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 = "250";
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}];
```

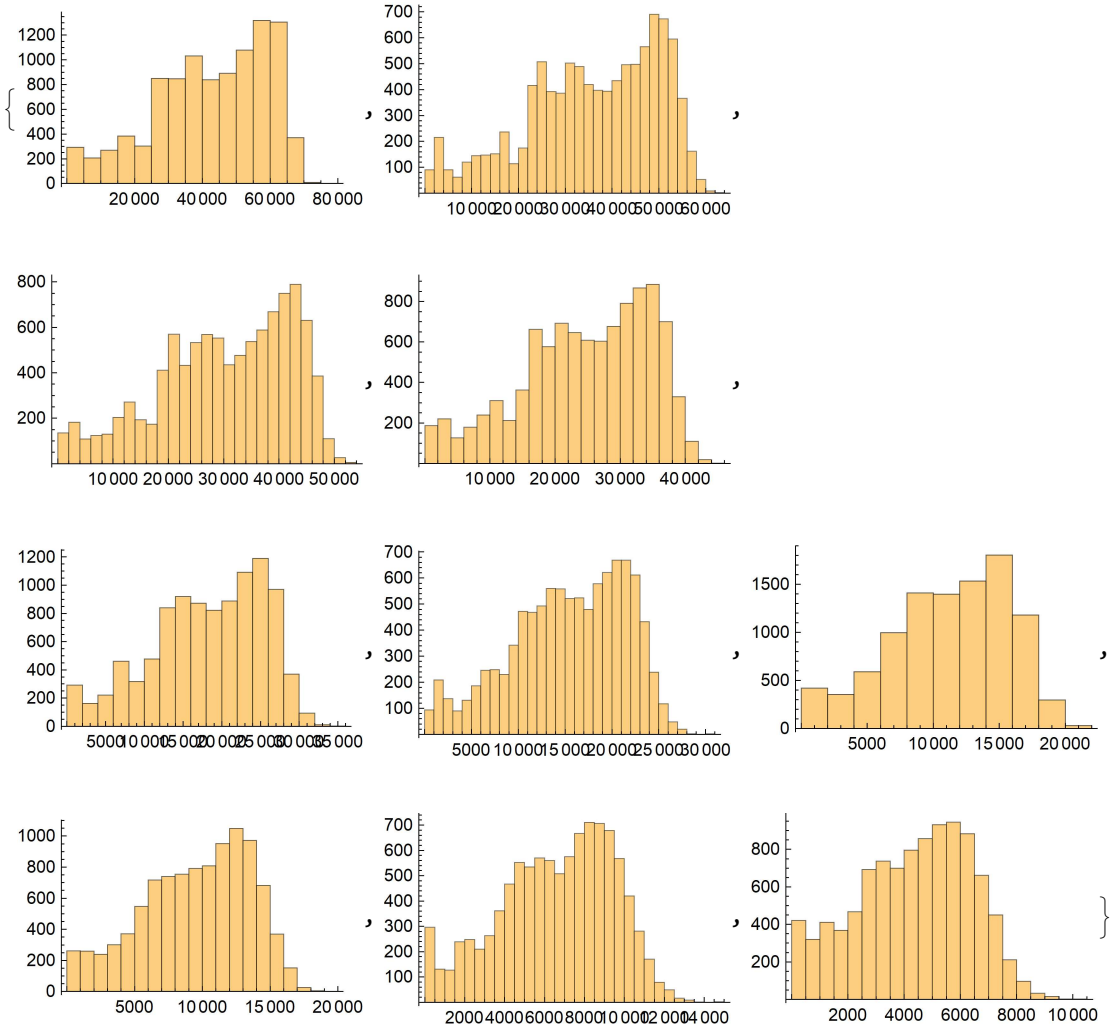
In[ ]:=
```
AbsoluteTiming[
 resultset = Table[Table[Chop[Table[Quiet@LinearProgramming[-objfunctions[[j, i]],
       stoichiometricmatrix, steadystatevector, k], {i, 50}],
    10^-5], {j, Length@objfunctions}], {k, boundariesa}];]
```

Out[ ]=
```
{5162.36, 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_-250and250_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}];*)

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

In[ ]:= AbsoluteTiming[featuredatalist =
           Table[MapThread[Dot, {objfunctionslist[[j]], solutionvectorslist[[j]]}], {j, 10}];]
Out[ ]= {2.71655, 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, 1700}, {2, 1400}, {3, 1200}, {4, 950},
    {5, 740}, {6, 650}, {7, 500}, {8, 440}, {9, 330}, {10, 220}};
Mean@thread[[All, 2]]
```

Out[ ]=
```
813
```

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}}
```

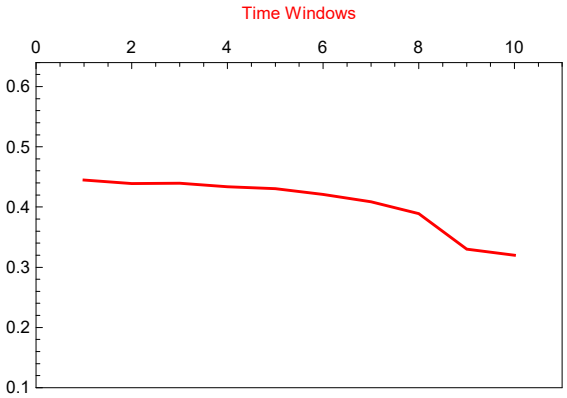
In[ ]:=
```
AbsoluteTiming[widthdataFixedstep2 =
    Table[snetworkdatabinned[3, i[[2]], datafulllist[[i[[1]]]]], {i, thread}];]
```

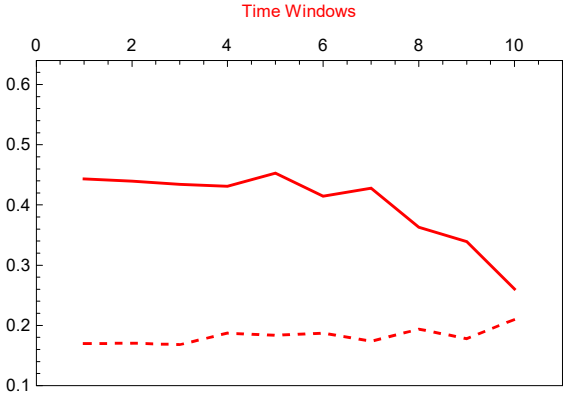
Out[ ]=
```
{8.13222, Null}
```

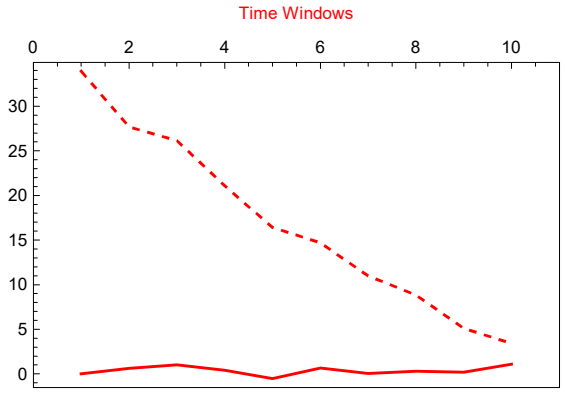
```
In[ ]:= graphsandnodenumbers12 = Table[snetworkgraph[widthdataFixedstep2[[i]][[1]],
          widthdataFixedstep2[[i]][[2]], 2, 7, 400, Green], {i, 10}];
        graphsandnodenumbers12[[All, 2]]
Out[ ]= {96, 81, 69, 58, 44, 39, 29, 25, 19, 13}

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[ ]= {117.524, Null}

In[ ]:= bucketnode12 = graphsandnodenumbers12[[All, 2]]
Out[ ]= {96, 81, 69, 58, 44, 39, 29, 25, 19, 13}
```

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.

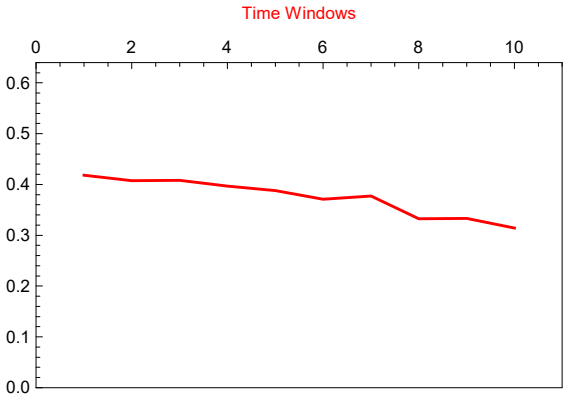
In[ ]:=
```
AbsoluteTiming[widthdataFixedbucket2 =
    Table[snetworkdatafxdbucket[3, bucketnode12[[i]], datafulllist[[i]]], {i, 10}];]
```

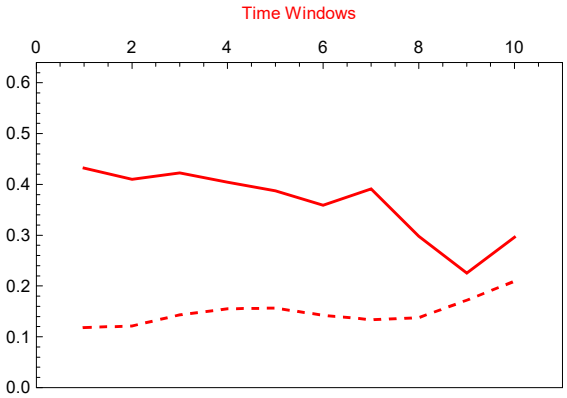
Out[ ]= {3.04263, Null}

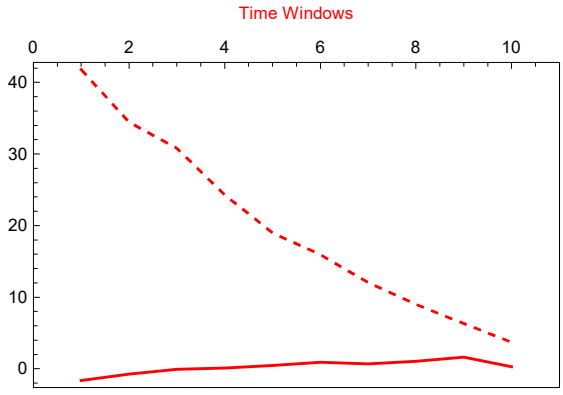
```
In[ ]:= graphsandnodenumbers32 = Table[snetworkgraph[widthdataFixedbucket2[[i]][[1]],
          widthdataFixedbucket2[[i]][[2]], 1.5, 7, 400, Green], {i, 10}];
        modularityvalues32 = Table[N@GraphAssortativity[graphsandnodenumbers32[[i]][[1]],
            FindGraphCommunities[graphsandnodenumbers32[[i]][[1]]], "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[ ]= {144.63, 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 <> "/-" <> 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/-250+250_quadrupled_(-1,1)-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-singrand-erd-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-singrand-comm-modularityvalues-fss.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-zscores-fss.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-singrand-erd-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-singrand-comm-modularityvalues-fbs.mx

Out[•]= plot_values/fxd_coeffs/-250+250_quadrupled_(-1,1)-zscores-fbs.mx
```