Bistable motif: parameter sampling

Finding the condition of multistationarity

Analysis of solutions and bifurcation analysis

In[1]:=
```
ClearAll["Global`*"];
A = Table[0, {11}, {6}];
A[[1]][[1]] = -1;
A[[1]][[3]] = -1;
A[[1]][[5]] = 1;
A[[2]] = -A[[1]];
A[[3]][[3]] = 1; A[[3]][[2]] = 1; A[[3]][[5]] = -1;
A[[4]][[1]] = -1;
A[[4]][[4]] = -1;
A[[4]][[6]] = 1;
A[[5]] = -A[[4]];
A[[6]][[4]] = 1;
A[[6]][[2]] = 1;
A[[6]][[6]] = -1;
A[[7]][[2]] = -1;
A[[7]][[1]] = 1;
A[[8]][[3]] = -1; A[[8]][[4]] = 1; A[[9]] = -A[[8]];
A[[10]][[5]] = -1; A[[10]][[6]] = 1; A[[11]] = -A[[10]];
stoiM = Transpose[A];
(* Now we construct the rate vector *)
ks = {k[1] × x[3] × x[1], k[2] × x[5], k[3] × x[5], k[4] × x[4] × x[1], k[5] × x[6],
   k[6] × x[6], k[7] × x[2], k[8] × x[3], k[9] × x[4], k[10] × x[5], k[11] × x[6]};
ssEqns = stoiM.ks;
mC = RowReduce[NullSpace[A]];
cons = {x[1] + x[2] + x[5] + x[6] - T[1], x[3] + x[4] + x[5] + x[6] - T[2]};
```

The parameters used

In[14]:=
```
pars1076 = {k[1] → 86.77935589, k[2] → 3.583044479, k[3] → 92.84145445,
    k[4] → 1.199993478, k[5] → 0.026263635, k[6] → 0.264415792, k[7] → 2.357404008,
    k[8] → 0.013100928, k[9] → 0.784202374, k[10] → 1.041346611,
    k[11] → 0.008056722, T[1] → 9.993526721(*,T[2]→2.113066106*)};
```

In[15]:=
```
(*k[1]=86.77935589;
k[2]=3.583044479;
k[3]=92.84145445;
k[4]=1.199993478;
k[5]=0.026263635;
k[6]=0.264415792;
k[7]=2.357404008;
k[8]=0.013100928;
k[9]=0.784202374;
k[10]=1.041346611;
k[11]=0.008056722;T[1]=9.993526721;T[2]=2.113066106;*)
k[1] = 86.77935589;
k[2] = 3.583044479;
k[3] = 92.84145445;
k[4] = 1.199993478;
k[5] = 0.026263635;
k[6] = 0.264415792;
k[7] = 2.357404008;
k[8] = 0.013100928;
k[9] = 0.784202374;
k[10] = 1.041346611;
k[11] = 0.008056722;
T[1] = 9.993526721;(*T[2]=2.113066106;*)
```

In[18]:=
```
ssEqns
```

Out[18]=
```
{2.3574 x[2] - 86.7794 x[1] x[3] - 1.19999 x[1] x[4] + 3.58304 x[5] + 0.0262636 x[6],
 -2.3574 x[2] + 92.8415 x[5] + 0.264416 x[6],
 -0.0131009 x[3] - 86.7794 x[1] x[3] + 0.784202 x[4] + 96.4245 x[5],
 0.0131009 x[3] - 0.784202 x[4] - 1.19999 x[1] x[4] + 0.290679 x[6],
 86.7794 x[1] x[3] - 97.4658 x[5] + 0.00805672 x[6],
 1.19999 x[1] x[4] + 1.04135 x[5] - 0.298736 x[6]}
```

Bifurcation analysis

Quantify the fluxes

Quantify the fluxes more

In[79]:=
```
(*k[1]=86.77935589;
k[2]=3.583044479;
k[3]=92.84145445;
k[4]=1.199993478;
k[5]=0.026263635;
k[6]=0.264415792;
k[7]=2.357404008;
k[8]=0.013100928;
k[9]=0.784202374;
k[10]=1.041346611;
k[11]=0.008056722;T[1]=9.993526721;T[2]=2.113066106;*)
k[1] = 86.77935589;
k[2] = 3.583044479;
k[3] = 92.84145445;
k[4] = 1.199993478;
k[5] = 0.026263635;
k[6] = 0.264415792;
k[7] = 2.357404008;
k[8] = 0.013100928;
k[9] = 0.784202374;
k[10] = 1.041346611;
k[11] = 0.008056722;
T[1] = 9.993526721;
(*T[2]=2.113066106;*)
```

In[82]:=
```
ssEqns
```

Out[82]=
$$\{2.3574\, x[2] - 86.7794\, x[1]\, x[3] - 1.19999\, x[1]\, x[4] + 3.58304\, x[5] + 0.0262636\, x[6],\\ -2.3574\, x[2] + 92.8415\, x[5] + 0.264416\, x[6],\\ -0.0131009\, x[3] - 86.7794\, x[1]\, x[3] + 0.784202\, x[4] + 96.4245\, x[5],\\ 0.0131009\, x[3] - 0.784202\, x[4] - 1.19999\, x[1]\, x[4] + 0.290679\, x[6],\\ 86.7794\, x[1]\, x[3] - 97.4658\, x[5] + 0.00805672\, x[6],\\ 1.19999\, x[1]\, x[4] + 1.04135\, x[5] - 0.298736\, x[6]\}$$

In[83]:=
```
sol1 = Solve[{ssEqns[[2]], ssEqns[[4]], ssEqns[[5]], ssEqns[[6]], cons[[1]]} == 0,
  {x[2], x[3], x[4], x[5], x[6]}]
```

Out[83]=
$$\left\{\left\{x[2] \to -\frac{0.292618\, \left(-178.797 + 7.89776\, x[1] + 1.\, x[1]^2\right)}{5.83555 + 1.\, x[1]},\right.\right.\\ x[3] \to -\frac{0.0060345\, \left(-244.702 + 14.4925\, x[1] + 1.\, x[1]^2\right)}{x[1]\, (5.83555 + 1.\, x[1])},\\ x[4] \to -\frac{0.170037\, \left(-0.145081 - 9.97901\, x[1] + 1.\, x[1]^2\right)}{x[1]\, (5.83555 + 1.\, x[1])},\\ x[5] \to -\frac{0.00543088\, \left(-242.159 + 14.238\, x[1] + 1.\, x[1]^2\right)}{5.83555 + 1.\, x[1]},\\ \left.\left.x[6] \to -\frac{0.701952\, \left(-6.67203 - 9.32589\, x[1] + 1.\, x[1]^2\right)}{5.83555 + 1.\, x[1]}\right\}\right\}$$

In[84]:=
```
poly1 = Numerator[Simplify[cons[[2]] /. sol1[[1]]]]
```

Out[84]=
$$1.50132 + (7.60792 - 5.83555\, T[2])\, x[1] + (6.29293 - 1.\, T[2])\, x[1]^2 - 0.707382\, x[1]^3$$

In[85]:=
```
polx1 = poly1 == 0 /. pars1076
```

Out[85]=
$$1.50132 + (7.60792 - 5.83555\, T[2])\, x[1] + (6.29293 - 1.\, T[2])\, x[1]^2 - 0.707382\, x[1]^3 == 0$$

In[88]:=
```
samplePoints =
 InputForm[Table[x[1] /. NSolve[{polx1} /. {T[2] → T2}, {x[1]}, Reals],
   {T2, {0.5, 1.0, 2.0, 2.2, 2.5, 3.0}}]]
```

Out[88]//InputForm=
```
{{8.956020038735588}, {7.836689628835086}, {5.006030442249345}, {0.40828702985109944, 1
  4.114272347979874}, {0.24657391714178972}, {0.15987931498014402}}
```

In[89]:=
```
x1s = {8.956020038735588, 7.836689628835086,
   5.006030442249345, 4.114272347979874, 1.263458691724523,
   0.40828702985109944, 0.24657391714178972, 0.15987931498014402}
```

Out[89]= {8.95602, 7.83669, 5.00603, 4.11427, 1.26346, 0.408287, 0.246574, 0.159879}

In[90]:=
```
x2 = x[2] /. sol1[[1]]
```

Out[90]=
$$-\frac{0.292618\left(-178.797+7.89776\,x[1]+1.\,x[1]^2\right)}{5.83555+1.\,x[1]}$$

In[91]:=
```
x2s = Table[x2 /. {x[1] → x1}, {x1, x1s}]
```

Out[91]= {0.551033, 1.18764, 3.0823, 3.80487, 6.89282, 8.2204, 8.5055, 8.66363}

In[92]:=
```
x3 = x[3] /. sol1[[1]]; x3s = Table[x3 /. {x[1] → x1}, {x1, x1s}]
```

Out[92]= {0.0015805, 0.0039264, 0.0163547,
 0.0247871, 0.151241, 0.564842, 0.970013, 1.52577}

In[93]:=
```
x4 = x[4] /. sol1[[1]]; x4s = Table[x4 /. {x[1] → x1}, {x1, x1s}]
```

Out[93]= {0.011946, 0.0268735, 0.0784495, 0.100828, 0.211507, 0.270314, 0.288537, 0.304217}

In[94]:=
```
x5 = x[5] /. sol1[[1]]; x5s = Table[x5 /. {x[1] → x1}, {x1, x1s}]
```

Out[94]= {0.0126422, 0.0274741, 0.0730469,
 0.0909633, 0.170273, 0.205428, 0.21304, 0.217271}

In[95]:=
```
x6 = x[6] /. sol1[[1]]; x6s = Table[x6 /. {x[1] → x1}, {x1, x1s}]
```

Out[95]= {0.473831, 0.941726, 1.83215, 1.98342, 1.66698, 1.15942, 1.02841, 0.952746}

In[96]:=
```
xValues = {x1s, x2s, x3s, x4s, x5s, x6s}
```

Out[96]= {{8.95602, 7.83669, 5.00603, 4.11427, 1.26346, 0.408287, 0.246574, 0.159879},
 {0.551033, 1.18764, 3.0823, 3.80487, 6.89282, 8.2204, 8.5055, 8.66363},
 {0.0015805, 0.0039264, 0.0163547, 0.0247871, 0.151241, 0.564842,
  0.970013, 1.52577}, {0.011946, 0.0268735, 0.0784495, 0.100828,
  0.211507, 0.270314, 0.288537, 0.304217}, {0.0126422, 0.0274741,
  0.0730469, 0.0909633, 0.170273, 0.205428, 0.21304, 0.217271},
 {0.473831, 0.941726, 1.83215, 1.98342, 1.66698, 1.15942, 1.02841, 0.952746}}

In[97]:=
```
xValuesT = Transpose[{x1s, x2s, x3s, x4s, x5s, x6s}]
```

Out[97]= {{8.95602, 0.551033, 0.0015805, 0.011946, 0.0126422, 0.473831},
 {7.83669, 1.18764, 0.0039264, 0.0268735, 0.0274741, 0.941726},
 {5.00603, 3.0823, 0.0163547, 0.0784495, 0.0730469, 1.83215},
 {4.11427, 3.80487, 0.0247871, 0.100828, 0.0909633, 1.98342},
 {1.26346, 6.89282, 0.151241, 0.211507, 0.170273, 1.66698},
 {0.408287, 8.2204, 0.564842, 0.270314, 0.205428, 1.15942},
 {0.246574, 8.5055, 0.970013, 0.288537, 0.21304, 1.02841},
 {0.159879, 8.66363, 1.52577, 0.304217, 0.217271, 0.952746}}

In[98]:=
```
kValues = {k[1] → 86.77935589, k[2] → 3.583044479,
    k[3] → 92.84145445, k[4] → 1.199993478, k[5] → 0.026263635,
    k[6] → 0.264415792, k[7] → 2.357404008, k[8] → 0.013100928,
    k[9] → 0.784202374, k[10] → 1.041346611, k[11] → 0.008056722};
```

In[100]:=
```
ksValuesT = Table[
  ks /. Flatten[{kValues, {x[1] → xValues[[1]][[p]], x[2] → xValues[[2]][[p]],
      x[3] → xValues[[3]][[p]], x[4] → xValues[[4]][[p]],
      x[5] → xValues[[5]][[p]], x[6] → xValues[[6]][[p]]}}], {p, 1, 8}]
```

Out[100]=
```
{{1.22836, 0.0452975, 1.17372, 0.128386, 0.0124445, 0.125288,
  1.29901, 0.0000207061, 0.00936808, 0.0131649, 0.00381753},
 {2.6702, 0.0984408, 2.55073, 0.252718, 0.0247331, 0.249007,
  2.79974, 0.0000514394, 0.0210742, 0.02861, 0.00758722},
 {7.10481, 0.26173, 6.78178, 0.471262, 0.0481189, 0.484449,
  7.26623, 0.000214262, 0.0615203, 0.0760671, 0.0147611},
 {8.84984, 0.325926, 8.44517, 0.497796, 0.0520919, 0.524448,
  8.96961, 0.000324734, 0.0790692, 0.0947243, 0.0159799},
 {16.5824, 0.610095, 15.8084, 0.320674, 0.043781, 0.440776,
  16.2492, 0.00198139, 0.165864, 0.177313, 0.0134304},
 {20.0129, 0.736057, 19.0722, 0.132438, 0.0304505, 0.306568,
  19.3788, 0.00739996, 0.211981, 0.213922, 0.00934109},
 {20.7559, 0.763333, 19.779, 0.0853743, 0.0270098, 0.271928,
  20.0509, 0.0127081, 0.226271, 0.221849, 0.00828561},
 {21.1688, 0.778492, 20.1718, 0.0583652, 0.0250226, 0.251921,
  20.4237, 0.019989, 0.238567, 0.226254, 0.00767601}}
```

In[101]:=
```
ksValues = Transpose[ksValuesT]
```

Out[101]=
```
{{1.22836, 2.6702, 7.10481, 8.84984, 16.5824, 20.0129, 20.7559, 21.1688},
 {0.0452975, 0.0984408, 0.26173, 0.325926,
  0.610095, 0.736057, 0.763333, 0.778492},
 {1.17372, 2.55073, 6.78178, 8.44517, 15.8084, 19.0722, 19.779, 20.1718},
 {0.128386, 0.252718, 0.471262, 0.497796, 0.320674, 0.132438,
  0.0853743, 0.0583652}, {0.0124445, 0.0247331, 0.0481189,
  0.0520919, 0.043781, 0.0304505, 0.0270098, 0.0250226},
 {0.125288, 0.249007, 0.484449, 0.524448, 0.440776, 0.306568, 0.271928, 0.251921},
 {1.29901, 2.79974, 7.26623, 8.96961, 16.2492, 19.3788, 20.0509, 20.4237},
 {0.0000207061, 0.0000514394, 0.000214262, 0.000324734, 0.00198139,
  0.00739996, 0.0127081, 0.019989}, {0.00936808, 0.0210742,
  0.0615203, 0.0790692, 0.165864, 0.211981, 0.226271, 0.238567},
 {0.0131649, 0.02861, 0.0760671, 0.0947243, 0.177313, 0.213922,
  0.221849, 0.226254}, {0.00381753, 0.00758722, 0.0147611,
  0.0159799, 0.0134304, 0.00934109, 0.00828561, 0.00767601}}
```

In[102]:=
```
fluxesT = Transpose[{ksValues[[1]] - ksValues[[2]], ksValues[[3]],
    ksValues[[4]] - ksValues[[5]], ksValues[[6]], ksValues[[7]],
    ksValues[[8]] - ksValues[[9]], ksValues[[10]] - ksValues[[11]]}]
```

Out[102]=
```
{{1.18307, 1.17372, 0.115941, 0.125288, 1.29901, -0.00934738, 0.00934738},
 {2.57176, 2.55073, 0.227984, 0.249007, 2.79974, -0.0210228, 0.0210228},
 {6.84308, 6.78178, 0.423143, 0.484449, 7.26623, -0.061306, 0.061306},
 {8.52391, 8.44517, 0.445704, 0.524448, 8.96961, -0.0787444, 0.0787444},
 {15.9723, 15.8084, 0.276893, 0.440776, 16.2492, -0.163883, 0.163883},
 {19.2768, 19.0722, 0.101987, 0.306568, 19.3788, -0.204581, 0.204581},
 {19.9925, 19.779, 0.0583646, 0.271928, 20.0509, -0.213563, 0.213563},
 {20.3903, 20.1718, 0.0333426, 0.251921, 20.4237, -0.218578, 0.218578}}
```