In[ ]:=
```
SetDirectory[
  "C:/Users/serha/OneDrive/Masaüstü/MyRepo/master_thesis_MMT003/210714_finalising/
    fxd_bounds"];
```

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[ ]:=
```
case = "bounds";
intvalues = {2, 4};
interval2 = "-5+5_quadrupled";

interval = "75percentdecreased_(" <>
   ToString@intvalues[[1]] <> "," <> ToString@intvalues[[2]] <> ")";
subsetpositionsforsequences = Import[
   "../cases/subsetpositionsforsequences_75percentdecreased.mx"];
boundaries = Import[
   "../cases/boundaries_for_deleted_reaction_series_-5and5_quadrupled.mx"];
boundariespos0 = Table[Position[boundaries[[i]], {0, 0}], {i, 10}];
boundariesposval = Table[Position[boundaries[[i]], {-5, 5}], {i, 10}];
boundariesa = Table[ReplacePart[
    (Table[ReplacePart[ConstantArray[{-500, 500}, fluxexchanges], MapThread[#1 → #2 &,
         {boundariespos0[[i]], ConstantArray[{0, 0}, Length@boundariespos0[[i]]]}]],
      {i, 10}])[[j]], MapThread[#1 → #2 &, {boundariesposval[[j]],
     ConstantArray[{-5, 5}, Length@boundariesposval[[j]]]}]], {j, 10}];
```

In[ ]:=
```
syntheticseqgenerator[stoichiometricmatrix_,
  steadystatevector_, boundaries_, fluxexchanges_, subsetpositions_] :=
 Module[{coefficients, objectivefunctions, solutionvectors},
  coefficients = Table[RandomReal[intvalues, 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,boundariesa}];]*)
```

In[ ]:=
```
(*Export["C:/Users/serha/NonDrive/OR_model-25.06.2021/solution_vectors/"<>
   interval<>"solutionvectors_fxd"<>case<>"_-5and5_quadrupled.mx",
  Table[Flatten[resultset[[i]][[All,2]],1],{i,10}]]

 Export["C:/Users/serha/NonDrive/OR_model-25.06.2021/objective_functions/"<>
   interval<>"objfunc_fxd"<>case<>"_-5and5_quadrupled.mx",
  Table[Flatten[resultset[[i]][[All,1]],1],{i,10}]]*)
```

In[ ]:=
```
(*solutionvectorslist=Table[Flatten[resultset[[i]][[All,2]],1],{i,10}];
objfunctionslist=Table[Flatten[resultset[[i]][[All,1]],1],{i,10}];*)
```

In[ ]:=
```
solutionvectorslist =
  Import["C:/Users/serha/NonDrive/OR_model-25.06.2021/solution_vectors/" <>
    interval <> "solutionvectors_fxd" <> case <> "_-5and5_quadrupled.mx"];
objfunctionslist = Import[
   "C:/Users/serha/NonDrive/OR_model-25.06.2021/objective_functions/" <>
    interval <> "objfunc_fxd" <> case <> "_-5and5_quadrupled.mx"];
```

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.0005611762650405114`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.0006052819385181111`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.0005584411820322412`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... General: Further output of LinearProgramming::lpipncv will be suppressed during this calculation.

```
In[ ]:= AbsoluteTiming[featuredatalist =
          Table[MapThread[Dot, {objfunctionslist[[j]], solutionvectorslist[[j]]}], {j, 10}];]
Out[ ]= {1.91333, 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}]
```

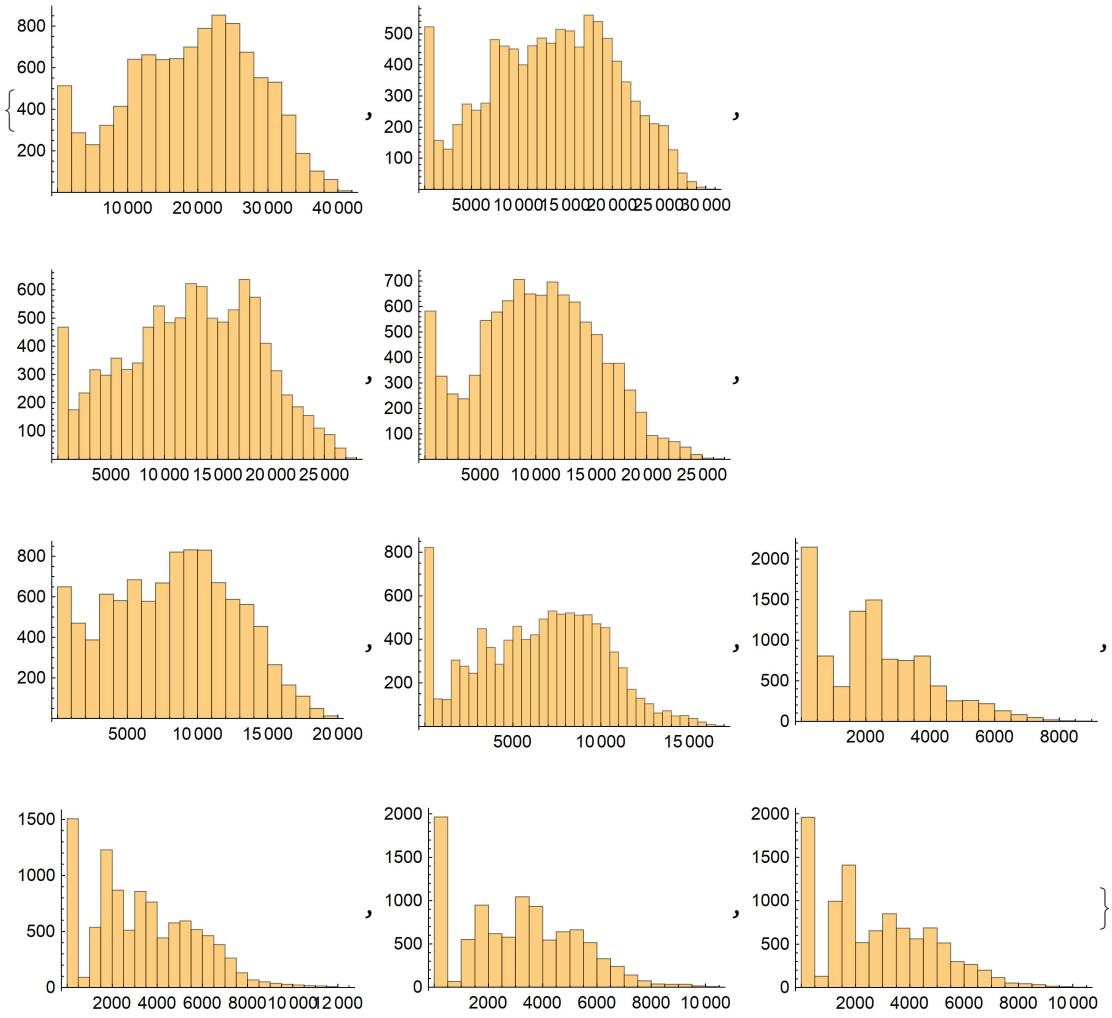
... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.0005611762650405114`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.000605281938518111`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.0005584411820322412`. The failure to converge might be because the problem is mildly infeasible. Setting the option Method -> RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

... General: Further output of LinearProgramming::lpipncv will be suppressed during this calculation.

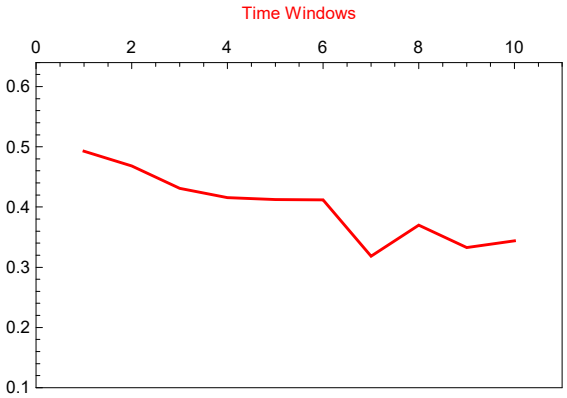
Out[ ]=

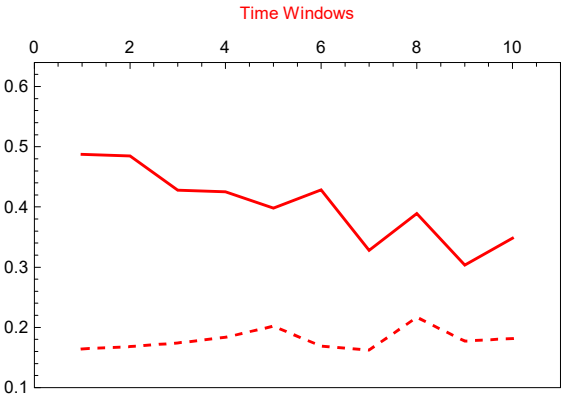


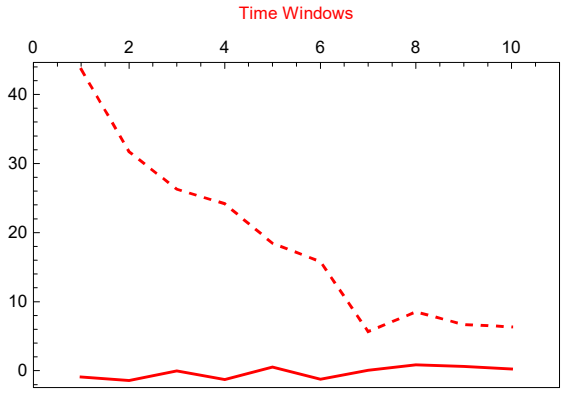
```
In[•]:= thread = {{1, 1000}, {2, 800}, {3, 700}, {4, 600},
           {5, 500}, {6, 400}, {7, 200}, {8, 250}, {9, 200}, {10, 220}};
         Mean@thread[[All, 2]]
Out[•]= 487

In[•]:= thread = Thread[{Range@10, 390}]
Out[•]= {{1, 390}, {2, 390}, {3, 390}, {4, 390},
          {5, 390}, {6, 390}, {7, 390}, {8, 390}, {9, 390}, {10, 390}}

In[•]:= AbsoluteTiming[widthdataFixedstep2 =
           Table[snetworkdatabinned[3, i[[2]], datafulllist[[i[[1]]]]], {i, thread}];]
Out[•]= {542.989, Null}

In[•]:= graphsandnodenumbers12 = Table[snetworkgraph[widthdataFixedstep2[[i]][[1]],
            widthdataFixedstep2[[i]][[2]], 2, 7, 400, Green], {i, 10}];
         graphsandnodenumbers12[[All, 2]]
Out[•]= {105, 78, 71, 68, 51, 44, 23, 32, 27, 27}

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[•]= {181.617, Null}

In[•]:= bucketnode12 = graphsandnodenumbers12[[All, 2]]
Out[•]= {105, 78, 71, 68, 51, 44, 23, 32, 27, 27}
```

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[ ]=







Degrees Fixed N.M.

Modularity N.M.

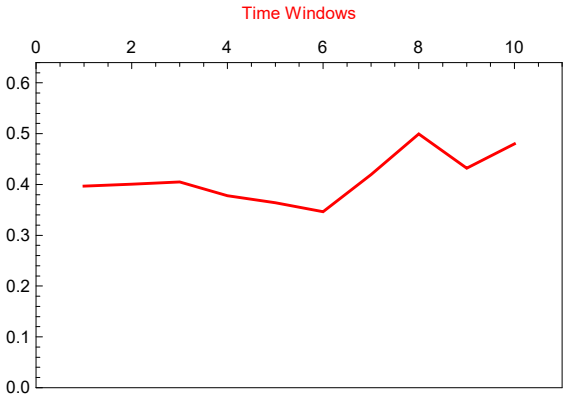
In[ ]:=
```
AbsoluteTiming[widthdataFixedbucket2 =
    Table[snetworkdatafxdbucket[3, bucketnode12[[i]], datafulllist[[i]]], {i, 10}];]
```

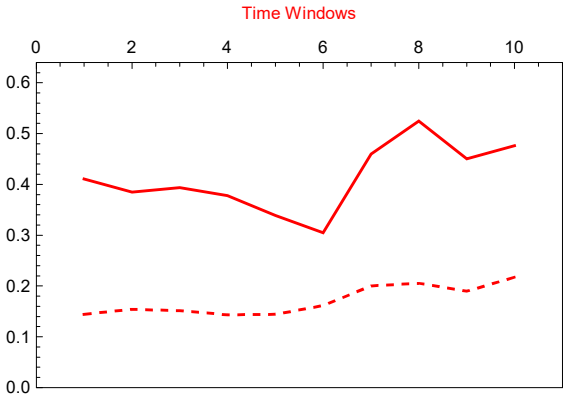
Out[ ]= {408.768, Null}

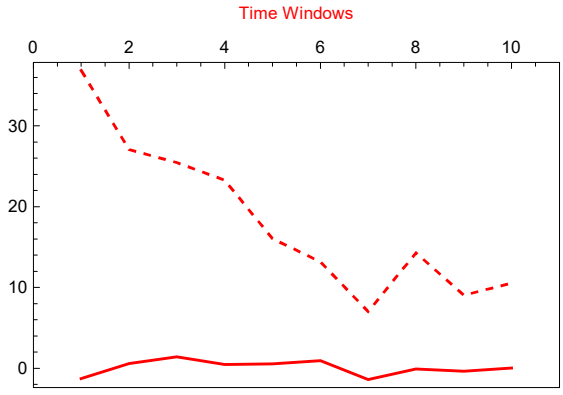
```
In[ ]:= graphsandnodenumbers32 = Table[snetworkgraph[widthdataFixedbucket2[[i]][[1]],
          widthdataFixedbucket2[[i]][[2]], 1.5, 7, 400, Green], {i, 10}];
        modularityvalues32 = Table[N@GraphAssortativity[graphsandnodenumbers32[[i]][[1]],
            FindGraphCommunities[graphsandnodenumbers32[[i]][[1]]], "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[ ]= {174.473, 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[ ]=







Degrees Fixed N.M.

Modularity N.M.

```
In[•]:= Export["plot_values/fxd_" <> case <> "/" <> interval <>
          "_" <> interval2 <> "-modularityvalues-fss.mx", modularityvalues12]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <>
          "-singrand-erd-modularityvalues-fss.mx", singlerandomerdrenmodularityvalues12]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <>
          "-singrand-comm-modularityvalues-fss.mx", singlerandomcommmodularityvalues12]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <> "-zscores-fss.mx",
         Zscoresmodularity12]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <>
          interval2 <> "-modularityvalues-fbs.mx", modularityvalues32]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <>
          "-singrand-erd-modularityvalues-fbs.mx", singlerandomerdrenmodularityvalues32]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <>
          "-singrand-comm-modularityvalues-fbs.mx", singlerandomcommmodularityvalues32]
        Export["plot_values/fxd_" <> case <> "/" <> interval <> "_" <> interval2 <> "-zscores-fbs.mx",
         Zscoresmodularity32]
Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-modularityvalues-fss.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-singrand-erd-
          modularityvalues-fss.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-singrand-comm-
          modularityvalues-fss.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-zscores-fss.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-singrand-erd-
          modularityvalues-fbs.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-singrand-comm-
          modularityvalues-fbs.mx

Out[•]= plot_values/fxd_bounds/75percentdecreased_(2,4)_-5+5_quadrupled-zscores-fbs.mx
```