

```

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

In[ ]:= Get["../../algorithm_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 = "50percentdecreased_("<>
    ToString@intvalues[[1]] <> ", " <> ToString@intvalues[[2]] <> ")";
  subsetpositionsforsequences = Import["../cases/subsetpositionsforsequences_half.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 $1.4901161193847656 \times 10^{-8}$. The best residual achieved is 0.000308883579924541 . The failure to converge might be because the problem is mildly infeasible. Setting the option Method \rightarrow RevisedSimplex should give a more definite answer, though large problems may take longer computing time.

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

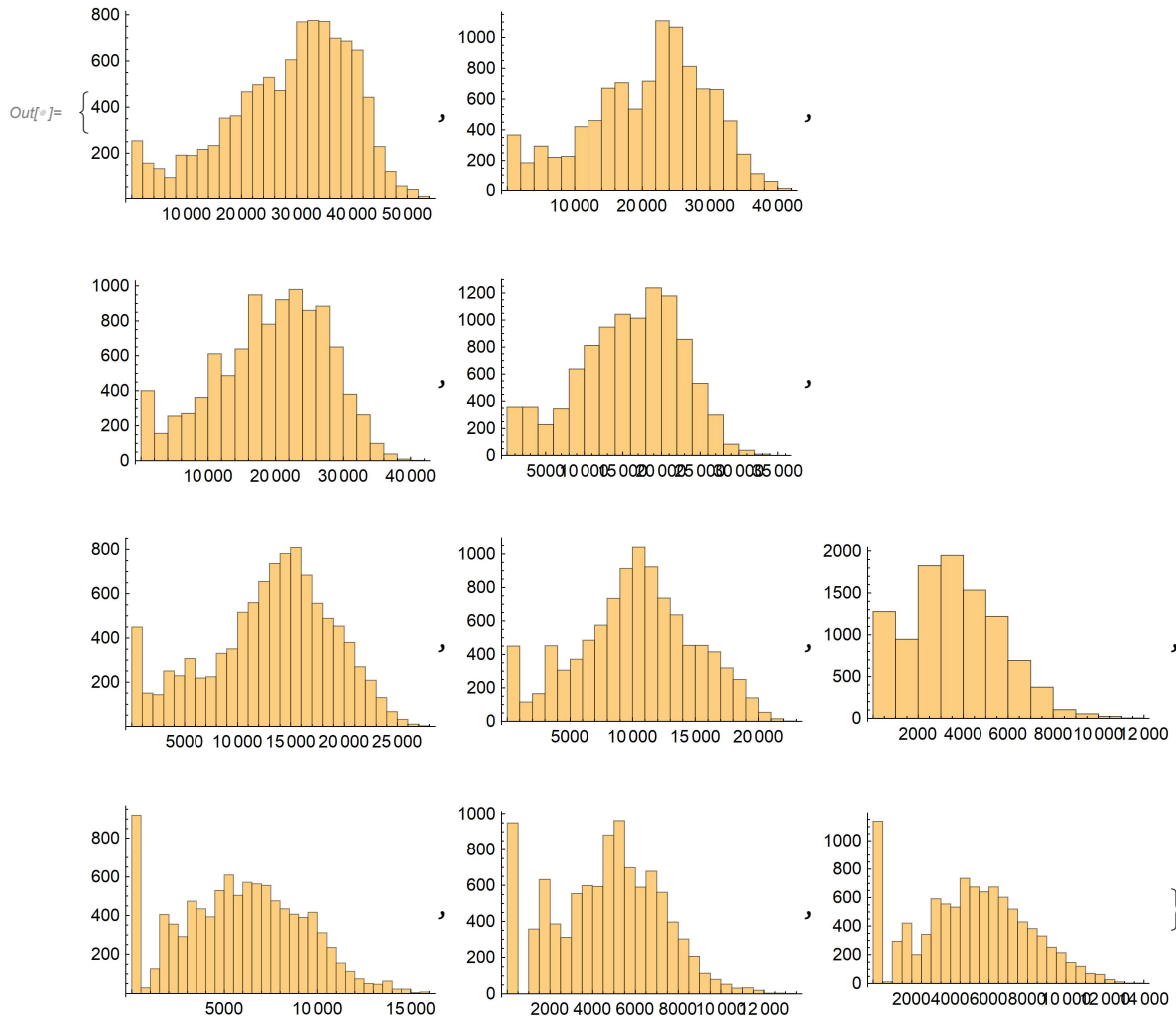
```
Out[ ]:= {1.99324, Null}
```

```

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 $1.4901161193847656 \times 10^{-8}$. The best residual achieved is 0.000308883579924541 . The failure to converge might be because the problem is mildly infeasible. Setting the option Method \rightarrow RevisedSimplex should give a more definite answer, though large problems may take longer computing time.



```

In[ ]:= thread = {{1, 1200}, {2, 900}, {3, 950}, {4, 850},
  {5, 650}, {6, 520}, {7, 260}, {8, 380}, {9, 280}, {10, 290}};
Mean@thread[[All, 2]]

```

Out[]:= 628

```

In[ ]:= thread = Thread[{Range@10, 505}]

```

```

Out[ ]:= {{1, 505}, {2, 505}, {3, 505}, {4, 505},
  {5, 505}, {6, 505}, {7, 505}, {8, 505}, {9, 505}, {10, 505}}

```

```

In[ ]:= AbsoluteTiming[widthdataFixedstep2 =
      Table[snetworkdatabin[3, i[[2]], datafulllist[[i[[1]]]], {i, thread}];]
Out[ ]:= {306.048, Null}

In[ ]:= graphsandnodenumbers12 = Table[snetworkgraph[widthdataFixedstep2[[i]][[1]],
      widthdataFixedstep2[[i]][[2]], 2, 7, 400, Green], {i, 10}];
graphsandnodenumbers12[[All, 2]]
Out[ ]:= {105, 83, 80, 69, 54, 43, 24, 32, 26, 28}

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[ ]:= {154.116, Null}

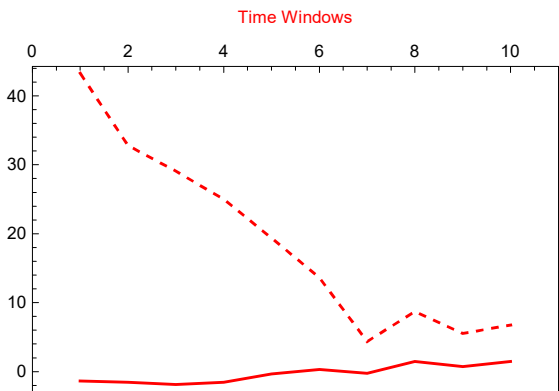
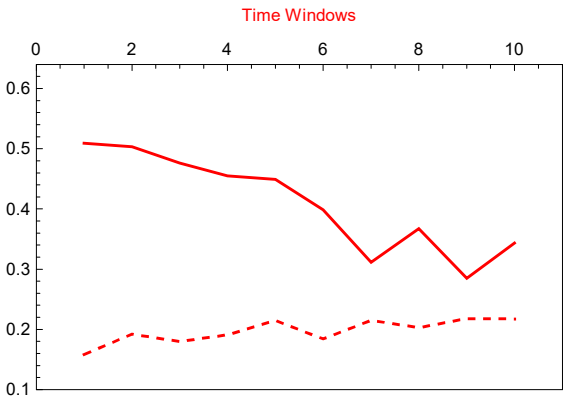
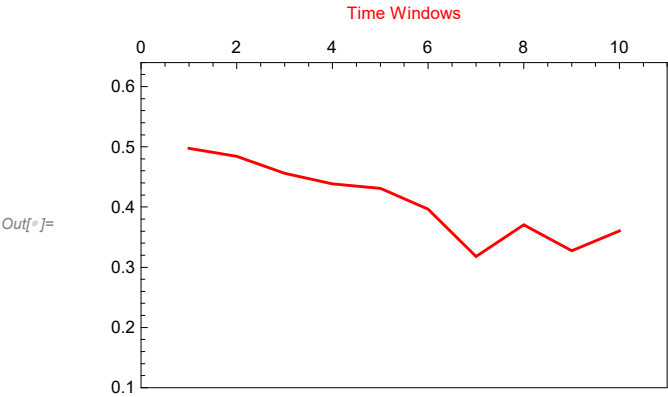
In[ ]:= bucketnode12 = graphsandnodenumbers12[[All, 2]]
Out[ ]:= {105, 83, 80, 69, 54, 43, 24, 32, 26, 28}

```

```

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]]

```



--- Degrees Fixed N.M.
— Modularity N.M.

```
In[*]:= AbsoluteTiming[widthdataFixedbucket2 =  
  Table[snetworkdatafxdbucket[3, bucketnode12[[i]], datafulllist[[i]]], {i, 10}];]  
Out[*]= {98.088, 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]]}];
singerandomerdrenmodularityvalues32 =
      Table[N@GraphAssortativity[singlerandomgraphsdegfxd32[[i]],
      FindGraphCommunities[singlerandomgraphsdegfxd32[[i]], "Normalized" -> False],
      {i, Length@singlerandomgraphsdegfxd32}];
singerandomgraphscomm32 = Table[randomizinggraphmod[i],
      {i, graphsandnodenumbers32[[All, 1]]}];
singerandomcommmodularityvalues32 =
      Table[N@GraphAssortativity[singlerandomgraphscomm32[[i]],
      FindGraphCommunities[singlerandomgraphscomm32[[i]], "Normalized" -> False],
      {i, Length@singlerandomgraphscomm32}];

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

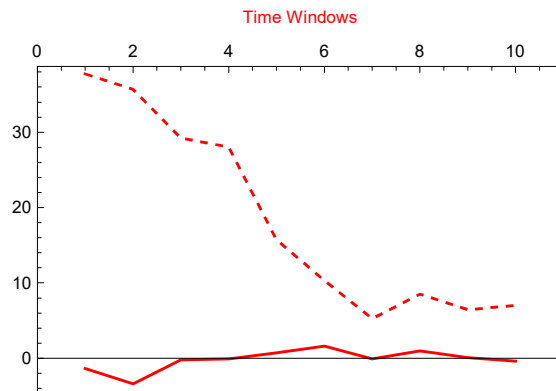
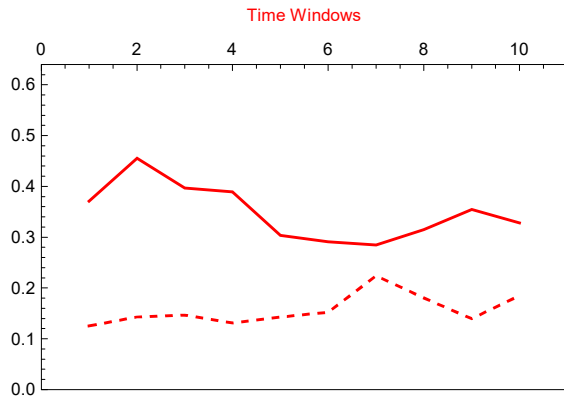
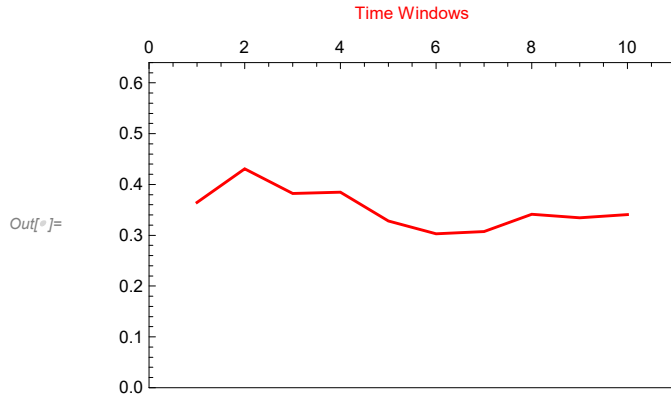
Out[ ]:= {139.229, Null}

```

```

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]]

```

--- 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/50percentdecreased_(2,4)_-5+5_quadrupled-modularityvalues-fss.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-singrand-erd-
  modularityvalues-fss.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-singrand-comm-
  modularityvalues-fss.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-zscores-fss.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-modularityvalues-fbs.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-singrand-erd-
  modularityvalues-fbs.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-singrand-comm-
  modularityvalues-fbs.mx

Out[ ]:= plot_values/fxd_bounds/50percentdecreased_(2,4)_-5+5_quadrupled-zscores-fbs.mx

```