Enumerate reaction networks composed with heteromultimer and single transformations
November 2014

This particular code is to enumerate all possible reaction networks (with certain dimensions, $n \times m$ where n is speciese number m is reaction number) composed of three types of interactions:

$$A + B \rightarrow C$$
$$\mathrm{D} \rightarrow E + F$$
$$G \rightarrow H$$

Those are heterodimerization, disassociation and single transformation.

With those three types of elementary reactions, we could construct a set of reaction networks, then we could use DSR graphs and bipartie to characteristic those networks if they are multistationary and has closed competition loop.

But before to go through such checking, we need to preclude situations that clearly not a complex balanced reaction network, by which mean it obeys the following three constraints:

0. Only allow elementary reactions described above, which is the starting point to construct the matrix;
   (more complex version should be including $I \rightarrow 2J$ and $2K \rightarrow L$ in future)
   list all possibly combinations and select m of those into matrix (sequence does not matter), then seperate into pos and neg matrices

1. Mass conservation;
   (it's very difficult to check, currently implemented without this checking but manual checking afterwards)

2. Complex banlanced: each species has at least one in flow and one out flow;
   (easy to check)
   Check pos matrix and neg matrix, (there is no zeros in columSum)

Then we need to:

4. check competition: there are at least one species has two -1 and there is another -1 in each of the according reactions;
   (in neg matrix, check if there are any two intersections of colSum and rowSum $\geqslant -2$ in a row are -1)
   find col indices, then get the other two species (competitors)

5. check loop: take indices of competitors, do the network searching, find the loop from one to another and then from the other to this one.

Cluster matrix into four categories: bistable with closed competition loop, bistable without closed competition loop, monostable with closed competition loop, monostable without closed competition loop.

Some functions might need:
sprintf(fmt, x1, ..., xn)
StringTools[Join](stringList, sep)
StringTools[CaseJoin](stringList)

mkdir(dirName)
FileTools[RemoveDirectory](dirName, options)
FileTools[Remove](file, file2, ...)
ListDirectory(dir, opt1, opt2, ...)
ArrayTools[AddAlongDimension](A,dim)

Initializations

```
> restart :
> interface(rtablesize = 400) :
> with(ListTools) :
> with(LinearAlgebra) :
> with(VectorCalculus) :
> with(GraphTheory) :
> with(combinat) :
> #with(MTM) :
> with(ArrayTools) :
> _Envsignum0 := 0 :
>
```

Functions for multistationality checking (execute before proceeding)

Step 1. Procedures to create the DSR-graph from the stoichiometric matrix

Find the matrix Z from the stoichiometric matrix A:

```
> findZ := proc(A)
    local Z, n, m, i, j :
     n := Dimension(A)[1] :
     m := Dimension(A)[2] :
     Z := Matrix(n, m) :
  for i from 1 to n by 1 do
    for j from 1 to m by 1 do
       if A[i, j] < 0 then Z[i, j] := z[i, j]; end if;      ### what is the z?
    end do;
  end do:
   return(Z) :
   end proc:

>
```

Find the DSR graph from labels, A and Z

```
> ##Create signed DSR graph: entries are two matrices and the labels of the nodes
  createDSRgraphsigned := proc(mynodes, A, Z)
    local G, n, m, Adj, varsZ, Zsign, varsA, Asign, X:
    n := Dimension(A)[1]: m := Dimension(A)[2]:
    X := Transpose(Z):
    varsZ := indets(X):
    Zsign := subs(seq(varsZ[i] = 1, i = 1..numelems(varsZ)), X):

   Adj := Matrix(n + m, n + m):
   Adj[[n + 1..n + m], [1..n]] := Transpose(map(signum, A)):
   Adj[[1..n], [n + 1..n + m]] := Transpose(Zsign):

    G := GraphTheory[Graph](mynodes, Adj, weighted = true):
    return(G):
  end proc:
```

Find the DSR graph from labels and A and return the list of edges:

```
> findedgesDSR := proc(mynodes, A)
    local G, Z:
    Z := findZ(A):
    G := createDSRgraphsigned(mylabels, A, Z):
    return(Edges(G, weights)):
  end proc:
```

```
>
```

Step 2. Procedures to test for multistationarity

Procedures

```
> ## compute Mtilde determinant
  computdet := proc(N, X)
   global Mt:
    local M, F, i, bigdet, n1, s1:
```

```
    n1 := Dimension(N)[1]: s1 := Rank(N):
    M := N.X:
    Mt := M:
    if s1 < n1 then
      F
        := ReducedRowEchelonForm(Transpose(Matrix([op(NullSpace(Transpose(
        N)))])))):
      for i from 1 by 1 to Dimension(F)[1] do
          Mt[ArrayTools[SearchArray](F[i])[1]] := F[i]:
      end do:
    end if:
    bigdet := expand(Determinant(Mt)):
    return(bigdet):
    end proc:
```

```
> ## compute Mtilde determinant
  computdet2 := proc(N, X)
    global Mt:
    local M, F, i, bigdet, n1, s1:
    n1 := Dimension(N)[1]: s1 := Rank(N):
    M := N.X:
    Mt := M:
    if s1 < n1 then
      F
        := ReducedRowEchelonForm(Transpose(Matrix([op(NullSpace(Transpose(
        N)))])))):
      for i from 1 by 1 to Dimension(F)[1] do
          Mt[ArrayTools[SearchArray](F[i])[1]] := F[i]:
      end do:
    end if:
    bigdet := expand(Determinant(Mt)):
    return(bigdet, Mt):
    end proc:
>
```

```
> ## injectivity check
  injective := proc(N, X)
    local det, signs, i, l, k:
    det := computdet(N, X):
    signs := ListTools[MakeUnique](map(sign, [coeffs(det)])):
    if det ≠ 0 then
        i := (-1)^(numelems(signs) + 1):
    else i := 0: end if:
    return(i, det):
    end proc:
> ## injectivity check
```

```
injectivePW := proc(N, X)
 local det, signs, i, n, m, X1, l, k :
n := Dimension(N)[1] : m := Dimension(N)[2] :
 X1 := DiagonalMatrix(Vector([seq(k_i, i = 1 ..m)])).X
     .DiagonalMatrix(Vector([seq(l_i, i = 1 ..n)])) :

 det := computdet(N, X1) :
 signs := ListTools[MakeUnique](map(sign, [coeffs(det)])) :
  if det ≠ 0 then
     i := (-1)^(numelems(signs) + 1) :
else i := 0 : end if:
  return(i, det) :
end proc:
```

```
> findV := proc(A)
   local V, n, m, i, j :
    n := Dimension(A)[1] :
    m := Dimension(A)[2] :
     V := Matrix(n, m) :
  for i from 1 to n by 1 do
    for j from 1 to m by 1 do
       if A[i,j] < 0 then V[i,j] := -A[i, j]; end if;
    end do;
  end do:
   return(Transpose(V)) :
   end proc:
```

```
> isinjective := proc(A)
    local V, i, det :
    V := findV(A) :
    i, det := injectivePW(A, V) :
    if i = 1 then return(1) :
    else
      return(0) :
   end if:
  end proc:
```

```
> ## compute Mtilde determinant with F given
  computdetF := proc(N, X, F)
   global Mt :
   local M, i, bigdet, n1, s1, sp :
   n1 := Dimension(N)[1] : s1 := Rank(N) : sp := Dimension(X)[2] :
   M := N.X :
```

```
    Mt := Matrix(sp, sp) :
     Mt[1..Dimension(F)[1]] := F :
     Mt[Dimension(F)[1]+1..sp] := M :

    bigdet := expand(Determinant(Mt)) :
    return(bigdet) :
   end proc:
```

```
> ## compute Mtilde determinant with F given
   computdetF2 := proc(N, X, F)
    local M, i, bigdet, n1, s1, sp, Mt :
    n1 := Dimension(N)[1] : s1 := Rank(N) : sp := Dimension(X)[2] :
    M := N.X :
    Mt := Matrix(sp, sp) :
     Mt[1..Dimension(F)[1]] := F :
     Mt[Dimension(F)[1]+1..sp] := M :

    bigdet := expand(Determinant(Mt)) :
    return(bigdet, Mt) :
   end proc:
```

```
> ## injectivity check with F given
   injectivePWF := proc(N, X, F)
    local det, signs, i, n, m, X1, l, k :
   n := Dimension(X)[2] : m := Dimension(X)[1] :
    X1 := DiagonalMatrix(Vector([seq(k_i, i=1..m)])).X
        .DiagonalMatrix(Vector([seq(l_i, i=1..n)])) :

    det := computdetF(N, X1, F) :
    signs := ListTools[MakeUnique](map(sign, [coeffs(det)])) :
     if det ≠ 0 then
        i := (-1)^(numelems(signs)+1) :
   else i := 0 : end if:
     return(i, det) :
   end proc:
```

```
> ## injectivity check with F given
   injectivePWF2 := proc(N, X, F)
    local det, signs, i, n, m, X1, l, k, Mt :
   n := Dimension(X)[2] : m := Dimension(X)[1] :
    X1 := DiagonalMatrix(Vector([seq(k_i, i=1..m)])).X
        .DiagonalMatrix(Vector([seq(l_i, i=1..n)])) :

    det, Mt := computdetF2(N, X1, F) :
    signs := ListTools[MakeUnique](map(sign, [coeffs(det)])) :
```

```
    if det ≠ 0 then
        i := (-1)^(numelems(signs)+1) :
    else i := 0 : end if:
    return(i, det, Mt) :
    end proc:


> ## check if after gauss reduction the system becomes injective: check all
    gaussinjallpos := proc(B, V, F)
        local m, myset, n, i, det, bigset, seenset, B2, V2, B1, myset2, control, control2 :
        m := Dimension(B)[2] : n := Dimension(B)[1] :
        myset := {seq(i, i = 1..n)} : control := 0 :
        bigset := {seq(i, i = 1..m)} :
        seenset := [myset] :

        while myset ≠ FAIL and control = 0 do
            B2 := B[.., [op(myset), op(bigset minus myset)]] :
            V2 := V[[op(myset), op(bigset minus myset)],..] :
            i, det, B1 := gaussinj(B2, V2, F) :
            if i = 1 then control := 1 : end if:  ## injective found
            if i = 2 then control := 2 : end if:  ## no positive steady states
            myset2 := { } :
            for i from 1 by 1 to Dimension(B1)[1] do
                myset2 := {op(myset2), ArrayTools[SearchArray](B1[i])[1]} :
            end do:
            seenset := [op(seenset), myset2] :
            seenset := [op(seenset), myset] :
            seenset := ListTools[MakeUnique](seenset) :
            while member(myset, seenset) and myset ≠ FAIL do
                myset := nextcomb(myset, m) :
            end do:
        end do:
        control2 := 0 :
        if control = 1 then
            while myset ≠ FAIL and control = 1 do
                B2 := B[.., [op(myset), op(bigset minus myset)]] :
                B1 := ReducedRowEchelonForm(B2) :
                control2 := gausssamesign(B1) :
                if control2 = 1 then control := 2 : end if:
                seenset := [op(seenset), myset] :
                seenset := ListTools[MakeUnique](seenset) :
                while member(myset, seenset) and myset ≠ FAIL do
                    myset := nextcomb(myset, m) :
                end do:
            end do:
        end if:
        return(control) :
    end proc:
```

```
>
```

```
> ## check if after gauss reduction the system becomes injective: check all
  gausssignall := proc(B)
     local m, myset, n, i, det, bigset, seenset, B2, V2, B1, myset2, control, control2 :
    m := Dimension(B)[2] : n := Dimension(B)[1] :
     myset := {seq(i, i = 1 ..n)} :
     bigset := {seq(i, i = 1 ..m)} :

   control2 := 0 :
      while myset ≠ FAIL and control2 = 0 do
        B2 := B[ .., [op(myset), op(bigset minus myset)]] :
        B1 := ReducedRowEchelonForm(B2) :
        control2 := gausssamesign(B1) :
        myset := nextcomb(myset, m) :
     end do:
   return(control2) :
  end proc:
>
```

```
> ## check if after gauss reduction the system becomes injective
  gaussinj := proc(N, V, F)
    local p, mysigns, control2, myset, B, i, m, n, maxcols, B1, B3, V3, j, maxcols2, count,
      indiceslist, mypos, B4, V4, control, M, Mt, det, signs, sp, det2, l, k :
   m := Dimension(N)[2] : n := Dimension(N)[1] : sp := Dimension(V)[2] :
   B1 := N :
   maxcols := numelems(ArrayTools[SearchArray](B1)) − n :
   B3 := Matrix(Dimension(B1)[1], maxcols) :
   V3 := Matrix(maxcols, sp) :

  count := 1 : indiceslist := [ ] :
  for i from 1 by 1 to Dimension(B1)[1] do
      maxcols2 := ArrayTools[SearchArray](B1[i]) :
      for j from 2 by 1 to numelems(maxcols2) do
        control := 0 :
        mypos := ListTools[Search](maxcols2[j], indiceslist) :
        if mypos ≠ 0 then
          ##print(i, j, mypos) :
           if Equal(V[maxcols2[j]] − V[maxcols2[1]], V3[mypos]) then
                B3[i, mypos] := -B1[i, maxcols2[j]] : control := 1 :
           end if:
        end if:
        if control = 0 then
            V3[count] := V[maxcols2[j]] − V[maxcols2[1]] :
            indiceslist := [op(indiceslist), maxcols2[j]] :
            B3[i, count] := -B1[i, maxcols2[j]] :
```

```
            count := count + 1 :
          end if:
        end do:

      end do:
      B4 := SubMatrix(B3, [1..Dimension(B3)[1]], [1..count - 1]) :
      V4 := SubMatrix(V3, [1..count - 1], [1..Dimension(V3)[2]]) :

      M := B4.DiagonalMatrix(Vector([seq(k_i, i = 1..Dimension(V4)[1])])).V4
        .DiagonalMatrix(Vector([seq(l_i, i = 1..Dimension(V4)[2])])) :
      Mt := Matrix(sp, sp) :
      Mt[1..Dimension(F)[1]] := F :
      Mt[Dimension(F)[1] + 1..sp] := M :

      ##injectivity test
      det := Determinant(Mt) :
      det2 := collect(det, indets(det),'distributed') :
      signs := ListTools[MakeUnique](map(sign, [coeffs(det2)])) :
      if det2 ≠ 0 then
        i := (-1)^(numelems(signs) + 1) :
      else i := 0 : end if:
      return(i, det, B1) :
    end proc:

> ## check if after gauss reduction the system becomes injective and return also the
      matrices
    gaussinjV := proc(N, V, F)
      local p, mysigns, control2, myset, B, i, m, n, maxcols, B1, B3, V3, j, maxcols2, count,
        indiceslist, mypos, B4, V4, control, M, Mt, det, sp, signs, det2 :
    m := Dimension(N)[2] : n := Dimension(N)[1] : sp := Dimension(V)[2] :
    B1 := N :
    maxcols := numelems(ArrayTools[SearchArray](B1)) - n :
    B3 := Matrix(Dimension(B1)[1], maxcols) :
    V3 := Matrix(maxcols, sp) :

    count := 1 : indiceslist := [ ] :
    for i from 1 by 1 to Dimension(B1)[1] do
      maxcols2 := ArrayTools[SearchArray](B1[i]) :
      for j from 2 by 1 to numelems(maxcols2) do
        control := 0 :
        mypos := ListTools[Search](maxcols2[j], indiceslist) :
        if mypos ≠ 0 then
          ##print(i, j, mypos) :
          if Equal(V[maxcols2[j]] - V[maxcols2[1]], V3[mypos]) then
            B3[i, mypos] := -B1[i, maxcols2[j]] : control := 1 :
          end if:
        end if:
        if control = 0 then
```

```
            V3[count] := V[maxcols2[j]] - V[maxcols2[1]]:
            indiceslist := [op(indiceslist), maxcols2[j]]:
            B3[i, count] := -B1[i, maxcols2[j]]:
            count := count + 1:
        end if:
    end do:

    end do:
    B4 := SubMatrix(B3, [1..Dimension(B3)[1]], [1..count - 1]):
    V4 := SubMatrix(V3, [1..count - 1], [1..Dimension(V3)[2]]):

    M := B4.DiagonalMatrix(Vector([seq(h_i, i = 1..Dimension(V4)[1])])).V4
      .DiagonalMatrix(Vector([seq(l_i, i = 1..Dimension(V4)[2])])):
    Mt := Matrix(sp, sp):
    Mt[1..Dimension(F)[1]] := F:
    Mt[Dimension(F)[1] + 1..sp] := M:
    ##injectivity test
    det := Determinant(Mt):
    det2 := collect(det, indets(det),'distributed'):
    signs := ListTools[MakeUnique](map(sign, [coeffs(det2)])):
    if det2 ≠ 0 then
        i := (-1)^(numelems(signs) + 1):
    else i := 0: end if:
    return(i, det, B4, V4):
end proc:
```

```
> ## check if after gauss reduction the system becomes injective: check all
gaussinjall := proc(B, V, F, myred)
    local m, myset, i, n, k, det, bigset, seenset, B2, V2, B1, myset2, myset3, control,
      control2:
    m := Dimension(B)[2]: n := Dimension(B)[1]:
    myset := {seq(i, i = 1..n)}: control := 0:
    bigset := {seq(i, i = 1..m)}:
    seenset := [myset]:

    while myset ≠ FAIL and control = 0 do
      B2 := B[.., [op(myset), op(bigset minus myset)]]:
      V2 := V[[op(myset), op(bigset minus myset)],..]:
      B1 := ReducedRowEchelonForm(B2):

      myset2 := {}:
      for k from 1 by 1 to n do
          myset2 := {op(myset2), ArrayTools[SearchArray](B1[k])[1]}:
      end do:
      myset3 := {op([op(myset), op(bigset minus myset)][[op(myset2)]])}:
      if not member(myset3, seenset) then
          i, det, B1 := gaussinj(B1, V2, F):
```

```
            if i = 1 then control := 1 : end if:  ## injective found
        end if:
        seenset := [op(seenset), myset3] :
        seenset := [op(seenset), myset] :
        seenset := ListTools[MakeUnique](seenset) :

        ##find new subset, filtered by seenset and the already known independent columns
       control2 := 0 :
       while control2 = 0 do
           control2 := 1 :
           myset := nextcomb(myset, m) :
          if myset ≠ FAIL then
             if member(myset, seenset) then control2 := 0 :
             else
              k := 1 :
              while k ≤ numelems(myred) and control2 = 1 do
                 if subset(myred[k], myset) then control2 := 0 : end if:
                 k := k + 1 :
               end do:
             end if:
          end if:
        end do:
     end do:  ##end big do, for myset and control

     return(control) :
    end proc:
>
```

```
> ## check if after gauss reduction the system becomes injective: check bistable
    Bistablecheck := proc(B)
       local m, n, j, k, control, control2, myrow, myvec, signvec :
      m := Dimension(B)[2] : n := Dimension(B)[1] :
      j := 1 :
      control2 := 0 :
      control := 2 :
      while control2 = 0 and j ≤ n do
          myrow := convert(ArrayTools[SearchArray](B[j]), list) :
         if numelems(myrow) ≤ 1 then control2 := 1 : control := 3 :
         else
            myvec := convert(B[j][myrow[2..numelems(myrow)]], list) :
            signvec := ListTools[MakeUnique](map(sign, myvec)) :
            if signvec ≠ [-1] then control2 := 1 : control := 0 :
            else
               k := 2 :
               while control2 = 0 and k ≤ numelems(myrow) do
                    if numelems(ArrayTools[SearchArray](B[.., myrow[k]])) ≠ 1
      then control2 := 1 : control := 0 : end if:
```

```
                    k := k + 1 :
                end do:
            end if:
        end if:
        j := j + 1 :
    end do:
    return(control) :
    end proc:
>
```

```
> ## check if after gauss reduction the system becomes injective: check bistable
    Bistablecheck2 := proc(B)
      local m, n, j, k, control, control2, myrow, myvec, signvec, disjsets, nonzerocols,
       totalcard :
      m := Dimension(B)[2] : n := Dimension(B)[1] :
      j := 1 : disjsets := [ ] :
      control2 := 0 :
      control := 2 :
      while control2 = 0 and j ≤ n do
          myrow := convert(ArrayTools[SearchArray](B[j]), list) :
          if numelems(myrow) ≤ 1 then control2 := 1 : control := 3 :
          else
              myvec := convert(B[j][myrow[2 ..numelems(myrow)]], list) :
              signvec := ListTools[MakeUnique](map(sign, myvec)) :
              if signvec ≠ [-1] then control2 := 1 : control := 0 :
              else k := 2 :
                  while control2 = 0 and k ≤ numelems(myrow) do
                      nonzerocols := ArrayTools[SearchArray](B[ .., myrow[k]]) :
                      if numelems(nonzerocols) > 1 then disjsets := [op(disjsets),
        convert(nonzerocols, list)] :
                      end if:
                      k := k + 1 :
                  end do:
              end if:
          end if:
          j := j + 1 :
      end do:
      disjsets := MakeUnique(disjsets) :
      totalcard := 0 :
      for k from 1 by 1 to numelems(disjsets) do  totalcard := totalcard
          + numelems(disjsets[k]) : end do:
      if numelems(MakeUnique(Flatten(disjsets))) ≠ totalcard then control := 0 : end
          if:

      return(control) :
      end proc:
```

```
> ## check if after gauss reduction the system becomes injective: check all
gaussinjallBi := proc(B, V, F, myred)
   local m, myset, i, n, k, det, bigset, seenset, B2, V2, B1, myset2, myset3, control,
    control2 :
   m := Dimension(B)[2] : n := Dimension(B)[1] :
    myset := {seq(i, i = 1 ..n)} : control := 0 :
    bigset := {seq(i, i = 1 ..m)} :
   seenset := [myset] :

  while myset ≠ FAIL and control = 0 do
    B2 := B[ .., [op(myset), op(bigset minus myset)]] :
    V2 := V[ [op(myset), op(bigset minus myset)],.. ] :
     B1 := ReducedRowEchelonForm(B2) :

     myset2 := { } :
     for k from 1 by 1 to n do
         myset2 := {op(myset2), ArrayTools[SearchArray](B1[k])[1]} :
    end do:
     myset3 := {op([op(myset), op(bigset minus myset)][[op(myset2)]])} :
    if not member(myset3, seenset) then
         i, det, B1 := gaussinj(B1, V2, F) :
         if i = 1 then control := 1 : end if:  ## injective found
         if i = -1 or i = 0 then
               control := Bistablecheck(B1) :
        end if:
    end if:
    seenset := [op(seenset), myset3] :
    seenset := [op(seenset), myset] :
    seenset := ListTools[MakeUnique](seenset) :

    ## find new subset, filtered by seenset and the already known independent columns
   control2 := 0 :
   while control2 = 0 do
      control2 := 1 :
      myset := nextcomb(myset, m) :
     if myset ≠ FAIL then
        if member(myset, seenset) then control2 := 0 :
        else
         k := 1 :
         while k ≤ numelems(myred) and control2 = 1 do
            if subset(myred[k], myset) then control2 := 0 : end if:
            k := k + 1 :
          end do:
        end if:
     end if:
    end do:
  end do:  ##end big do, for myset and control
```

```
    return(control) :
  end proc:
>
```

```
> gaussinjallBi2 := proc(B, V, F, myred)
    local m, myset, i, n, k, det, bigset, seenset, B2, V2, B1, myset2, myset3, control,
     control2, lastseen, myseen :
    m := Dimension(B)[2] : n := Dimension(B)[1] :
    myset := {seq(i, i = 1 ..n)} : control := 0 :
    bigset := {seq(i, i = 1 ..m)} :
    seenset := [ ] :
    myseen := [ ] :

    while myset ≠ FAIL and control = 0 do
      B2 := B[ .., [op(myset), op(bigset minus myset)]] :
      V2 := V[[op(myset), op(bigset minus myset)],..] :
      B1 := ReducedRowEchelonForm(B2) :
      lastseen := myset : myseen := [op(myseen), myset] :
      myset2 := { } :
      for k from 1 by 1 to n do
          myset2 := {op(myset2), ArrayTools[SearchArray](B1[k])[1]} :
      end do:
      myset3 := {op([op(myset), op(bigset minus myset)][[op(myset2)]])} :
      if not member(myset3, seenset) then
          i, det, B1 := gaussinj(B1, V2, F) :
          if i = 1 then control := 1 : end if:  ## injective found
          if i = -1 or i = 0 then
                control := Bistablecheck2(B1) :
          end if:
      end if:
      seenset := [op(seenset), myset3] :
      seenset := [op(seenset), myset] :
      seenset := ListTools[MakeUnique](seenset) :

      ## find new subset, filtered by seenset and the already known independent columns
      control2 := 0 :
      while control2 = 0 do
         control2 := 1 :
         myset := nextcomb(myset, m) :
        if myset ≠ FAIL then
          if member(myset, seenset) then control2 := 0 :
          else
           k := 1 :
           while k ≤ numelems(myred) and control2 = 1 do
              if subset(myred[k], myset) then control2 := 0 : end if:
              k := k + 1 :
            end do:
```

```
            end if:
          end if:
        end do:
      end do:  ##end big do, for myset and control

      return(control, myset, B1, lastseen, myseen) :
    end proc:
```

```
> isinjectiveextended := proc(A)
    local V, M, F, i, n1, s1, B, toexclude, myred, control, myset, B1, lastseen, myseen :
    myred := { } :
    V := findV(A) :
    n1 := Dimension(A)[1] : s1 := Rank(A) :
    toexclude := [ ] :
    if s1 < n1 then
      F
      := ReducedRowEchelonForm(Transpose(Matrix([op(NullSpace(Transpose(
      A)))])))) :
      for i from 1 by 1 to Dimension(F)[1] do
        toexclude := [op(toexclude), ArrayTools[SearchArray](F[i])[1]] :
      end do:
    else
      F := [ ] :
    end if:
    B := SubMatrix(A, [op({seq(i, i = 1 .. n1)} minus {op(toexclude)})], [1
      ..Dimension(A)[2]]) :
    if Dimension(B)[1] < Dimension(B)[2] then
      control, myset, B1, lastseen, myseen := gaussinjallBi2(B, V, F, myred) :
      return(control) :
    else
      return(0) :
    end if:
  end proc:
```

```
>
```

Step 3. Finding the positive feedback loops for multistationary networks

Auxiliary procedures

```
> addlist := proc(mylist, myaddlist)
    local i, newlist :
    newlist := [op(mylist), op(myaddlist)] :
    return newlist :
  end proc:
```

This procedure computes the polynomial $p_{A,Z}$ in the main text. The input are the matrices A and Z (in the function denoted N and X).

```
> ## compute Mtilde determinant
  computdetS := proc(N, X)
   global Mt :
   local M, F, i, bigdet, n1, s1 :
   n1 := Dimension(N)[1] : s1 := Rank(N) :
   M := N.Transpose(X) :
   Mt := M :
   if s1 < n1 then
     F
       := ReducedRowEchelonForm(Transpose(Matrix([op(NullSpace(Transpose(
      N)))])))) :
     for i from 1 by 1 to Dimension(F)[1] do
        Mt[ArrayTools[SearchArray](F[i])[1]] := F[i] :
     end do:
   end if:
   bigdet := expand(Determinant(Mt)) :
   return(bigdet) :
  end proc:
```

This function returns the list of monomials that have the wrong sign. The input are the determinant and the wrong sign.

```
> ##Given a determinant and a wrong sign, return the list of wrong monomials
  badterms := proc(deter, mysign)
      local vars, coeflist, monomlist, coeflistsign, wterms, i :
       vars := indets(deter) :
      coeflist := [coeffs(deter, vars, 't')] :
       monomlist := [t] :
      coeflistsign := map(sign, coeflist) :
      wterms := [ ] :
      for i from 1 by 1 to numelems(coeflistsign) do
          if mysign = coeflistsign[i] then wterms := [op(wterms), monomlist[i]] : end
        if:
      end do:
      return(wterms) :

   end proc:
```

Given a monomial on the entries of a matrix Amatrix, this function finds a matrix from Amatrix such that the variables in the monomial become 1 and the rest are zero.

```
> ##Find submatrix of a matrix corresponding to a monomial
findmatrix := proc(wmonom, Amatrix)
    local vars, wvarscomp, Anew, i, Anew1 :
    vars := indets(wmonom) :
    wvarscomp := indets(Amatrix) minus vars :
    Anew := subs(seq(wvarscomp[i] = 0, i = 1 ..numelems(wvarscomp)), Amatrix) :
    Anew1 := subs(seq(vars[i] = 1, i = 1 ..numelems(vars)), Anew) :
   return(Anew1) :
  end proc:
```

Find the two submatrices of A and Z corresponding to the monomial, and make A symbolic by introducing a new variable x.

```
> ## Find the two matrices A,Z corresponding to a monomial
twomatrices := proc(wmonom)
    global A, Z :
    local vars, wvarscomp, Zembed, i, row, col, Aembed, Aembedx, nZ, X :
   X := Transpose(Z) :
    vars := indets(wmonom) :
    wvarscomp := indets(X) minus vars :
    Zembed := subs(seq(wvarscomp[i] = 0, i = 1 ..numelems(wvarscomp)), X) :
    row, col := ArrayTools[SearchArray](Zembed) :
    Zembed := Zembed[convert(row, list), convert(col, list)] :
     nZ := numelems(vars) :
    Aembed := A[convert(col, list), convert(row, list)] :
   Aembed := map(signum, Aembed) :
   row, col := ArrayTools[SearchArray](Aembed) :
   Aembedx := Matrix(nZ, nZ) :
   for i from 1 by 1 to numelems(col) do
     Aembedx[row[i], col[i]] := Aembed[row[i], col[i]]·x_i :
   end do:
   return(Aembedx, Zembed) :
end proc:
```

Extract the indices of the species and the reaction in the given monomial in the variables of Z

```
> ## Extract indices of species and reaction in the monomial from Z
extractsr := proc(wmonom)
    global Z :
    local vars, wvarscomp, Zembed, i, row, col, X :
    X := Transpose(Z) :
     vars := indets(wmonom) :
    wvarscomp := indets(X) minus vars :
      ## indeterminates not in the monomial
    Zembed := subs(seq(wvarscomp[i] = 0, i = 1 ..numelems(wvarscomp)), X) :
```

```
    ##set the entries of the indeterminates not in the monomial to zero
    row, col := ArrayTools[SearchArray](Zembed) :
    ##find the nonzero entries of the resulting matrix.
    return(row, col) :  ##return the species and reaction indices
  end proc:
```

```
> ##Create DSR graph: entries are two matrices and the labels of the nodes
  createDSRgraph := proc(mynodes, A, Z)
    local G, n, m, Adj, varsZ, Zsign, varsA, Asign, X :
    n := Dimension(A)[1] : m := Dimension(A)[2] :
    X := Transpose(Z) :
    varsZ := indets(X) :
    Zsign := subs(seq(varsZ[i] = 1, i = 1 ..numelems(varsZ)), X) :
    varsA := indets(A) :
    Asign := subs(seq(varsA[i] = 1, i = 1 ..numelems(varsA)), A) :

   Adj := Matrix(n + m, n + m) :
   Adj[[n + 1 ..n + m], [1 ..n]] := Transpose(map(signum, Asign)) :
   Adj[[1 ..n], [n + 1 ..n + m]] := Transpose(Zsign) :

    G := GraphTheory[Graph](mynodes, Adj, weighted = true) :
    return(G) :
  end proc:
>
```

This function selects the subgraphs that give rise to the monomials with the wrong sign.

```
> ## Select the subgraphs that correspond to the wrong terms of A and Z
  graphlist := proc(mydet)
   global A, Z :
   local srlist, row, col, Gsub, s, wsign, wrongterms, k, wcurrent, Aembedx, Zembed,
       detZ, detAx, wsignA, wrongtermsA, wcurrentA, j, Aembedx1, mynodes :
  Gsub := [ ]:
   srlist := [ ]:
   s := Rank(A) :
  wsign := (-1)^(s + 1) :                    ## find wrong sign
  wrongterms := badterms(mydet, wsign) :
       ## select the monomials with the wrong sign
   for k from 1 by 1 to numelems(wrongterms) do
       ## for each such monomial, find the associated subgraph
       wcurrent := wrongterms[k] :
       row, col := extractsr(wcurrent) :
       ## find the indices of the species and the reactions in the monomial
       mynodes := [seq(S_col[i], i = 1 ..numelems(col)), seq(R_row[i], i = 1
        ..numelems(row))] :
       Aembedx, Zembed := twomatrices(wcurrent) :
```

```
        ## the returned Zembed is giving half of the edges of the subgraphs
        detZ := subs(seq(indets(Zembed)[i] = 1, i = 1 ..numelems(indets(Zembed))),
         Determinant(Zembed)) :
        detAx := expand(Determinant(Aembedx)) :
        wsignA := wsign·detZ :
        wrongtermsA := badterms(detAx, wsignA) :
        ## select the monomials with the wrong sign of the subsystem
        for j from 1 by 1 to numelems(wrongtermsA) do
            wcurrentA := wrongtermsA[j] :
            Aembedx1 := findmatrix(wcurrentA, Aembedx) :
        ## find the other half of the edges of the subgraphs
            Gsub := [op(Gsub), createDSRgraph(mynodes, Aembedx1, Zembed)] :
        end do:
    end do:
    return(Gsub) :  ##return the list of graphs
end proc:
```

Given a list of edges that form a loop, the function returns the edges ordered such that connected they form the loop.

```
> ## Order the edges to have a loop
orderedge := proc(myedges)
    local orderededges, endpoint, total, control, k :
    orderededges := [myedges[1]] :
    endpoint := myedges[1][1][2] :
    total := numelems(myedges) :
    while numelems(orderededges) < total do
        control := 0 : k := 2 :
        while control = 0 do
            if endpoint = myedges[k][1][1] then
                orderededges := [op(orderededges), myedges[k]] :
                control := 1 :
                endpoint := myedges[k][1][2] :

            end if:
            k := k + 1 :
        end do:
    end do:
    return(orderededges) :
end proc:
```

Find the sequence of signs of the loop

```
> ##Extract the  sequence  of signs of a loop
extractsign := proc(orderededges)
    local graphsign, i :
    graphsign := [ ] :
    for i from 1 by 1 to numelems(orderededges) do
```

```
    graphsign := [op(graphsign), orderededges[i][2]]:
  end do:
  return(graphsign):
end proc:
```

Given a list of graphs, we find the positive feedback loops that they contain and return the sign pattern of each positive feedback loop as well (as those given in Table 1 in the main text).

```
> ##Find the positive feedback loops in the list of graphs
positivefeed := proc(Gsub)
    local selected, j, mygraph, Gsubcomp, k, mycomp, newgraph, wedges, myprod, i,
     signcycle:
    selected := []:
   signcycle := []:
   Gsubcomp := []:
   for j from 1 by 1 to numelems(Gsub) do
     mygraph := Gsub[j]:
    Gsubcomp := ConnectedComponents(mygraph):
    for k from 1 by 1 to numelems(Gsubcomp) do
      mycomp := Gsubcomp[k]:
     newgraph := InducedSubgraph(mygraph, mycomp):
     wedges := Edges(newgraph, weights):
     myprod := mul(wedges[i][2], i = 1..numelems(wedges)):
     if myprod = 1 then              ##if the loop is positive, select it
        selected := [op(selected), [op(wedges)]]:
    end if:
   end do:
  end do:
  selected := ListTools[MakeUnique](selected):
  for k from 1 by 1 to numelems(selected) do
    selected[k] := orderedge(selected[k]):
    signcycle := [op(signcycle), extractsign(selected[k])]:
  end do:
  return(selected, signcycle):
end proc:
```

The main procedure to find the positive loop is the following:

```
> ##main program: find the positive loops
findloops := proc( )
  global A, Z:
  local Gsub, selected, signcycle, mydet:
```

```
    mydet := computdetS(A, Z) :  ## find the polynomial p_{A, Z}
    Gsub := graphlist(mydet) :
      ## find the list of subgraphs corresponding to the wrong signs
    selected, signcycle := positivefeed(Gsub) :
      ## find the positive feedback loops and their sign pattern
    return(selected) :
  end proc:
```

The second main procedure of the method is the function that draws the selected positive feedback loops. It requires a list with the names of the nodes (see the examples below)

```
> ## draw the positive feedback loops
drawloops := proc(selected, speciesord)
  local loops, i, vertices, speciesdic, selected2 :
 loops := [ ] :
 speciesdic := {seq(S_i = speciesord[i], i = 1 ..numelems(speciesord))} :
 selected2 := subs(speciesdic, selected) :
for i from 1 by 1 to numelems(selected2) do
     vertices := ListTools[MakeUnique]([seq(op(selected2[i][j][1]), j = 1
     ..numelems(selected2[i]))]) :
     loops := [op(loops), Digraph(vertices, {op(selected2[i])})] :
 end do:
DrawGraph(loops, style = circle);

 end proc:
```

Functions for constructing stoichiomatric matrix and examine the existence of competition and closed loop.

1. constructing stoichiomatric vectors based on the certain reaction patterns

List all reaction types based on the number of species. $R_n = \binom{n}{2} \cdot 2 + \binom{n}{3} \cdot 6$

```
> listRs := proc(n)
      local R, r, se, i, j, k, sign, l :
      r := binom(n, 2)·2 + binom(n, 3)·6 :
      R := Matrix(r, n) :
```

```
    # Now construct the reaction pattern matrix
    i := 1 :

    # here we first consider single transformation
    for se from -1 to 1 by 2 do
      for j from 1 to n by 1 do
        for k from j + 1 to n by 1 do
          R[i, j] := se :
          R[i, k] := -se :
          i := i + 1 :
        end do:
      end do:
    end do:

    # now consider heterodimerization and disassociation
    for sign from -1 to 1 by 2 do
      for j from 1 to n by 1 do
        for k from j + 1 to n by 1 do
          for l from k + 1 to n by 1 do
            R[i, j] := sign :
            R[i, k] := -sign :
            R[i, l] := -sign :
            i := i + 1 :
            R[i, j] := sign :
            R[i, k] := sign :
            R[i, l] := -sign :
            i := i + 1 :
            R[i, j] := sign :
            R[i, k] := -sign :
            R[i, l] := sign :
            i := i + 1 :
          end do:
        end do:
      end do:
    end do:

    # in this case we don't consider homodimerization and disassociation

    # Here transpose the R
    # R := Transpose(R) :
     # no need to ranspose, need to assign rows to untransposed A's rows
    return(R) :
  end proc:
```

Here is a long function to enumerate first two reaction pattern (will reduce large mount of symmetric reactions).

```
> listR2 := proc(n)
    local R2, r2, R3, r3, R4, r4 :
    if n ≥ 4 then
      r2 := 29·2 :
      R2 := Matrix(r2, 4) :

      # in this case we don't consider homodimerization and disassociation

      ## now we construct the reaction pattern with n = 4
      R2[1] := ⟨1,-1⟩ : R2[2] := ⟨0, 0, 1,-1⟩ :
      R2[3] := ⟨1,-1⟩ : R2[4] := ⟨0, 1,-1⟩ :
      R2[5] := ⟨1,-1⟩ : R2[6] := ⟨1, 0,-1⟩ :
      R2[7] := ⟨1,-1⟩ : R2[8] := ⟨0,-1, 1⟩ :
      R2[9] := ⟨1,-1⟩ : R2[10] := ⟨-1, 0, 1⟩ :
      R2[11] := ⟨1,-1⟩ : R2[12] := ⟨-1, 1⟩ :
      R2[13] := ⟨1,-1⟩ : R2[14] := ⟨0, 1,-1,-1⟩ :
      R2[15] := ⟨1,-1⟩ : R2[16] := ⟨1, 0,-1,-1⟩ :
      R2[17] := ⟨1,-1⟩ : R2[18] := ⟨0,-1, 1,-1⟩ :
      R2[19] := ⟨1,-1⟩ : R2[20] := ⟨-1, 0, 1,-1⟩ :
      R2[21] := ⟨1,-1⟩ : R2[22] := ⟨0, 1, 1,-1⟩ :
      R2[23] := ⟨1,-1⟩ : R2[24] := ⟨1, 0, 1,-1⟩ :
      R2[25] := ⟨1,-1⟩ : R2[26] := ⟨0,-1, 1, 1⟩ :
      R2[27] := ⟨1,-1⟩ : R2[28] := ⟨-1, 0, 1, 1⟩ :
      R2[29] := ⟨1,-1⟩ : R2[30] := ⟨-1,-1, 1⟩ :
      R2[31] := ⟨1,-1⟩ : R2[32] := ⟨1, 1,-1⟩ :
      R2[33] := ⟨1,-1,-1⟩ : R2[34] := ⟨0, 1,-1,-1⟩ :
      R2[35] := ⟨1,-1,-1⟩ : R2[36] := ⟨1, 0,-1,-1⟩ :
      R2[37] := ⟨1,-1,-1⟩ : R2[38] := ⟨0,-1,-1, 1⟩ :
      R2[39] := ⟨1,-1,-1⟩ : R2[40] := ⟨-1,-1, 0, 1⟩ :
      R2[41] := ⟨1,-1,-1⟩ : R2[42] := ⟨0, 1, 1,-1⟩ :
      R2[43] := ⟨1,-1,-1⟩ : R2[44] := ⟨1, 1, 0,-1⟩ :
      R2[45] := ⟨1,-1,-1⟩ : R2[46] := ⟨0, 1,-1, 1⟩ :
      R2[47] := ⟨1,-1,-1⟩ : R2[48] := ⟨-1, 1, 0, 1⟩ :
      R2[49] := ⟨1,-1,-1⟩ : R2[50] := ⟨-1, 1, 1⟩ :
      R2[51] := ⟨1, 1,-1⟩ : R2[52] := ⟨0, 1, 1,-1⟩ :
      R2[53] := ⟨1, 1,-1⟩ : R2[54] := ⟨1, 1, 0,-1⟩ :
      R2[55] := ⟨1, 1,-1⟩ : R2[56] := ⟨0, 1,-1, 1⟩ :
      R2[57] := ⟨1, 1,-1⟩ : R2[58] := ⟨1,-1, 0, 1⟩ :


      if n ≥ 5 then
        ## now we add the reaction pattern with n = 5

        r3 := 43·2 :
        R3 := Matrix(r3, 5) :
        R3[1..r2] := R2[ ] :

        R3[59] := ⟨1,-1⟩ : R3[60] := ⟨0, 0, 1,-1,-1⟩ :
```

```
        R3[61] := ⟨1,-1⟩ : R3[62] := ⟨0, 0, 1, 1,-1⟩ :
        R3[63] := ⟨1,-1,-1⟩ : R3[64] := ⟨0, 0, 1,-1,-1⟩ :
        R3[65] := ⟨1,-1,-1⟩ : R3[66] := ⟨1, 0, 0,-1,-1⟩ :
        R3[67] := ⟨1,-1,-1⟩ : R3[68] := ⟨0, 0,-1, 1,-1⟩ :
        R3[69] := ⟨1,-1,-1⟩ : R3[70] := ⟨-1, 0, 0, 1,-1⟩ :
        R3[71] := ⟨1,-1,-1⟩ : R3[72] := ⟨0, 0, 1, 1,-1⟩ :
        R3[73] := ⟨1,-1,-1⟩ : R3[74] := ⟨1, 0, 0, 1,-1⟩ :
        R3[75] := ⟨1,-1,-1⟩ : R3[76] := ⟨0, 0,-1, 1, 1⟩ :
        R3[77] := ⟨1,-1,-1⟩ : R3[78] := ⟨-1, 0, 0, 1, 1⟩ :
        R3[79] := ⟨1, 1,-1⟩ : R3[80] := ⟨0, 0, 1, 1,-1⟩ :
        R3[81] := ⟨1, 1,-1⟩ : R3[82] := ⟨1, 0, 0, 1,-1⟩ :
        R3[83] := ⟨1, 1,-1⟩ : R3[84] := ⟨0, 0,-1, 1, 1⟩ :
        R3[85] := ⟨1, 1,-1⟩ : R3[86] := ⟨-1, 0, 0, 1, 1⟩ :

        if n ≥ 6 then
          ## now we add the reaction pattern with n = 6

          r4 := 46·2 :
          R4 := Matrix(r4, n) :
          R4[1..r3] := R3[ ] :

          R4[87] := ⟨1,-1,-1⟩ : R4[88] := ⟨0, 0, 0, 1,-1,-1⟩ :
          R4[89] := ⟨1,-1,-1⟩ : R4[90] := ⟨0, 0, 0, 1, 1,-1⟩ :
          R4[91] := ⟨1, 1,-1⟩ : R4[92] := ⟨0, 0, 0, 1, 1,-1⟩ :

          return(R4) :
        else
          return(R3) :
        end if:
      else
        return(R2) :
      end if:
    else
      error "ERROR: n is smaller than 4"
    end if:

  end proc:
```

2. Now we can construct stoichiomatric matrix based on the reaction patterns, and examine their properties.

Here, we construct the stoichiomatric matrices.

The total number of stoichiomatric matrices is $\binom{R_n}{m}$, which is still a huge number. But currently there seems no other better options.

We only consider when $m \leq 6$.

The function(s) to examine existence of competition and loops a stoichiomatric matrix.

```
>
```

The function to check if the stoichiomatric matrix is mass conserved.

First check the passed matrix $A_{m\times n}$ (must be in a consistent form)

```
> ismassconserved := proc(A)
    local R, N, NS, m, n, absAdd, Add, x, y, z, e, i, nsAdd, nsAbsAdd, a, b, c :
    m := 0 :
    n := Dimension(A)[2] :
    absAdd := AddAlongDimension(|A|, 1) :
    z := Search(0, absAdd) :
    if z = 0 then
      Add := AddAlongDimension(A, 1) :
      x := Search(0, VectorAdd(absAdd, Add, 1, -1)) :
      if x = 0 then
        y := Search(0, VectorAdd(absAdd, Add, 1, 1)) :
        if y = 0 then
          N := NullSpace(A) :
          e := numelems(N) :
          if e > 0 then
            NS := Matrix(e, n) :
            for i from 1 to e by 1 do
              NS[i] := N[i] :
            end do:
            nsAbsAdd := AddAlongDimension(|NS|, 1) :
            a := Search(0, nsAbsAdd) :
            if a = 0 then
              nsAdd := AddAlongDimension(NS, 1) :
              b := Search(0, VectorAdd(nsAbsAdd, nsAdd, 1, 1)) :
              if b = 0 then
                m := 1 :
              end if:
            end if:
          end if:
        end if:
      end if:
    end if:
    return(m) :
  end proc:
```

Construct and examine the properties of all stoichiomatric matrices.

```
> constrM := proc(n, m)
    local R, A, r, g, h, i, j, k, l, total, right, mc, V, R2, r2, inject, inject0, inject1, injectEx,
```

```
injectEx0, injectEx1, injectEx2, injectEx3, fileName, matrixData, tA, interV :
r := binomial(n, 2)·2 + binomial(n, 3)·6 :

A := Matrix(m, n) :

R := listRs(n) :
R2 := listR2(n) :

if n = 4  then  r2 := 29·2 : end if:
if n = 5  then  r2 := 43·2 : end if:
if n ≥ 6  then  r2 := 46·2 : end if:
if n < 4 then error "ERROR: n is smaller than 4" end if:

total := r2/2 · binomial(r, m − 2) :

# here we use some variable to count how many reactions are correct.
right := 0 : inject0 := 0 : inject1 := 0 : injectEx0 := 0 : injectEx1 := 0 : injectEx2
  := 0 : injectEx3 := 0 :
for l from 1 to r2 − 1 by 2 do
   A[1] := R2[l] :
   A[2] := R2[l + 1] :
   for g from 1 to r by 1 do
      # here we should check whether this is duplicate of the fixed two reactions.
      #######
      A[3] := R[g] :
      for h from g + 1 to r by 1 do
         A[4] := R[h] :
         for i from h + 1 to r by 1 do
            A[5] := R[i] :
            #for j from i+1 to r by 1 do
               #A[6] := R[j] :

               # now we have matrix A, we need to exam A with constraints.
               mc := ismassconserved(A) :
               if mc = 1 then


# before this we should preclude the reactions violating mass conservation!

### the idea is construct a sequence of species based on the mass (sorted by
reactions)

### if there is any species with two different positions then it violates mass
conservation.
                  ### Or just record the sequential position for each species,
                  ### then find if there are species with two or more position numbers
```

```
                right := right + 1 :

                tA := Transpose(A) :

                inject := isinjective(tA) :
                if inject = 0 then
                   inject0 := inject0 + 1 :
                   fileName
 := sprintf("%1dspecies/injectivity/noninjective_%d.csv", n, inject0) :
                   ExportMatrix(fileName, tA, target = csv, format = rectangular,
mode = ascii) :

                   injectEx := isinjectiveextended(tA) :
                   if injectEx = 0 then
                      injectEx0 := injectEx0 + 1 :
                      fileName
 := sprintf("%1dspecies/bistability/needToolbox_%d.csv", n, injectEx0) :
                      ExportMatrix(fileName, tA, target = csv, format = rectangular,
mode = ascii) :

                   elif injectEx = 1 then
                      injectEx1 := injectEx1 + 1 :

                   elif injectEx = 2 then
                      injectEx2 := injectEx2 + 1 :
                      fileName := sprintf("%1dspecies/bistability/bistable_%d.csv",
n, injectEx2) :
                      ExportMatrix(fileName, tA, target = csv, format = rectangular,
mode = ascii) :

                   elif injectEx = 3 then
                      injectEx3 := injectEx3 + 1 :
                   else
                      error "ERROR: injectivity extended of A is not any of 0 to 3."
                   end if:
                elif inject = 1 then
                   inject1 := inject1 + 1 :
                else
                   error "ERROR: the injectivity of A is neither 0 nor 1."
                end if:
             end if:
          #end do:
       end do:
    end do:
  end do:

V := [injectEx0, injectEx1, injectEx2, injectEx3, inject0, inject1, right, total, r, r2] :
return(V) :
```

```
end proc:
>
```

Testing

Here we test all functions:

```
> V := constrM(5, 5) # just count right matrices ~ 2360s (40 mins) (9.29s to 2359.41s)
```

$$V := [0, 0, 0, 0, 0, 0, 9229, 3532880, 80, 86] \quad \textbf{(3.1)}$$

```
> #V:=constrM(5, 5) # also count injective matrices ~
> #V:=constrM(5, 5) # also count injective matrices and export noninjective matrices ~
> #V:=constrM(5, 5) # also count injective extended matrices ~
> V := constrM(5, 5)
      # also count injective extended matrices and export bistable matrices ~ 2716s
                                                          #(45 mins) (4621.73 s
      to 7337.76 s)
```

$$V := [65, 578, 87, 3977, 4707, 4522, 9229, 3532880, 80, 86] \quad \textbf{(3.2)}$$

```
>
>
>
```