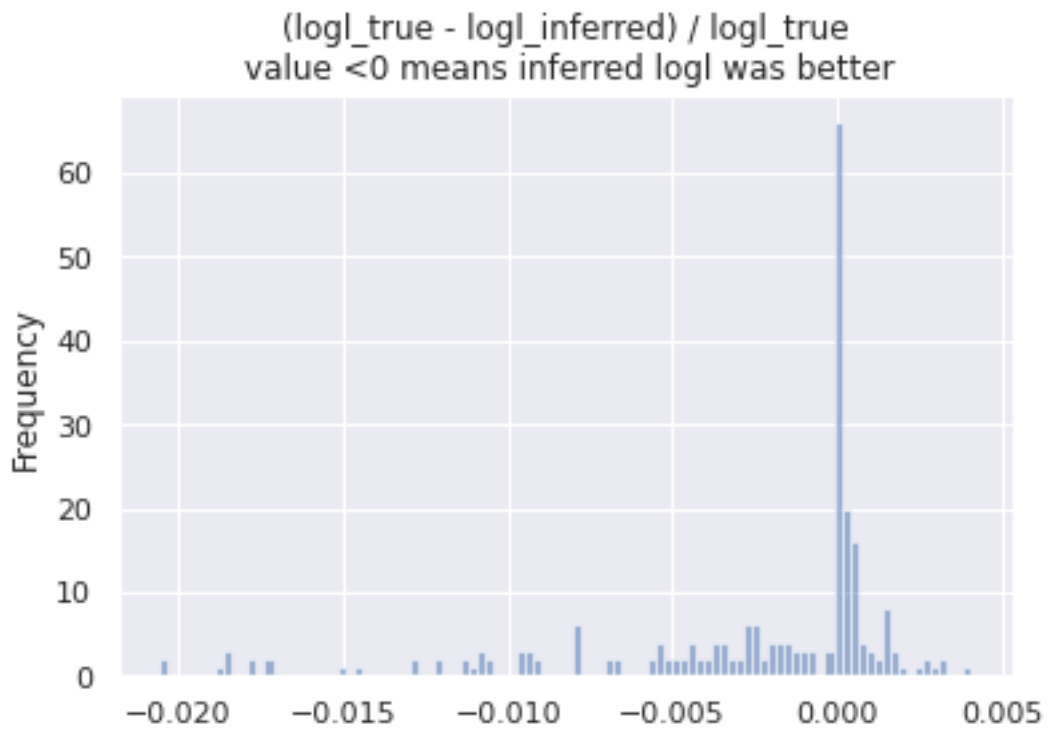
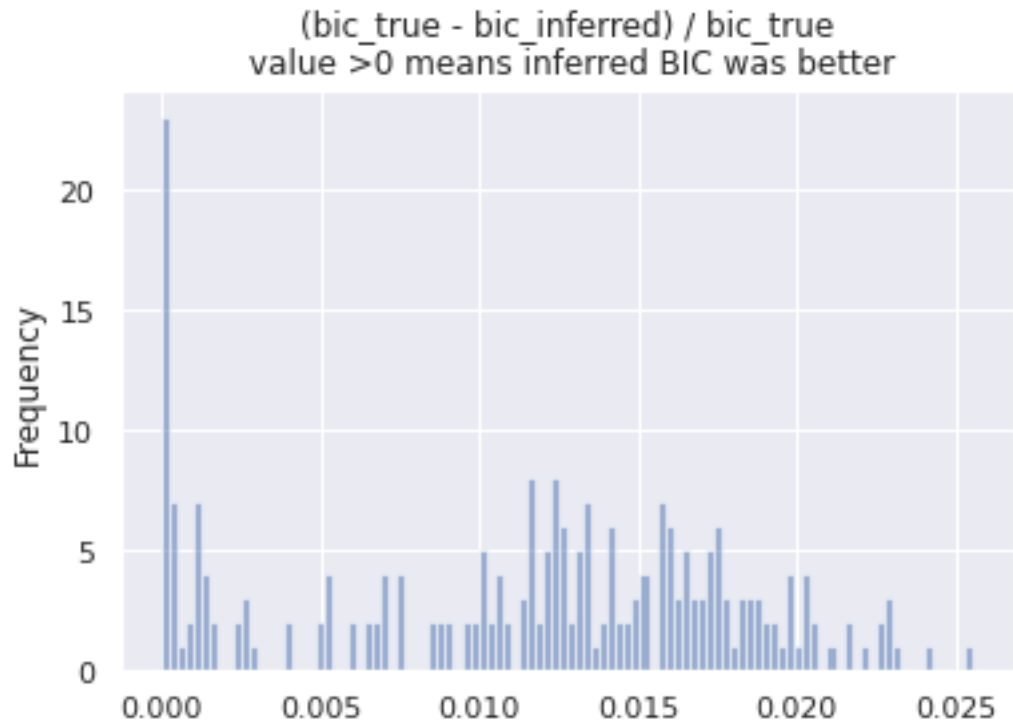
2.2 Plots for MSA_size ~ 200*n_trees

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

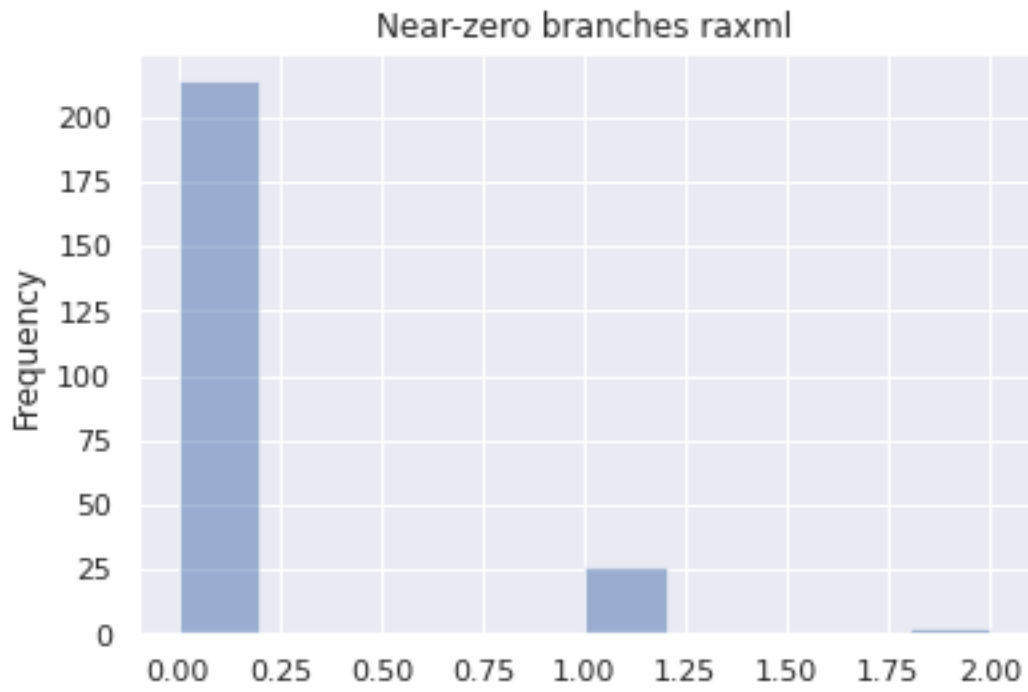
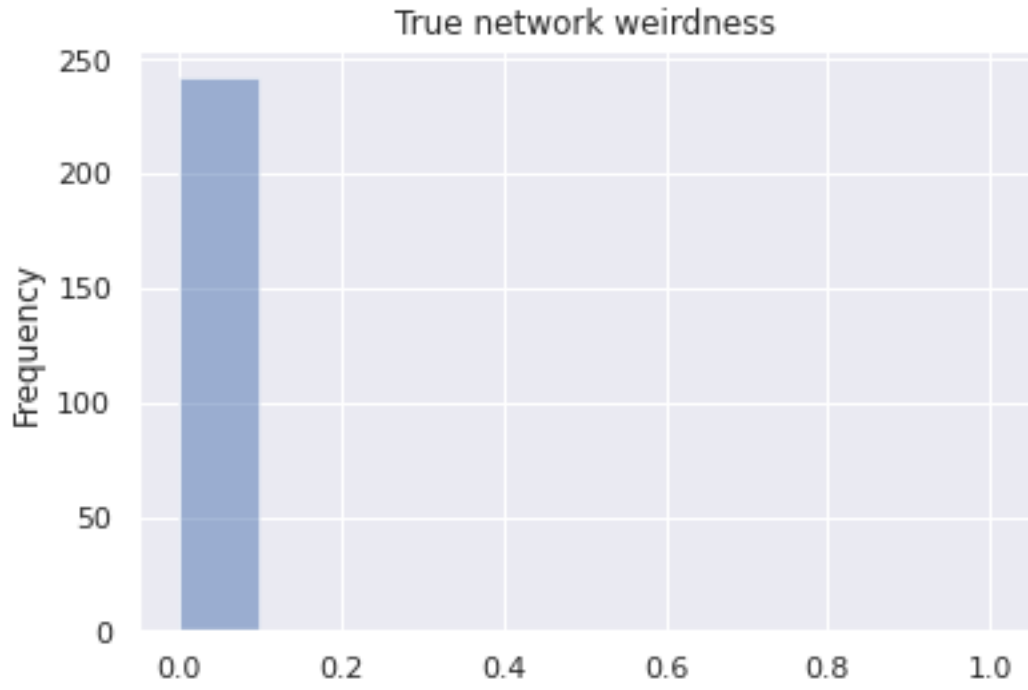
Inferred BIC better or equal: 239
Inferred BIC worse: 3

Inferred loglh better or equal: 120
Inferred loglh worse: 122

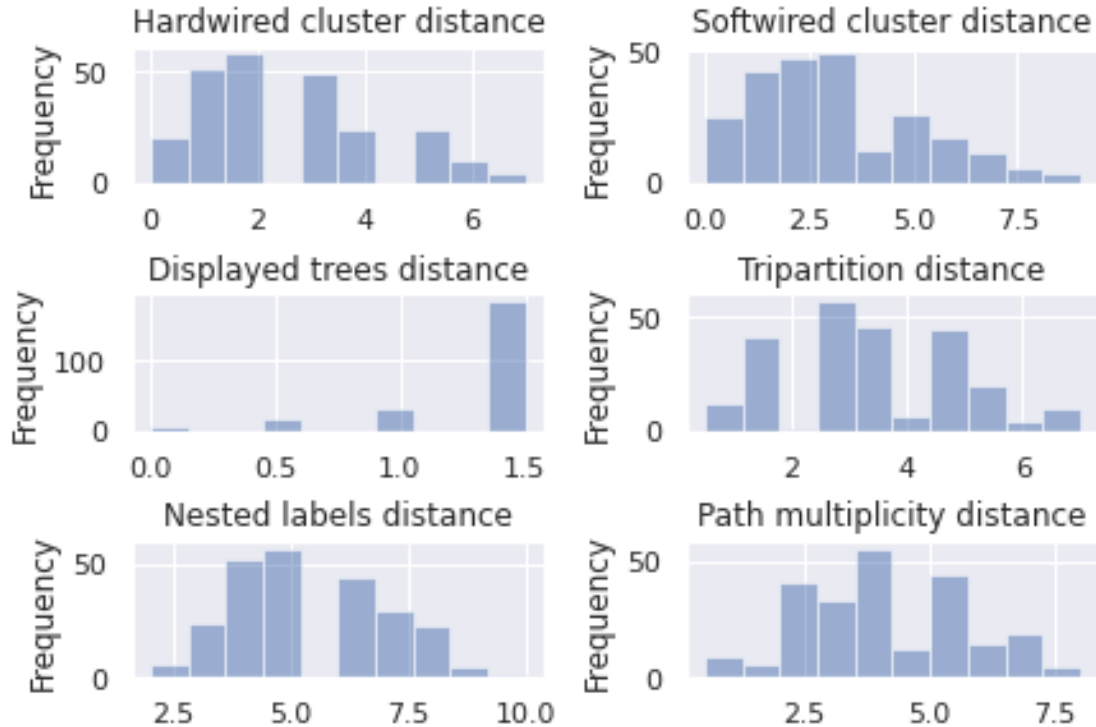
Inferred n_reticulations less: 200
Inferred n_reticulations equal: 42
Inferred n_reticulations more: 0



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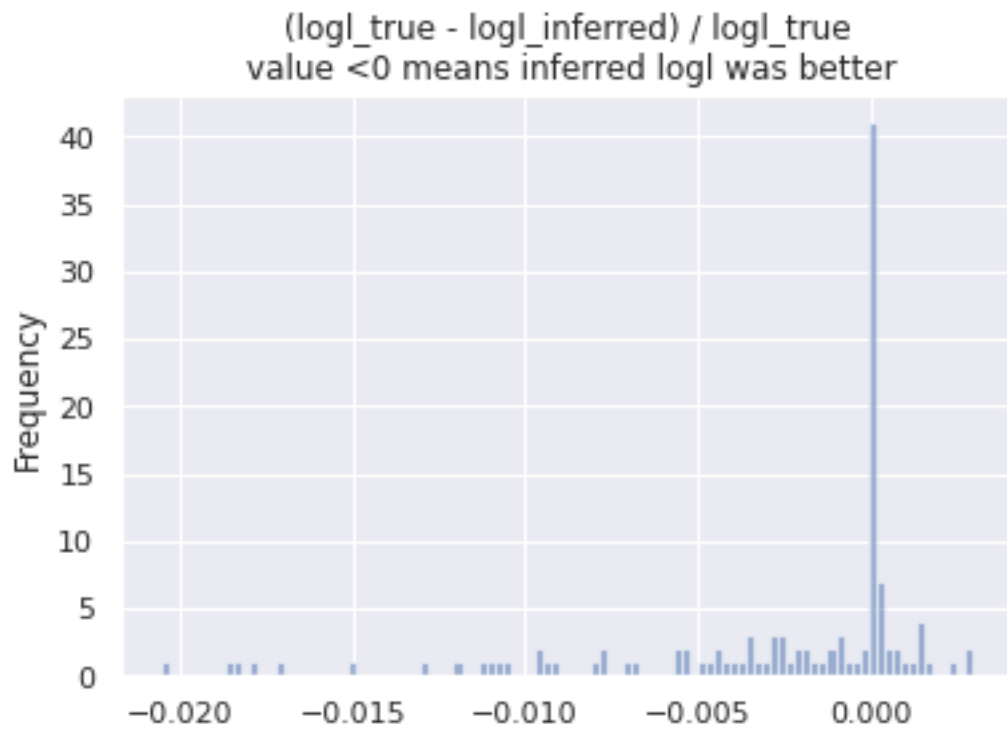
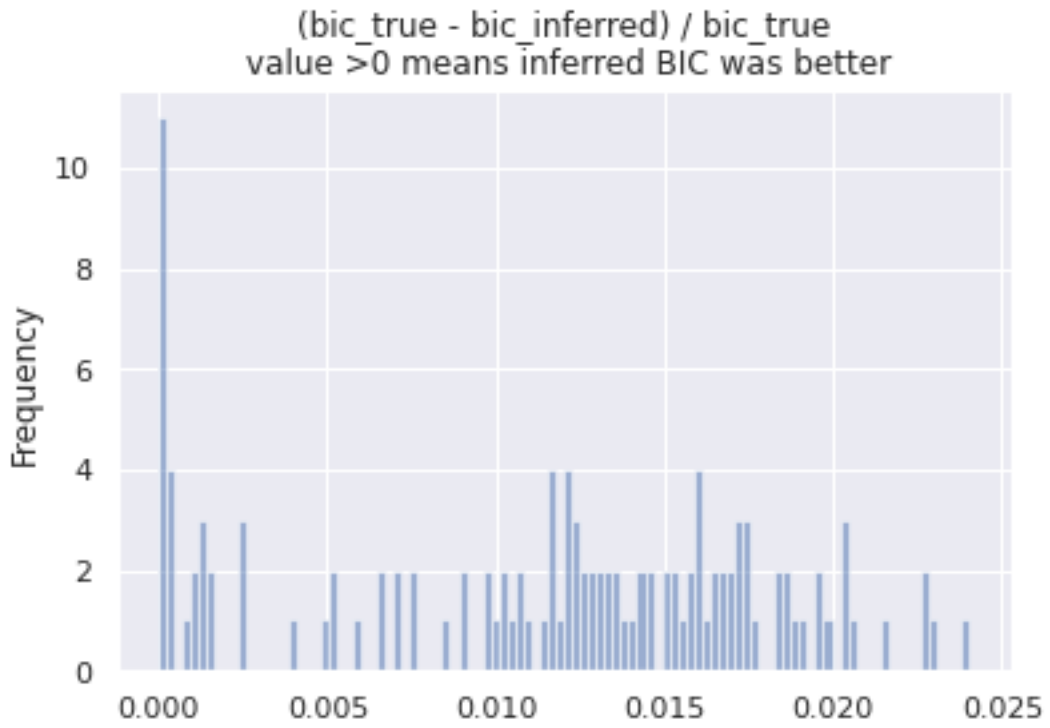
2.2.1 Plots for LikelihoodType.AVERAGE

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

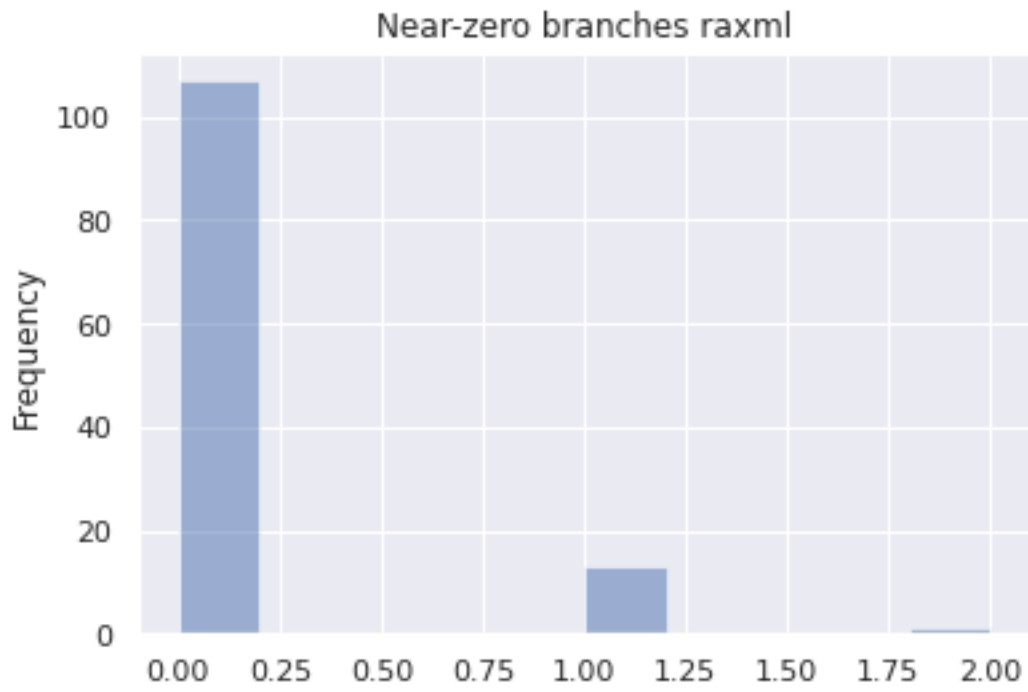
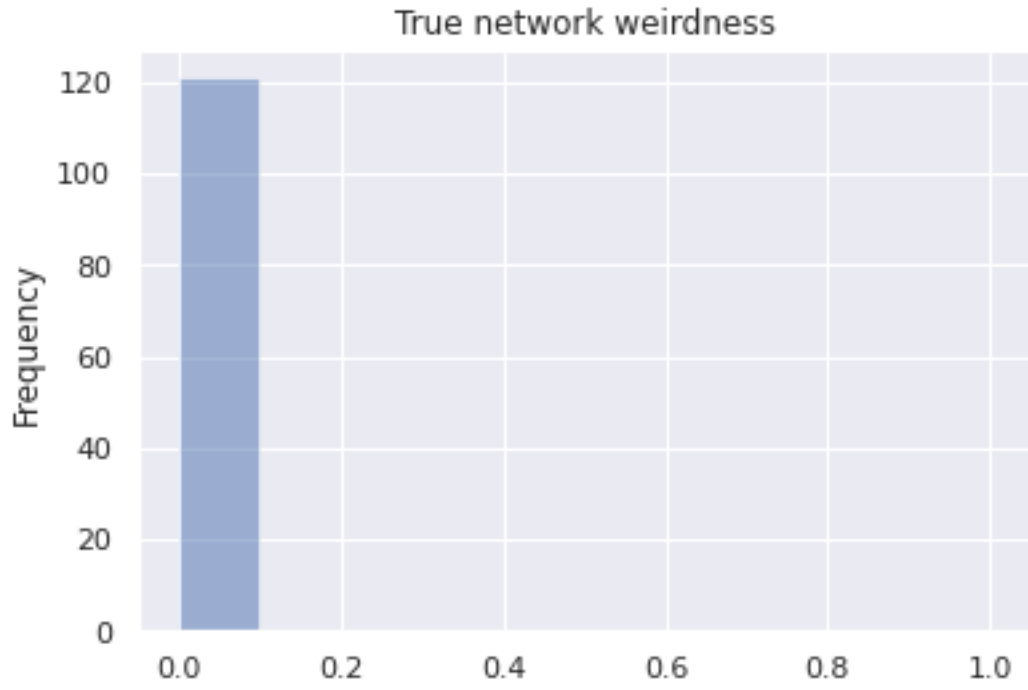
Inferred BIC better or equal: 120
Inferred BIC worse: 1

Inferred loglh better or equal: 56
Inferred loglh worse: 65

Inferred n_reticulations less: 100
Inferred n_reticulations equal: 21
Inferred n_reticulations more: 0



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<Figure size 432x288 with 0 Axes>



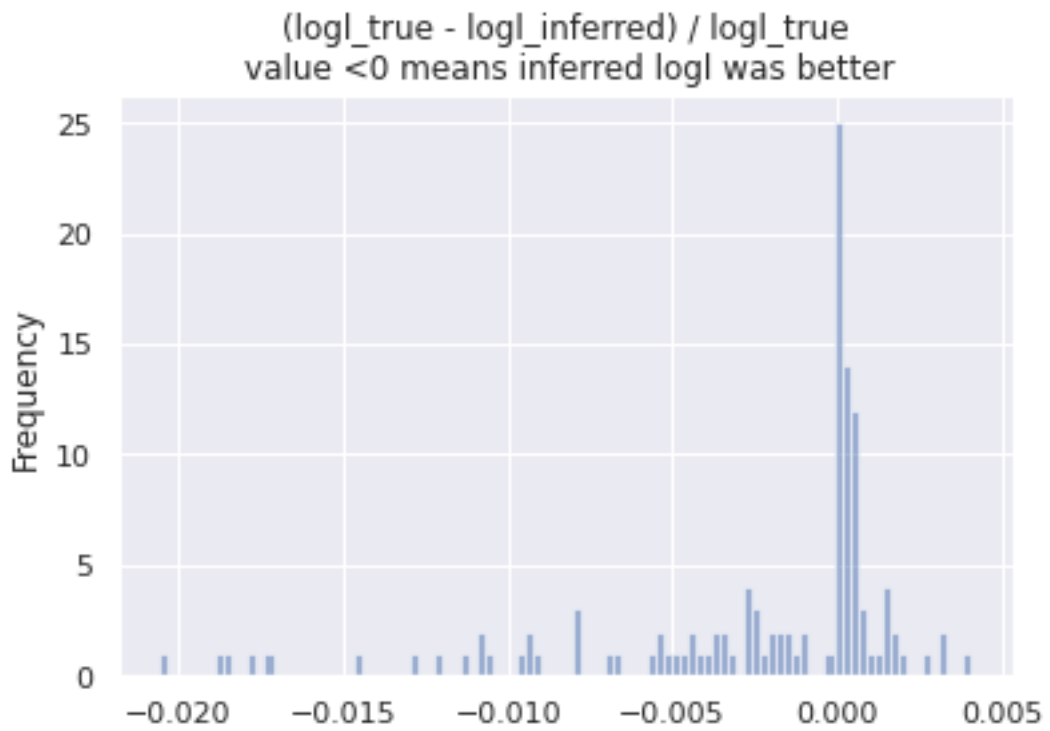
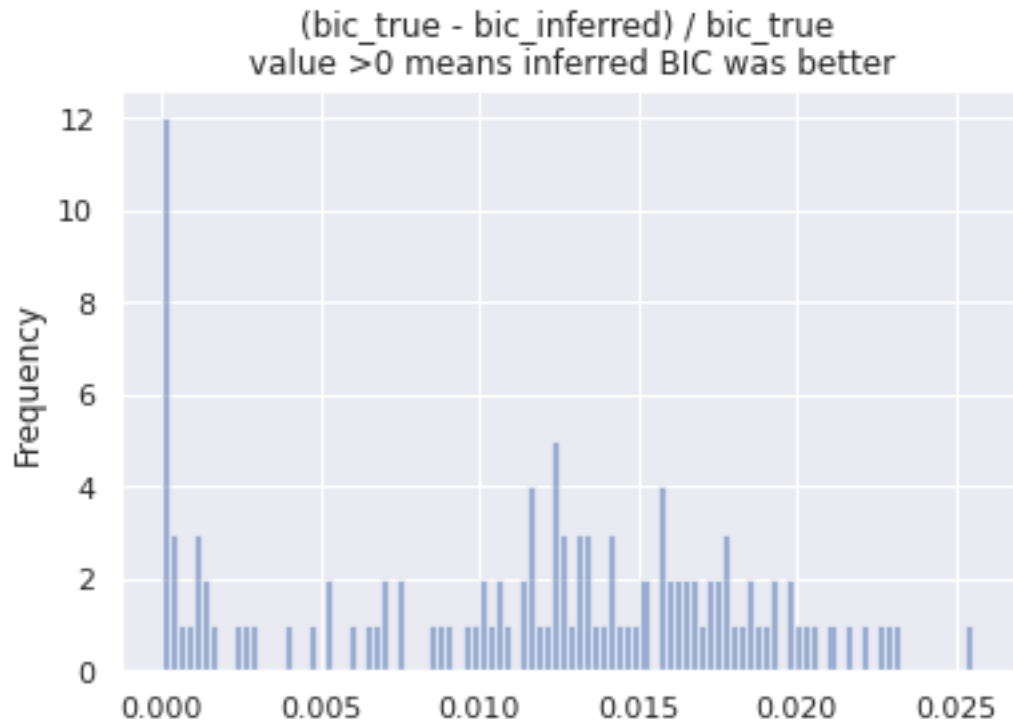
2.2.2 Plots for LikelihoodType.BEST

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

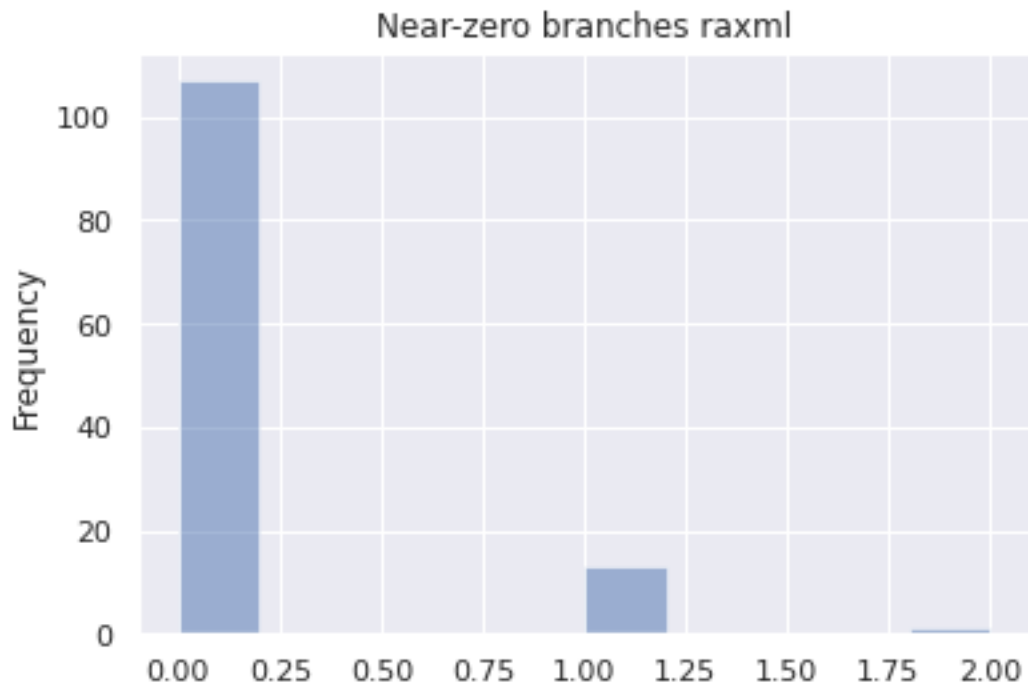
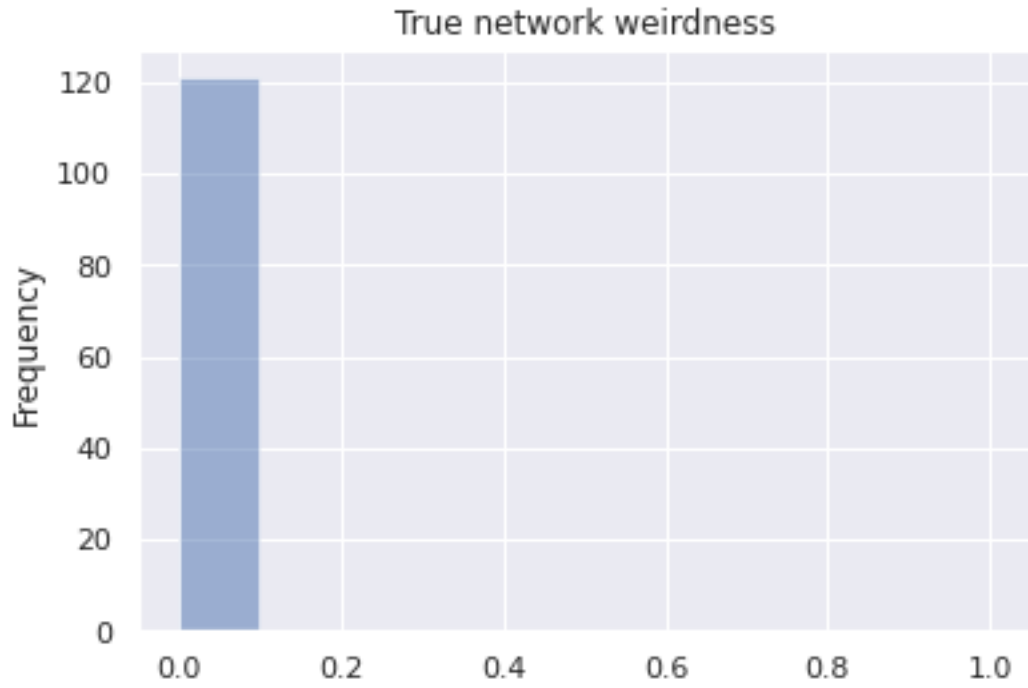
Inferred BIC better or equal: 119
Inferred BIC worse: 2

Inferred loglh better or equal: 64
Inferred loglh worse: 57

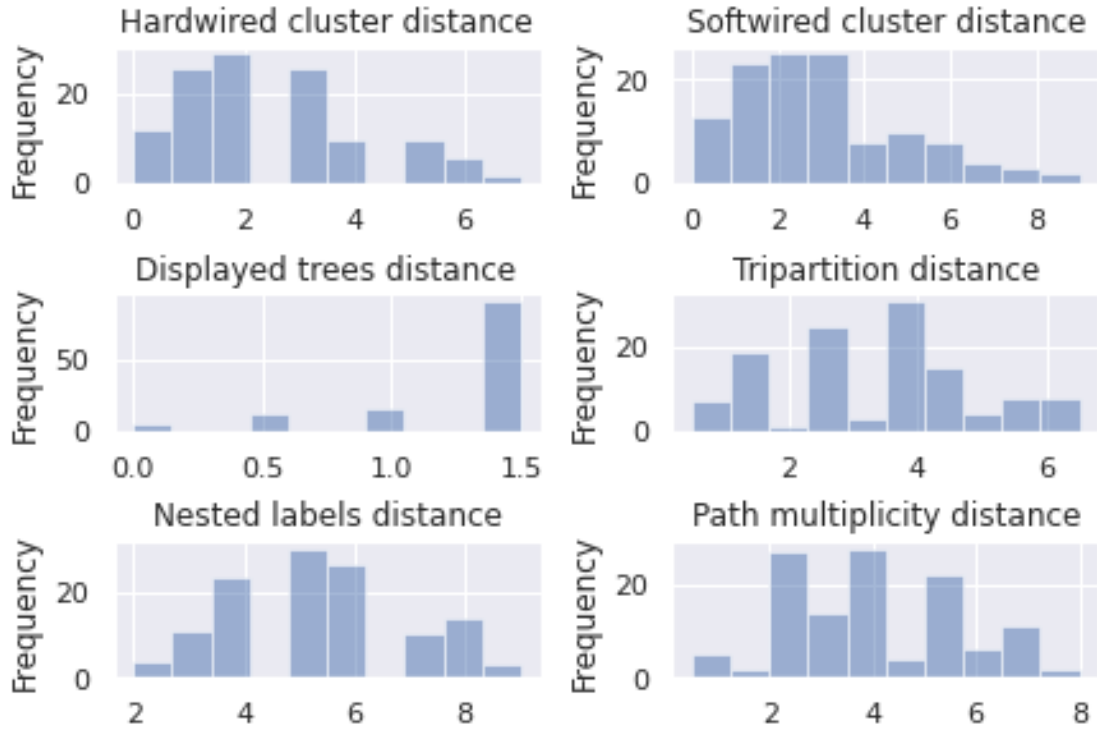
Inferred n_reticulations less: 100
Inferred n_reticulations equal: 21
Inferred n_reticulations more: 0



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[]:

