```
> # Execute every statement in order
> restart :
>
> # for 2-species networks with 1 reversible reaction and 1 irreversible
    reaction, polynomials from the ODE system are:
```

$$f_1 := (b_{11} - a_{11}) \cdot k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} + (a_{11} - b_{11}) \cdot k_2 \cdot x_1^{b_{11}} \cdot x_2^{b_{21}} + (b_{12} - a_{12}) \cdot k_3 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} :$$

$$f_2 := (b_{21} - a_{21}) \cdot k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} + (a_{21} - b_{21}) \cdot k_2 \cdot x_1^{b_{11}} \cdot x_2^{b_{21}} + (b_{22} - a_{22}) \cdot k_3 \cdot x_1^{a_{12}} \cdot x_2^{a_{22}} :$$

```
> # if the network has one-dimensional sthoichiometric subspace, then the above
    two polynomials can be simplified:
  # K = lambda·k_3
```

$$f_1 := (b_{11} - a_{11}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} - k_2 \cdot x_1^{b_{11}} \cdot x_2^{b_{21}} - K \cdot x_1^{a_{12}} \cdot x_2^{a_{22}}\right) :$$

$$f_2 := (b_{21} - a_{21}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} - k_2 \cdot x_1^{b_{11}} \cdot x_2^{b_{21}} - K \cdot x_1^{a_{12}} \cdot x_2^{a_{22}}\right) :$$

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

$$h_1 := (b_{11} - a_{11}) \cdot \left(k_1 \cdot x_1^{a_{11}} \cdot x_2^{a_{21}} - k_2 \cdot x_1^{b_{11}} \cdot x_2^{b_{21}} - K \cdot x_1^{a_{12}} \cdot x_2^{a_{22}}\right) :$$

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

```
> g := subs(x_2 = solve(h_2, x_2), h_1) :
  tr := diff(f_1, x_1) + diff(f_2, x_2) :
> sol := [0, 0, 0] : evasol := [0, 0, 0] : evatr := [0, 0, 0] :
>
>
> # below, we show witness of multistability for networks in Rows (7) − (10)
    in Table 4 (see main manuscript)
> # ------------------------------
  # Row(7) [a_11, a_21, b_11, b_21, a_12, a_22] = [0, 1, 1, 0, 2, 1]

  co := [0, 1, 1, 0, 2, 1] : unassign('b_12', 'b_22') :
  a_11 := co[1] : a_21 := co[2] : b_11 := co[3] : b_21 := co[4] :
  a_12 := co[5] : a_22 := co[6] : b_12 := b_12 : b_22 := b_22 :
  h_1; h_2;
```

$$-K\, x_1^2\, x_2 + k_1\, x_2 - k_2\, x_1$$

$$-x_1 - x_2 - c_1 \qquad (1)$$

```
> # choose witness
```

$coepick := \left[c_1 = -9,\ k_1 = \frac{1}{2},\ k_2 = 16,\ K = -\frac{3}{2}\right]:$

$sh[1] := subs\left(coepick,\ h_1\right);$

$sh[2] := subs\left(coepick,\ h_2\right);$

$$sh_1 := \frac{3}{2}\ x_1^{\ 2}\ x_2 - 16\ x_1 + \frac{1}{2}\ x_2$$

$$sh_2 := -x_1 - x_2 + 9 \qquad (2)$$

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

$shsol := solve\left(subs\left(x_2 = solve\left(sh[2],\ x_2\right),\ sh[1]\right),\ x_1\right):$

for n **from** 1 **to** 3 **do**

$sol[n] := \left[x_1 = shsol[n],\ x_2 = subs\left(x_1 = shsol[n],\ solve\left(sh[2],\ x_2\right)\right)\right];$

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

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

end do:

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

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

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

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

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

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

$$\left[\left[x_1 = 4 - \sqrt{13},\ x_2 = 5 + \sqrt{13}\right],\ \left[x_1 = 0.3944,\ x_2 = 8.6056\right],\ if\_tr = -6.5513\right]$$

$$\left[\left[x_1 = 1,\ x_2 = 8\right],\ \left[x_1 = 1.,\ x_2 = 8.\right],\ if\_tr = 6.\right]$$

$$\left[\left[x_1 = 4 + \sqrt{13},\ x_2 = 5 - \sqrt{13}\right],\ \left[x_1 = 7.6056,\ x_2 = 1.3944\right],\ if\_tr = -71.453\right] \qquad (3)$$

```
>
>
> # --------------------------
```

> # $Row(8)$ $\left[a_{11},\ a_{21},\ b_{11},\ b_{21},\ a_{12},\ a_{22}\right] = [1,\ 0,\ 0,\ 2,\ 2,\ 1]$

$co := [1,\ 0,\ 0,\ 2,\ 2,\ 1]:\ unassign\left('b_{12}',\ 'b_{22}'\right):$

$a_{11} := co[1]:\ a_{21} := co[2]:\ b_{11} := co[3]:\ b_{21} := co[4]:$

$a_{12} := co[5]:\ a_{22} := co[6]:\ b_{12} := b_{12}:\ b_{22} := b_{22}:$

$h_1;\ h_2;$

$$K\,x_1^{\,2}\,x_2 + k_2\,x_2^{\,2} - k_1\,x_1$$
$$2\,x_1 + x_2 - c_1 \tag{4}$$

```
> # choose witness
```

$coepick := \left[c_1 = 6,\ k_1 = 16,\ k_2 = \frac{1}{8},\ K = \frac{7}{2}\right]:$

$sh[1] := subs(coepick,\ h_1);$

$sh[2] := subs(coepick,\ h_2);$

$$sh_1 := \frac{7}{2}\,x_1^{\,2}\,x_2 + \frac{1}{8}\,x_2^{\,2} - 16\,x_1$$
$$sh_2 := 2\,x_1 + x_2 - 6 \tag{5}$$

```
>
```

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

$shsol := solve(subs(x_2 = solve(sh[2],\ x_2),\ sh[1]),\ x_1):$

for n **from** 1 **to** 3 **do**

$sol[n] := [x_1 = shsol[n],\ x_2 = subs(x_1 = shsol[n],\ solve(sh[2],\ x_2))];$

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

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

end do:

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

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

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

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

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

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

$$\left[\left[x_1 = \frac{29}{28} - \frac{\sqrt{337}}{28},\ x_2 = \frac{55}{14} + \frac{\sqrt{337}}{14}\right],\ [x_1 = 0.38006,\ x_2 = 5.2399],\ if\_tr = -5.6906\right]$$

$$[[x_1 = 1,\ x_2 = 4],\ [x_1 = 1.,\ x_2 = 4.],\ if\_tr = 3.]$$

$$\left[\left[x_1 = \frac{29}{28} + \frac{\sqrt{337}}{28},\ x_2 = \frac{55}{14} - \frac{\sqrt{337}}{14}\right],\ [x_1 = 1.6913,\ x_2 = 2.6173],\ if\_tr = -6.3464\right] \tag{6}$$

```
>
>
> # -------------------------
```

```
> # Row(9) [a_11, a_21, b_11, b_21, a_12, a_22] = [1, 2, 0, 0, 2, 0]

  co := [1, 2, 0, 0, 2, 0] : unassign('b_12', 'b_22') :
  a_11 := co[1] : a_21 := co[2] : b_11 := co[3] : b_21 := co[4] :
  a_12 := co[5] : a_22 := co[6] : b_12 := b_12 : b_22 := b_22 :
  h_1; h_2;
```

$$-k_1\ x_1\ x_2^2 + K\ x_1^2 + k_2$$

$$-2\ x_1 + x_2 - c_1 \tag{7}$$

```
> # choose witness
  coepick := [c_1 = 6, k_1 = 1, k_2 = 1, K = 63] :
  sh[1] := subs(coepick, h_1);
  sh[2] := subs(coepick, h_2);
```

$$sh_1 := -x_1\ x_2^2 + 63\ x_1^2 + 1$$

$$sh_2 := -2\ x_1 + x_2 - 6 \tag{8}$$

```
>
> # 3 positive steady states
  # stable, if tr<0;
  shsol := solve(subs(x_2 = solve(sh[2], x_2), sh[1]), x_1) :
  for n from 1 to 3 do
  sol[n] := [x_1 = shsol[n], x_2 = subs(x_1 = shsol[n], solve(sh[2], x_2))];
  evasol[n] := evalf(sol[n], 5);
  evatr[n] := if_tr = evalf(subs(sol[n][1], sol[n][2], coepick, 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]];
```

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

$$\left[\left[x_1 = \frac{35}{8} - \frac{\sqrt{1209}}{8},\ x_2 = \frac{59}{4} - \frac{\sqrt{1209}}{4}\right],\ [x_1 = 0.0286,\ x_2 = 6.0572],\ if\_tr = -33.77\right]$$

$$[[x_1 = 1,\ x_2 = 8],\ [x_1 = 1.,\ x_2 = 8.],\ if\_tr = 30.]$$

$$\left[\left[x_1 = \frac{35}{8} + \frac{\sqrt{1209}}{8},\ x_2 = \frac{59}{4} + \frac{\sqrt{1209}}{4}\right],\ [x_1 = 8.7214,\ x_2 = 23.443],\ if\_tr \tag{9}$$

$= -268.51]$

>

>

> # --------------------------------

> # Row(10) $[a_{11}, a_{21}, b_{11}, b_{21}, a_{12}, a_{22}] = [1, 2, 0, 1, 2, 0]$

```
co := [1, 2, 0, 1, 2, 0] : unassign('b12', 'b22') :
a11 := co[1] : a21 := co[2] : b11 := co[3] : b21 := co[4] :
a12 := co[5] : a22 := co[6] : b12 := b12 : b22 := b22 :
h1; h2;
```

$$-k_1 x_1 x_2^2 + K x_1^2 + k_2 x_2$$
$$-x_1 + x_2 - c_1 \tag{10}$$

> # choose witness

```
coepick := [c1 = 3, k1 = 1, k2 = 1, K = 12] :
sh[1] := subs(coepick, h1);
sh[2] := subs(coepick, h2);
```

$$sh_1 := -x_1 x_2^2 + 12 x_1^2 + x_2$$
$$sh_2 := -x_1 + x_2 - 3 \tag{11}$$

>

> # 3 positive steady states

```
# stable, if tr<0;
shsol := solve(subs(x2 = solve(sh[2], x2), sh[1]), x1) :
for n from 1 to 3 do
sol[n] := [x1 = shsol[n], x2 = subs(x1 = shsol[n], solve(sh[2], x2))];
evasol[n] := evalf(sol[n], 5);
evatr[n] := if_tr = evalf(subs(sol[n][1], sol[n][2], coepick, 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*)]

$$\left[\left[x_1=\frac{5}{2}-\frac{\sqrt{13}}{2},\ x_2=\frac{11}{2}-\frac{\sqrt{13}}{2}\right],\ \left[x_1=0.6972,\ x_2=3.6972\right],\ if\_tr=-1.091\right]$$

$$\left[\left[x_1=1,\ x_2=4\right],\ \left[x_1=1.,\ x_2=4.\right],\ if\_tr=1.\right]$$

$$\left[\left[x_1=\frac{5}{2}+\frac{\sqrt{13}}{2},\ x_2=\frac{11}{2}+\frac{\sqrt{13}}{2}\right],\ \left[x_1=4.3028,\ x_2=7.3028\right],\ if\_tr=-11.913\right] \tag{12}$$

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