In[ ]:=
```
SetDirectory[
  "C:/Users/serha/OneDrive/Masaüstü/MyRepo/master_thesis_MMT003/210628_finalising/
    fxd_coefficients"];
```

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 = "coeffs";
interval = "(-1,1)";
val = "5";
val2 = "quadrupled";

objfunctions =
  Import["C:/Users/serha/NonDrive/OR_model-25.06.2021/objective_functions/" <>
    interval <> "objfunc_fxd" <> case <> ".mx"];
boundaries = Import["../cases/boundaries_for_deleted_reaction_series_-5and5_" <>
    val2 <> ".mx"];
subsetpositionsforsequences = Import["../cases/subsetpositionsforsequences.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[{-ToExpression@val,
        ToExpression@val}, Length@boundariesposval[[j]]]}]], {j, 10}];
```

In[ ]:=
```
AbsoluteTiming[
 resultset = Table[Table[Chop[Table[Quiet@LinearProgramming[-objfunctions[[j, i]],
          stoichiometricmatrix, steadystatevector, k], {i, 50}],
       10^-5], {j, Length@objfunctions}], {k, boundariesa}];]
```

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.00018993671588177886`. 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 0.00047679552134372976`. 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.

Out[ ]=
```
{5314.6, Null}
```

In[ ]:=
```
Export["C:/Users/serha/NonDrive/OR_model-25.06.2021/solution_vectors/" <> interval <>
  "solutionvectors_fxd" <> case <> "_-" <> val <> "and" <> val <> "_" <> val2 <> "pcs.mx",
 Table[Flatten[resultset[[i]], 1], {i, 10}]]
```

Out[ ]=
```
C:/Users/serha/NonDrive/OR_model-25.06.2021/solution_vectors/(-1,1)
  solutionvectors_fxdcoeffs_-5and5_quadrupledpcs.mx
```

In[ ]:=
```
solutionvectorslist =
  Import["C:/Users/serha/NonDrive/OR_model-25.06.2021/solution_vectors/" <> interval <>
    "solutionvectors_fxd" <> case <> "_-" <> val <> "and" <> val <> "_" <> val2 <> "pcs.mx"];
(*solutionvectorslist=Table[Flatten[resultset[[i]],1],{i,10}];*)
```

... LinearProgramming: The interior point algorithm cannot converge to the tolerance of 1.4901161193847656`*^-8. The best residual achieved is 0.00018993671588177886`. 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 0.00047679552134372976`. 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.

In[ ]:=
```
objfunctionslist = Table[Flatten[objfunctions, 1], {i, 10}];
```

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

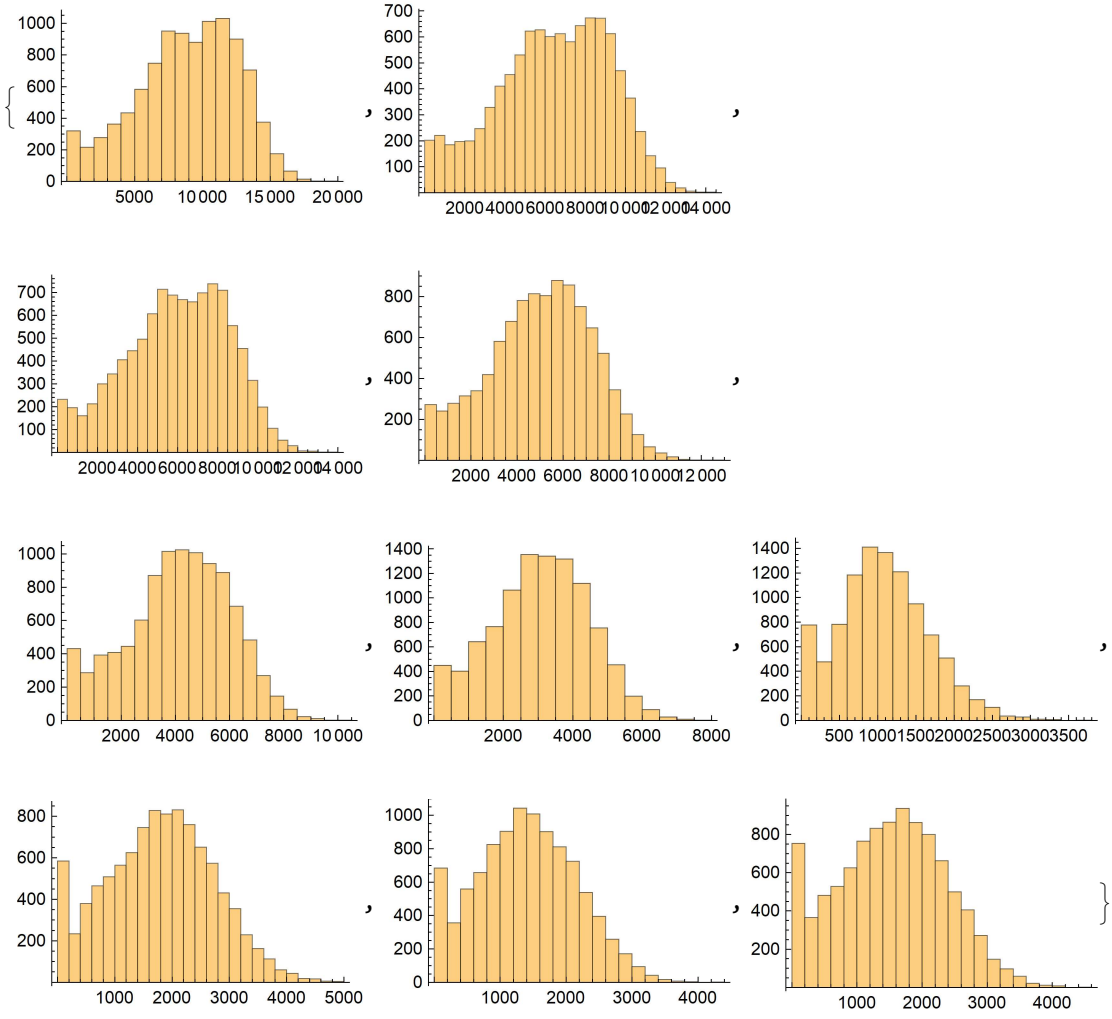
Out[ ]=
```
{2.37461, Null}
```

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 0.00018993671588177886`. 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 0.00047679552134372976`. 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.

Out[ ]=



In[ ]:=
```
thread = {{1, 450}, {2, 330}, {3, 320}, {4, 310},
   {5, 240}, {6, 170}, {7, 70}, {8, 110}, {9, 100}, {10, 100}};
Mean@thread[[All, 2]]
```

Out[ ]=
```
220
```

```
In[ ]:= thread = Thread[{Range@10, 780}]
```

```
Out[ ]= {{1, 780}, {2, 780}, {3, 780}, {4, 780},
  {5, 780}, {6, 780}, {7, 780}, {8, 780}, {9, 780}, {10, 780}}
```

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

```
Out[ ]= {344.899, Null}
```

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

```
Out[ ]= {25, 19, 18, 17, 14, 10, 5, 7, 6, 6}
```

```
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]]}];]
```

```
••• Power: Infinite expression 1/0. encountered.
```

```
Out[ ]= {104.516, Null}
```

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

```
Out[ ]= {25, 19, 18, 17, 14, 10, 5, 7, 6, 6}
```

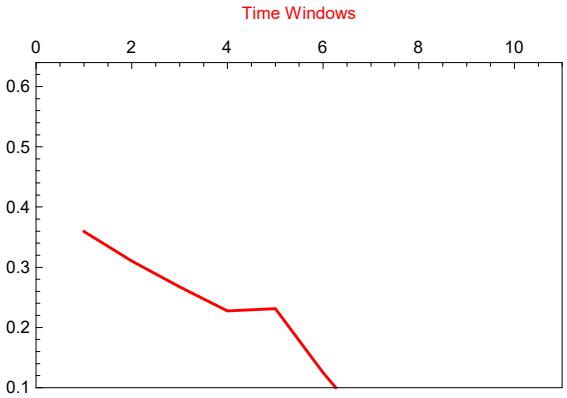
In[ ]:=
```
modularityvaluestimewinsmall = modularityvalues12;
randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues12;
randommodtimewinsmallcomm = singlerandomcommmodularityvalues12;
Zscoretimewinsmall = Zscoresmodularity12;
modularityplotrange = {0.1, 0.64};
(*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
  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}]
```

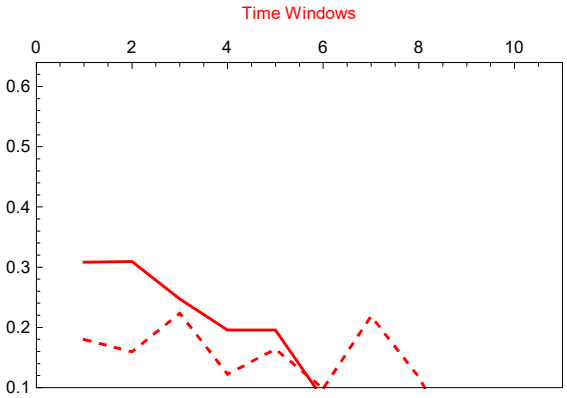
... Min: Invalid comparison with ComplexInfinity attempted.

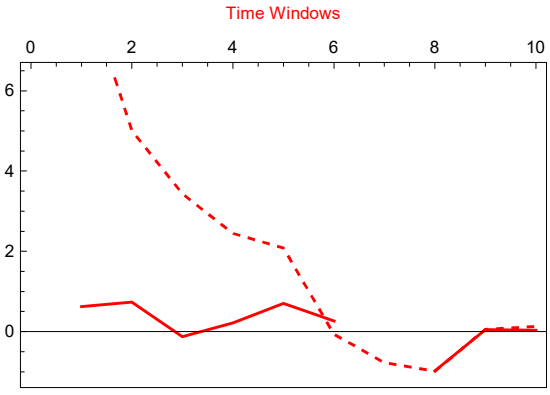
... Max: Invalid comparison with ComplexInfinity attempted.

... ListLinePlot: Value of option PlotRange –> {{0, 11}, {–1 + Min[–0.988425, ComplexInfinity], 1 + Max[8.88798, ComplexInfinity]}} is not All, Full, Automatic, a positive machine number, or an appropriate list of range specifications.

Out[•]=







Degrees Fixed N.M.

Modularity N.M.

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

Out[•]= {414.724, Null}

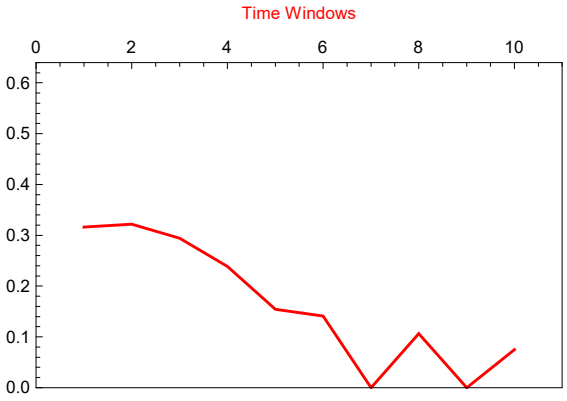
```
In[ ]:= graphsandnodenumbers32 = Table[snetworkgraph[widthdataFixedbucket2[[i]][[1]],
          widthdataFixedbucket2[[i]][[2]], 1.5, 7, 400, Green], {i, 10}];
        modularityvalues32 = Table[N@GraphAssortativity[graphsandnodenumbers32[[i]][[1]],
            FindGraphCommunities[graphsandnodenumbers32[[i]][[1]]],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

  ... Power: Infinite expression 1/0. encountered.

  ... Infinity: Indeterminate expression 0. ComplexInfinity encountered.

  ... Power: Infinite expression 1/0. encountered.

  ... Infinity: Indeterminate expression 0. ComplexInfinity encountered.
```

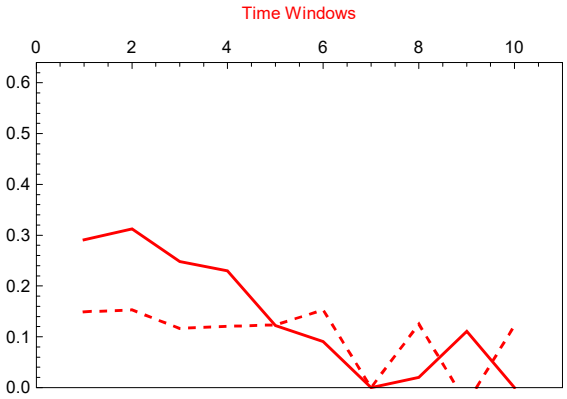
Out[ ]= {42.2979, Null}

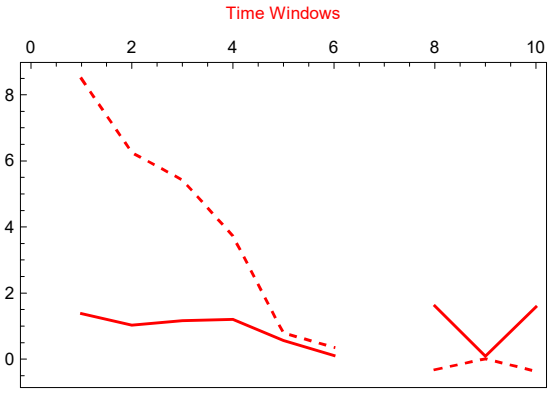
In[ ]:=
```
modularityvaluestimewinsmall = modularityvalues32;
randommodtimewinsmalldegreefxd = singlerandomerdrenmodularityvalues32;
randommodtimewinsmallcomm = singlerandomcommmodularityvalues32;
Zscoretimewinsmall = Zscoresmodularity32;
modularityplotrange = {0, 0.64};
(*MinMax[{modularityvalues1,singlerandomcommmodularityvalues1,
  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}]
```

ListLinePlot: Value of option PlotRange –> {{0, 11}, {Indeterminate, Indeterminate}} is not All, Full, Automatic, a positive machine number, or an appropriate list of range specifications.

Out[•]=







Degrees Fixed N.M.

Modularity N.M.

```
In[•]:= Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-modularityvalues-fss.mx", modularityvalues12]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-singrand-erd-modularityvalues-fss.mx",
         singlerandomerdrenmodularityvalues12]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-singrand-comm-modularityvalues-fss.mx",
         singlerandomcommmodularityvalues12]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-zscores-fss.mx", Zscoresmodularity12]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <> val2 <>
          "_" <> interval <> "-modularityvalues-fbs.mx", modularityvalues32]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-singrand-erd-modularityvalues-fbs.mx",
         singlerandomerdrenmodularityvalues32]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-singrand-comm-modularityvalues-fbs.mx",
         singlerandomcommmodularityvalues32]
        Export["plot_values/fxd_" <> case <> "/-" <> val <> "+" <> val <> "_" <>
          val2 <> "_" <> interval <> "-zscores-fbs.mx", Zscoresmodularity32]
Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-singrand-erd-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-singrand-comm-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-zscores-fss.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-singrand-erd-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-singrand-comm-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-5+5_quadrupled_(-1,1)-zscores-fbs.mx
```