```
> # Execute every statement in order
> restart;
>
> # for 3-species networks with exactly 2 reactions, polynomials from the ODE
    system are:
```

$f_1 := (x_1, x_2, x_3) \to (b_{11}-a_{11}) \cdot k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} + (b_{12}-a_{12}) \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}:$

$f_2 := (x_1, x_2, x_3) \to (b_{21}-a_{21}) \cdot k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} + (b_{22}-a_{22}) \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}:$

$f_3 := (x_1, x_2, x_3) \to (b_{31}-a_{31}) \cdot k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} + (b_{32}-a_{32}) \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}:$

```
> # if the network has one-dimensional sthoichiometric subspace, then the above
    three polynomials can be simplified:
```

$f_1 := (x_1, x_2, x_3) \to (b_{11}-a_{11}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} - lambda \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}\right):$

$f_2 := (x_1, x_2, x_3) \to (b_{21}-a_{21}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} - lambda \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}\right):$

$f_3 := (x_1, x_2, x_3) \to (b_{31}-a_{31}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} - lambda \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}\right):$

```
> # below, we combine the conservation law equation
```

$h_1 := (x_1, x_2, x_3) \to (b_{11}-a_{11}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} \cdot x_3^{a_{31}} - lambda \cdot k_2 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} \cdot x_3^{a_{32}}\right):$

$h_2 := (x_1, x_2) \to (b_{21}-a_{21}) \cdot x_1 - (b_{11}-a_{11}) \cdot x_2 - c_1:$

$h_3 := (x_1, x_3) \to (b_{31}-a_{31}) \cdot x_1 - (b_{11}-a_{11}) \cdot x_3 - c_2:$

```
> # stability criterion
```

$tr := D[1](f_1)(x_1, x_2, x_3) + D[2](f_2)(x_1, x_2, x_3) + D[3](f_3)(x_1, x_2, x_3):$

```
>
> sol := [0, 0, 0] : evasol := [0, 0, 0] : evatr := [0, 0, 0] :
>
> # below, we show witness of multistability for networks in Row (3) and Row (7)
    in Table 2 (see main manuscript)
> # ------------------------------------------------
  # Row (3)

  # X1 + 3X2       →      4 X2 + X3
  #      X2 + X3  →  X1
>
```

$\# \; X_1 + 3X_2 \to 4\,X_2 + X_3$

$\# \; X_2 + X_3 \to X_1$

```
> a11 := 1 : a21 := 3 : a31 := 0 : a12 := 0 : a22 := 1 : a32 := 1 :
  b11 := 0 : b21 := 4 : b31 := 1 : b12 := 1 : b22 := 0 : b32 := 0 :
  h1(x1, x2, x3) ; h2(x1, x2) ; h3(x1, x3) ;
```

$$-k_1\ x_1\ x_2^3 + \lambda\ k_2\ x_2\ x_3$$
$$x_1 + x_2 - c_1$$
$$x_1 + x_3 - c_2 \tag{1}$$

```
> # choose witness
  lambda := 1 : k1 := 9 : k2 := 50 : c1 := 6 : c2 := 59/10 :
  h1(x1, x2, x3) ; h2(x1, x2) ; h3(x1, x3) ;
```

$$-9\ x_1\ x_2^3 + 50\ x_2\ x_3$$
$$x_1 + x_2 - 6$$
$$x_1 + x_3 - \frac{59}{10} \tag{2}$$

```
> # 3 positive steady states
  # stable, if tr<0;
  shsol := solve(h1(x1, solve(h2(x1, x2), x2), solve(h3(x1, x3), x3)), x1) :
  for n from 2 to 4 do
  sol[n − 1] := [x1 = shsol[n], x2 = solve(h2(shsol[n], x2), x2), x3
      = solve(h3(shsol[n], x3), x3)];
  evasol[n − 1] := evalf(sol[n − 1], 5);
  evatr[n − 1] := if_tr = evalf(subs(sol[n − 1][1], sol[n − 1][2], sol[n − 1][3], tr),
      5);
  end do:

  # 1st column: Solutions; 2nd column: Approximate Values; 3rd column: Trace of
      Jacobian(f).
  [Steady States, Approximate Values, Trace of Jacobian(f)];
  [sol[2], evasol[2], evatr[2]];
  [sol[1], evasol[1], evatr[1]];
  [sol[3], evasol[3], evatr[3]];
```

[Steady States, Approximate Values, Trace of Jacobian(f)]

$$\left[\left[x_1 = \frac{7}{2} - \frac{\sqrt{205}}{6},\ x_2 = \frac{5}{2} + \frac{\sqrt{205}}{6},\ x_3 = \frac{12}{5} + \frac{\sqrt{205}}{6}\right],\ [x_1 = 1.1136,\ x_2 = 4.8864,\ x_3 = 4.7864],\ if\_tr = -815.74\right]$$

$$\left[\left[x_1=5,\ x_2=1,\ x_3=\frac{9}{10}\right],\ \left[x_1=5.,\ x_2=1.,\ x_3=0.90000\right],\ if\_tr=31.\right]$$

$$\left[\left[x_1=\frac{7}{2}+\frac{\sqrt{205}}{6},\ x_2=\frac{5}{2}-\frac{\sqrt{205}}{6},\ x_3=\frac{12}{5}-\frac{\sqrt{205}}{6}\right],\ \left[x_1=5.8864,\ x_2=0.1136,\ x_3=0.0136\right],\ if\_tr=-4.32\right] \quad (3)$$

```
>
>
> # ------------------------------------------------------
  # Row (7)
```

$\#\ X_1+2\,X_2+X_3 \rightarrow \qquad b_{21}X_2$

$\#\qquad 3\,X_3 \rightarrow b_{12}X_1+b_{22}X_2+b_{32}X_3$

$\#\ b_{21}=0$

```
>
```

> $unassign('b_{12}', 'b_{22}', 'b_{32}');$
> $a_{11}:=1:\ a_{21}:=2:\ a_{31}:=1:\ a_{12}:=0:\ a_{22}:=0:\ a_{32}:=3:$
> $b_{11}:=0:\ b_{21}:=0:\ b_{31}:=0:\ b_{12}:=b_{12}:\ b_{22}:=2\cdot b_{12}:\ b_{32}:=b_{12}+2:$
> $h_1(x_1,x_2,x_3);\ h_2(x_1,x_2);\ h_3(x_1,x_3);$

$$-9\,x_1\,x_2^2\,x_3+50\,x_3^3$$
$$-2\,x_1+x_2-6$$
$$-x_1+x_3-\frac{59}{10} \quad (4)$$

> # choose witness
> $lambda:=b_{12}:\ k_1:=1:k_2:=\frac{48}{b_{12}}:c_1:=\frac{13}{2}:c_2:=\frac{1}{4}:$
> $h_1(x_1,x_2,x_3);\ h_2(x_1,x_2);\ h_3(x_1,x_3);$

$$-x_1\,x_2^2\,x_3+48\,x_3^3$$
$$-2\,x_1+x_2-\frac{13}{2}$$
$$-x_1+x_3-\frac{1}{4} \quad (5)$$

> # 3 positive steady states
> # stable, if tr<0;
> $shsol:=solve(h_1(x_1, solve(h_2(x_1,x_2),x_2), solve(h_3(x_1,x_3),x_3)), x_1):$
> for n from 2 to 4 do
> $sol[n-1]:=[x_1=shsol[n],\ x_2=solve(h_2(shsol[n],x_2),x_2),\ x_3$

```
    = solve(h_3(shsol[n], x_3), x_3)];
evasol[n - 1] := evalf(sol[n - 1], 5);
evatr[n - 1] := if_tr = evalf(subs(sol[n - 1][1], sol[n - 1][2], sol[n - 1][3], tr),
    5);
end do:

# 1st column: Solutions; 2nd column: Approximate Values; 3rd column: Trace of
    Jacobian(f).
[Steady States, Approximate Values, Trace of Jacobian(f)];
[sol[2], evasol[2], evatr[2]];
[sol[1], evasol[1], evatr[1]];
[sol[3], evasol[3], evatr[3]];
```

$$[\mathit{Steady\ States},\ \mathit{Approximate\ Values},\ \mathit{Trace\ of\ Jacobian}(f)]$$

$$\left[\left[x_1=\frac{19}{8}-\frac{3\sqrt{33}}{8},\ x_2=\frac{45}{4}-\frac{3\sqrt{33}}{4},\ x_3=\frac{21}{8}-\frac{3\sqrt{33}}{8}\right],\ [x_1=0.2208,\ x_2=6.9416,\ x_3=0.4708],\ \mathit{if\_tr}=-4.293\right]$$

$$\left[\left[x_1=\frac{3}{4},\ x_2=8,\ x_3=1\right],\ [x_1=0.75000,\ x_2=8.,\ x_3=1.],\ \mathit{if\_tr}=8.\right]$$

$$\left[\left[x_1=\frac{19}{8}+\frac{3\sqrt{33}}{8},\ x_2=\frac{45}{4}+\frac{3\sqrt{33}}{4},\ x_3=\frac{21}{8}+\frac{3\sqrt{33}}{8}\right],\ [x_1=4.5292,\ x_2=15.558,\ x_3=4.7792],\ \mathit{if\_tr}=-311.1\right] \tag{6}$$

```
>
>
> # -----------------------------------------------------
# Row (7)

# X_1 + 2 X_2 + X_3 →           b_21 X_2
#             3 X_3 → b_12 X_1 + b_22 X_2 + b_32 X_3
# b_21 = 1
>
> unassign('b_12', 'b_22', 'b_32');
a_11 := 1 : a_21 := 2 : a_31 := 1 : a_12 := 0 : a_22 := 0 : a_32 := 3 :
b_11 := 0 : b_21 := 1 : b_31 := 0 : b_12 := b_12 : b_22 := b_12 : b_32 := b_12 + 2 :
h_1(x_1, x_2, x_3); h_2(x_1, x_2); h_3(x_1, x_3);
```

$$-x_1\ x_2^{\ 2}\ x_3+48\ x_3^{\ 3}$$

$$-x_1+x_2-\frac{13}{2}$$

$$-x_1+x_3-\frac{1}{4} \qquad (7)$$

```
> # choose witness
```

$lambda := b_{12} : k_1 := 1 : k_2 := \frac{12}{b_{12}} : c_1 := \frac{13}{4} : c_2 := \frac{1}{4} :$

$h_1(x_1, x_2, x_3); h_2(x_1, x_2); h_3(x_1, x_3);$

$$-x_1 x_2^2 x_3 + 12 x_3^3$$

$$-x_1+x_2-\frac{13}{4}$$

$$-x_1+x_3-\frac{1}{4} \qquad (8)$$

```
> # 3 positive steady states
# stable, if tr<0;
```

$shsol := solve(h_1(x_1, solve(h_2(x_1, x_2), x_2), solve(h_3(x_1, x_3), x_3)), x_1) :$

for n from 2 to 4 do

$sol[n-1] := [x_1 = shsol[n], x_2 = solve(h_2(shsol[n], x_2), x_2), x_3 = solve(h_3(shsol[n], x_3), x_3)];$

$evasol[n-1] := evalf(sol[n-1], 5);$

$evatr[n-1] := if\_tr = evalf(subs(sol[n-1][1], sol[n-1][2], sol[n-1][3], tr), 5);$

end do:

```
# 1st column: Solutions; 2nd column: Approximate Values; 3rd column: Trace of Jacobian(f).
```

[Steady States, Approximate Values, Trace of Jacobian(f)];

[sol[2], evasol[2], evatr[2]];

[sol[1], evasol[1], evatr[1]];

[sol[3], evasol[3], evatr[3]];

[Steady States, Approximate Values, Trace of Jacobian(f)]

$$\left[\left[x_1=\frac{19}{8}-\frac{3\sqrt{33}}{8}, x_2=\frac{45}{8}-\frac{3\sqrt{33}}{8}, x_3=\frac{21}{8}-\frac{3\sqrt{33}}{8}\right], [x_1=0.2208, x_2=3.4708, x_3=0.4708], if\_tr=-1.0733\right]$$

$$\left[\left[x_1=\frac{3}{4}, x_2=4, x_3=1\right], [x_1=0.75000, x_2=4., x_3=1.], if\_tr=2.\right]$$

$$\left[\left[x_1=\frac{19}{8}+\frac{3\sqrt{33}}{8}, x_2=\frac{45}{8}+\frac{3\sqrt{33}}{8}, x_3=\frac{21}{8}+\frac{3\sqrt{33}}{8}\right], [x_1=4.5292, x_2 \qquad (9)$$

$= 7.7792, \; x_3 = 4.7792 \,], \; if\_tr = -77.81 \,]$

>

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