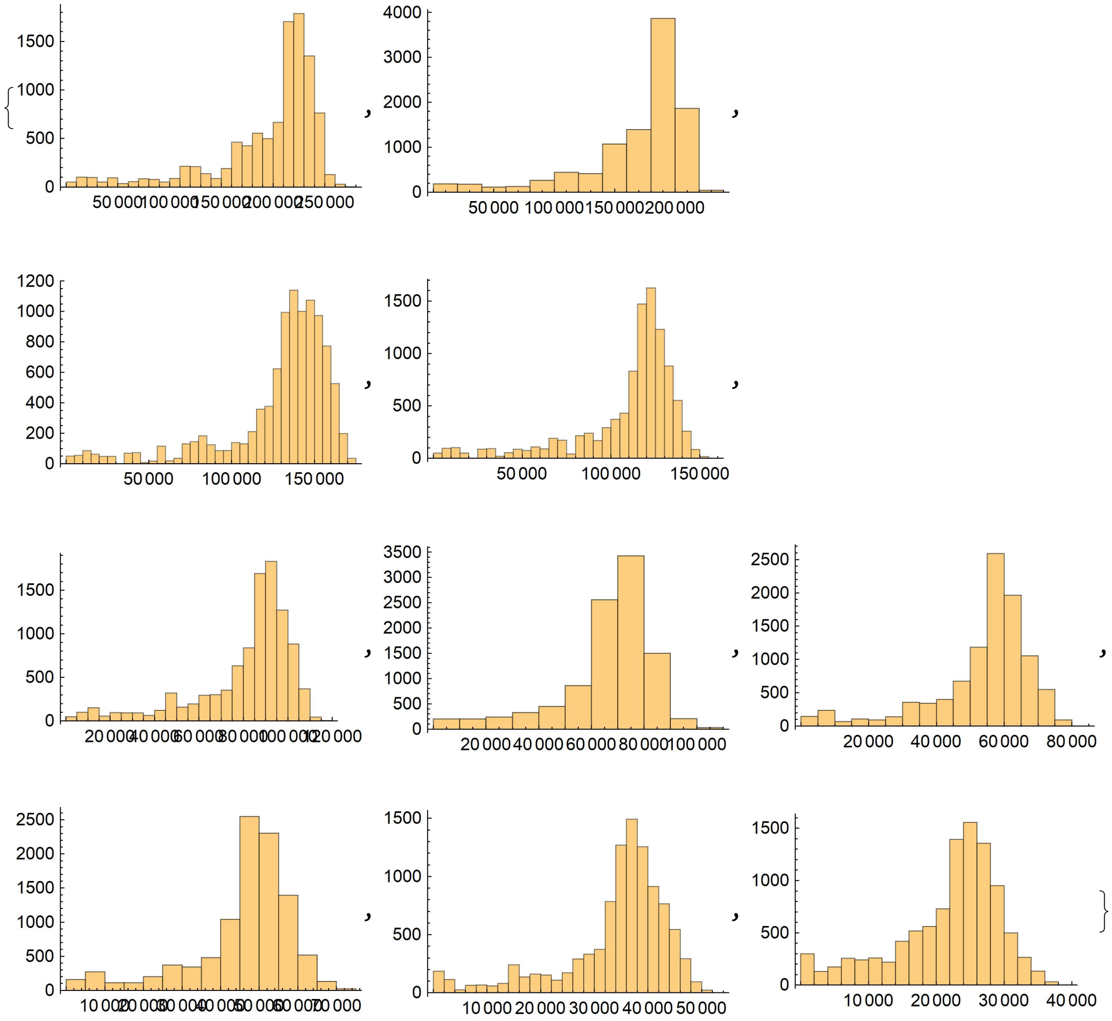
```
In[ ]:= SetDirectory[
          "C:/Users/serha/OneDrive/Masaüstü/MyRepo/master_thesis_MMT003/210603_bar_charts_and_OR
            _model/deleting_reactions"];

In[ ]:= Get["../../algoritm_packages/SingleNetworks-algorithm-package-2.wl"]
        (* ?SingleNetworks`* *)

In[ ]:= stoichioforhomosapiens =
          Drop[Import["../../210324_disc_time_windows_and_OR_model/iAT_PLT_636_stoichiomat.csv",
            HeaderLines → 1], None, {1}];
        SparseArray@stoichioforhomosapiens

Out[ ]= SparseArray[ ⊞  Specified elements: 4006
                        Dimensions: {738, 1008} ]

In[ ]:= stoichiometricmatrix = stoichioforhomosapiens;
        metabolites = 738;
        fluxexchanges = 1008;
        steadystatevector = ConstantArray[{0, 0}, metabolites];
        first[a_] := First /@ GatherBy[Ordering@a, a[[#]] &] // Sort;

In[ ]:= subsetpositionsforsequences =
          Import["../cases/subsetpositionsforsequences_10percentincreased.mx"];
        boundaries = Import["../cases/boundaries_for_deleted_reaction_series_-5and5_105.mx"];

In[ ]:= syntheticseqgenerator[stoichiometricmatrix_,
          steadystatevector_, boundaries_, fluxexchanges_, subsetpositions_] :=
         Module[{coefficients, objectivefunctions, solutionvectors},
          coefficients = Table[RandomReal[{2, 4}, Length@subsetpositions], 50];
          objectivefunctions = Table[ReplacePart[ConstantArray[0., fluxexchanges],
             MapThread[#1 → #2 &, {subsetpositions, coefficients[[i]]}]], {i, 50}];
          solutionvectors = Chop[Table[LinearProgramming[-objectivefunctions[[i]],
              stoichiometricmatrix, steadystatevector, boundaries],
             {i, Length@objectivefunctions}], 10^-5];
          {objectivefunctions, solutionvectors}]

In[ ]:= AbsoluteTiming[resultset =
           Table[Quiet@Table[syntheticseqgenerator[stoichiometricmatrix, steadystatevector,
               j, fluxexchanges, i], {i, subsetpositionsforsequences}], {j, boundaries}];]

Out[ ]= {5477.64, Null}
```

```
In[•]:= Export["C:/Users/serha/NonDrive/OR_model-deleted_reactions/solution_vectors/10
           perincobjfuncterms_+2+4solutionvectors_fxdbounds_-5and5_105pcs.mx",
         Table[Flatten[resultset[[i]][[All, 2]], 1], {i, 10}]]
        Export["C:/Users/serha/NonDrive/OR_model-deleted_reactions/objective_functions/10
           perincobjfuncterms_+2+4objfunc_fxdbounds_-5and5_105pcs.mx",
         Table[Flatten[resultset[[i]][[All, 1]], 1], {i, 10}]]

Out[•]= C:/Users/serha/NonDrive/OR_model-deleted_reactions/solution_vectors/10
          perincobjfuncterms_+2+4solutionvectors_fxdbounds_-5and5_105pcs.mx

Out[•]= C:/Users/serha/NonDrive/OR_model-deleted_reactions/objective_functions/10
          perincobjfuncterms_+2+4objfunc_fxdbounds_-5and5_105pcs.mx

In[•]:= (*solutionvectorslist=
         Import["C:/Users/serha/NonDrive/OR_model-deleted_reactions/solution_vectors/10
            perincobjfuncterms_+2+4solutionvectors_fxdbounds_-5and5_105pcs.mx"];
        objfunctionslist=
         Import["C:/Users/serha/NonDrive/OR_model-deleted_reactions/objective_functions/10
            perincobjfuncterms_+2+4objfunc_fxdbounds_-5and5_105pcs.mx"];*)

In[•]:= solutionvectorslist = Table[Flatten[resultset[[i]][[All, 2]], 1], {i, 10}];
        objfunctionslist = Table[Flatten[resultset[[i]][[All, 1]], 1], {i, 10}];

In[•]:= AbsoluteTiming[featuredatalist =
           Table[MapThread[Dot, {objfunctionslist[[j]], solutionvectorslist[[j]]}], {j, 10}];]

Out[•]= {1.59827, Null}
```

```
In[ ]:= datafulllist = Table[Join[Partition[Range@10000, 1],
           Partition[Flatten@Table[ConstantArray[i, 50], {i, 200}], 1],
           Partition[featuredatalist[[j]], 1], 2], {j, 10}];
        Table[Histogram@datafulllist[[i]][[All, 3]], {i, 10}]
```

Out[ ]=



```
In[ ]:= thread = {{1, 6500}, {2, 5200}, {3, 3600}, {4, 3200},
          {5, 2800}, {6, 2300}, {7, 1900}, {8, 1800}, {9, 1200}, {10, 900}};
```

```
In[ ]:= AbsoluteTiming[widthdataFixedstep2 =
          Table[snetworkdatabinned[3, i[[2]], datafulllist[[i[[1]]]]], {i, thread}];]

Out[ ]= {8.40213, Null}
```

```
In[ ]:= graphsandnodenumbers12 = Table[snetworkgraph[widthdataFixedstep2[[i]][[1]],
           widthdataFixedstep2[[i]][[2]], 2, 7, 400, Green], {i, 10}];
        graphsandnodenumbers12[[All, 2]]

Out[ ]= {42, 43, 47, 49, 42, 47, 43, 41, 45, 44}
```

```
In[ ]:= modularityvalues12 = Table[N@GraphAssortativity[graphsandnodenumbers12[[i]][[1]],
            FindGraphCommunities[graphsandnodenumbers12[[i]][[1]]], "Normalized" → False],
          {i, Length@graphsandnodenumbers12}];
```

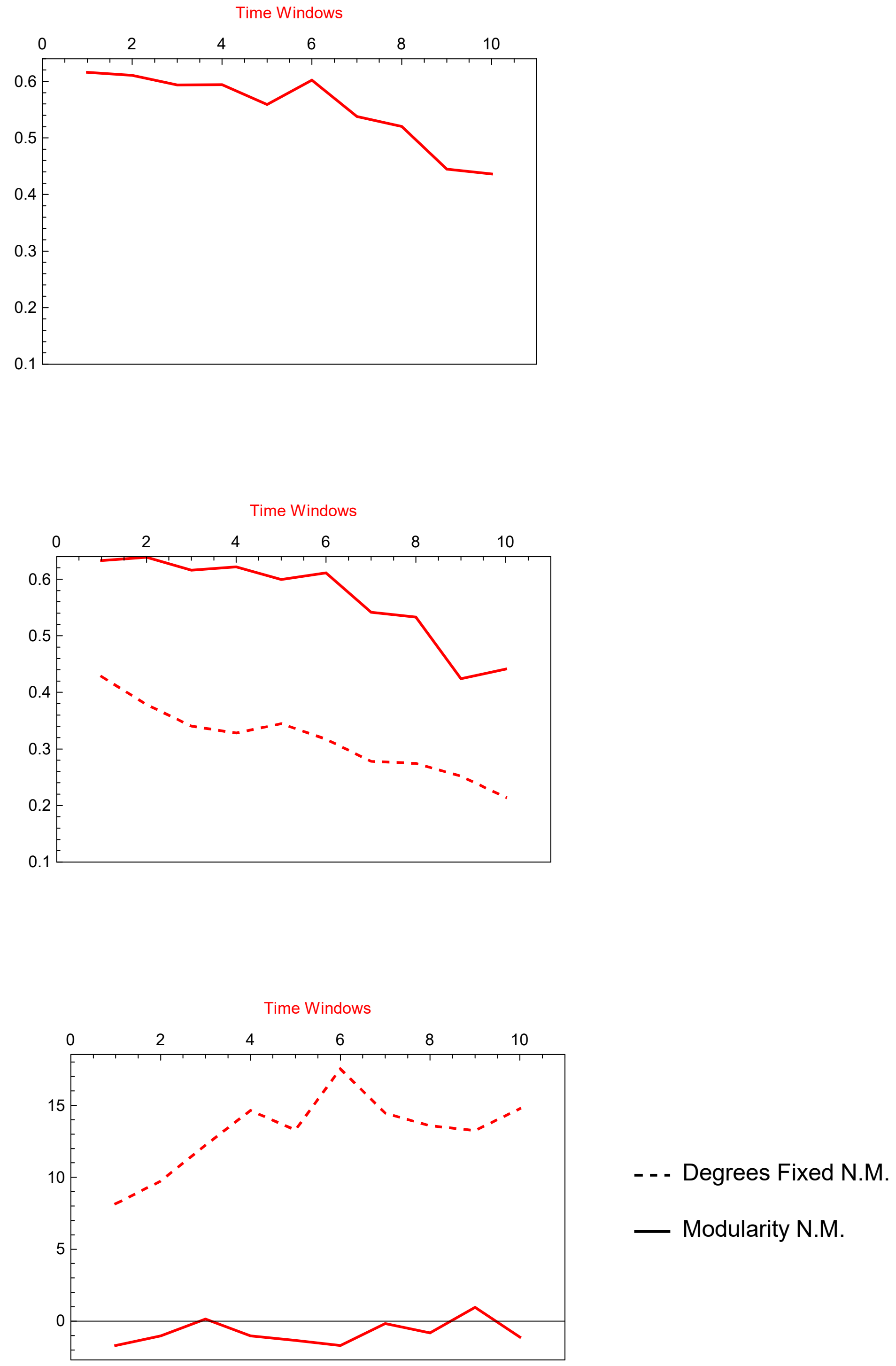
```
In[ ]:= singlerandomgraphsdegfxd12 =
          Table[randomizinggraphdegfxd[i], {i, graphsandnodenumbers12[[All, 1]]}];
        singlerandomerdrenmodularityvalues12 =
          Table[N@GraphAssortativity[singlerandomgraphsdegfxd12[[i]],
             FindGraphCommunities[singlerandomgraphsdegfxd12[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphsdegfxd12}];
        singlerandomgraphscomm12 = Table[randomizinggraphmod[i],
           {i, graphsandnodenumbers12[[All, 1]]}];
        singlerandomcommmodularityvalues12 =
          Table[N@GraphAssortativity[singlerandomgraphscomm12[[i]],
             FindGraphCommunities[singlerandomgraphscomm12[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphscomm12}];
```

```
In[ ]:= AbsoluteTiming[Zscoresmodularity12 =
           Table[zscorefunctionfortwonullmodels[i], {i, graphsandnodenumbers12[[All, 1]]}];]

Out[ ]= {137.055, Null}
```

```
In[ ]:= bucketnode12 = graphsandnodenumbers12[[All, 2]]

Out[ ]= {42, 43, 47, 49, 42, 47, 43, 41, 45, 44}
```

```
In[•]:= modularityvaluestimewinsmall = modularityvalues12;
        randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues12;
        randommodtimewinsmallcomm = singlerandomcommmodularityvalues12;
        Zscoretimewinsmall = Zscoresmodularity12;
        modularityplotrange = {0.1, 0.64};
        (*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
          singlerandomerdrenmodularityvalues1,modularityvalues12}]*)
        padding = 38;
        win2 = 10;
        Row[{ListLinePlot[Thread[{Range@win2, modularityvaluestimewinsmall}],
           Frame → True, ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
           FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}}, PlotStyle → Red,
           ImageSize → 350, PlotRange → {{0, win2 + 1}, modularityplotrange}],
          Row[{ListLinePlot[{Thread[{Range@win2, randommodtimewinsmalldegreefxd}],
               Thread[{Range@win2, randommodtimewinsmallcomm}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, modularityplotrange}],
             ListLinePlot[{Thread[{Range@win2, Zscoretimewinsmall[[All, 1]]}],
               Thread[{Range@win2, Zscoretimewinsmall[[All, 2]]}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, MinMax[Flatten[Zscoretimewinsmall], 1]}]}],
          LineLegend[{Dashed, Black}, {"Degrees Fixed N.M.", "Modularity N.M."},
           LegendMargins → 0, LegendMarkerSize → {20, 20}], Spacer@0.1}]
```

Out[]=



```
In[]:= AbsoluteTiming[widthdataFixedbucket2 =
          Table[snetworkdatafxdbucket[3, bucketnode12[[i]], datafulllist[[i]]], {i, 10}];]
Out[]= {3.24594, Null}
```

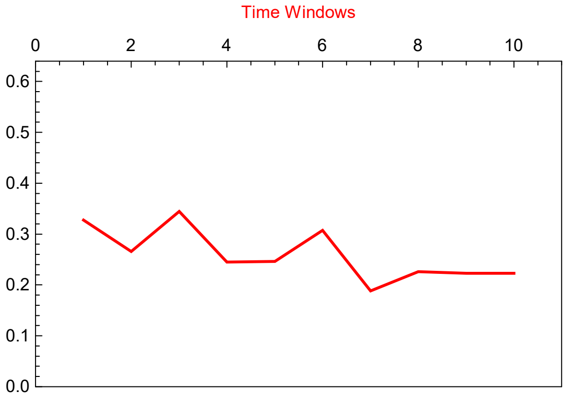
```
In[ ]:= graphsandnodenumbers32 = Table[snetworkgraph[widthdataFixedbucket2[[i]][[1]],
            widthdataFixedbucket2[[i]][[2]], 1.5, 7, 400, Green], {i, 10}];
        modularityvalues32 = Table[N@GraphAssortativity[graphsandnodenumbers32[[i]][[1]],
             FindGraphCommunities[graphsandnodenumbers32[[i]][[1]]], "Normalized" → False],
           {i, Length@graphsandnodenumbers32}];
```

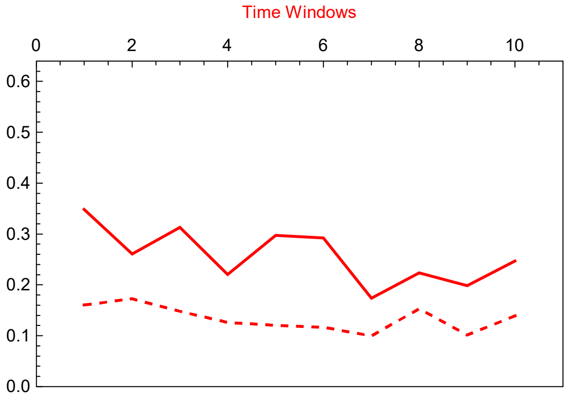
```
In[ ]:= singlerandomgraphsdegfxd32 =
          Table[randomizinggraphdegfxd[i], {i, graphsandnodenumbers32[[All, 1]]}];
        singlerandomerdrenmodularityvalues32 =
          Table[N@GraphAssortativity[singlerandomgraphsdegfxd32[[i]],
             FindGraphCommunities[singlerandomgraphsdegfxd32[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphsdegfxd32}];
        singlerandomgraphscomm32 = Table[randomizinggraphmod[i],
           {i, graphsandnodenumbers32[[All, 1]]}];
        singlerandomcommmodularityvalues32 =
          Table[N@GraphAssortativity[singlerandomgraphscomm32[[i]],
             FindGraphCommunities[singlerandomgraphscomm32[[i]]], "Normalized" -> False],
           {i, Length@singlerandomgraphscomm32}];
```

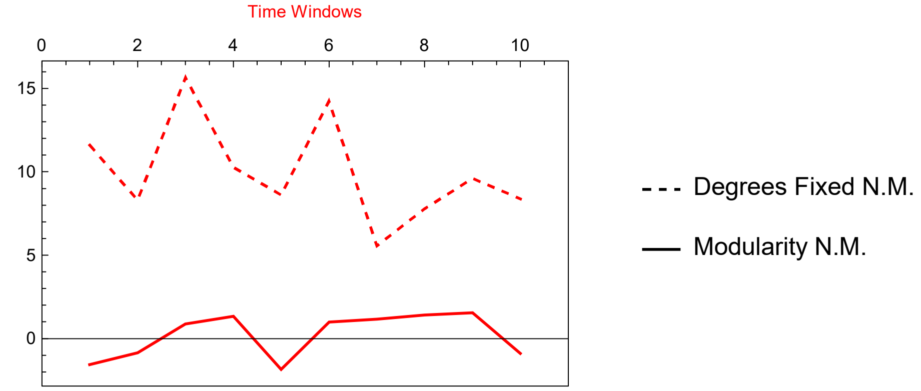
```
In[ ]:= AbsoluteTiming[Zscoresmodularity32 =
           Table[zscorefunctionfortwonullmodels[i], {i, graphsandnodenumbers32[[All, 1]]}];]

Out[ ]= {85.316, Null}
```

```
In[ ]:= modularityvaluestimewinsmall = modularityvalues32;
        randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues32;
        randommodtimewinsmallcomm = singlerandomcommmodularityvalues32;
        Zscoretimewinsmall = Zscoresmodularity32;
        modularityplotrange = {0, 0.64};
        (*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
          singlerandomerdrenmodularityvalues1,modularityvalues12}]*)
        padding = 38;
        win2 = 10;
        Row[{ListLinePlot[Thread[{Range@win2, modularityvaluestimewinsmall}],
            Frame → True, ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
            FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}}, PlotStyle → Red,
            ImageSize → 350, PlotRange → {{0, win2 + 1}, modularityplotrange}],
          Row[{ListLinePlot[{Thread[{Range@win2, randommodtimewinsmalldegreefxd}],
                Thread[{Range@win2, randommodtimewinsmallcomm}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, modularityplotrange}],
            ListLinePlot[{Thread[{Range@win2, Zscoretimewinsmall[[All, 1]]}],
                Thread[{Range@win2, Zscoretimewinsmall[[All, 2]]}]}, Frame → True,
              ImagePadding → padding, FrameTicks → {{All, None}, {None, All}},
              FrameLabel → {{None, None}, {None, Style["Time Windows", Red]}},
              PlotStyle → {{Dashed, Red}, Red}, ImageSize → 350,
              PlotRange → {{0, win2 + 1}, MinMax[Flatten[Zscoretimewinsmall], 1]}]}],
          LineLegend[{Dashed, Black}, {"Degrees Fixed N.M.", "Modularity N.M."},
            LegendMargins → 0, LegendMarkerSize → {20, 20}], Spacer@0.1}]
```

Out[∘]=


Time Windows
0
2
4
6
8
10
0.6
0.5
0.4
0.3
0.2
0.1
0.0


Time Windows
0
2
4
6
8
10
0.6
0.5
0.4
0.3
0.2
0.1
0.0


Time Windows
0
2
4
6
8
10
15
10
5
0
Degrees Fixed N.M.
Modularity N.M.

```
In[∘]:= Export["plot_values/10per_inc_obj-funcs/(2,4)-modularityvalues-fss.mx",
          modularityvalues12]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-singrand-erd-modularityvalues-fss.mx",
          singlerandomerdrenmodularityvalues12]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-singrand-comm-modularityvalues-fss.mx",
          singlerandomcommmodularityvalues12]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-zscores-fss.mx", Zscoresmodularity12]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-modularityvalues-fbs.mx",
          modularityvalues32]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-singrand-erd-modularityvalues-fbs.mx",
          singlerandomerdrenmodularityvalues32]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-singrand-comm-modularityvalues-fbs.mx",
          singlerandomcommmodularityvalues32]
        Export["plot_values/10per_inc_obj-funcs/(2,4)-zscores-fbs.mx", Zscoresmodularity32]

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-modularityvalues-fss.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-singrand-erd-modularityvalues-fss.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-singrand-comm-modularityvalues-fss.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-zscores-fss.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-modularityvalues-fbs.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-singrand-erd-modularityvalues-fbs.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-singrand-comm-modularityvalues-fbs.mx

Out[∘]= plot_values/10per_inc_obj-funcs/(2,4)-zscores-fbs.mx
```