Structural identifiability of reaction-diffusion processes in mathematical biology

Chemotaxis model

In[ ]:=
```
(* Define equations*)
sys1 = {
    D[ρ[x, t], t] - (Dρ * D[ρ[x, t], {x, 2}] -
        χ D[c[x, t], {x, 2}] * ρ[x, t] - χ D[c[x, t], x] * D[ρ[x, t], x]),
    D[c[x, t], t] - (Dc * D[c[x, t], {x, 2}] - k * c[x, t] + α * ρ[x, t])
   };
```

In[ ]:=
```
(* Obtain parameters in the above expression *)
params = Quiet[Complement[Variables[sys1], Join[{ρ[x, t], c[x, t]},
     Select[Variables[sys1], #[[0]][[1]] === ρ || #[[0]][[1]] === c &]]]]
```

Out[ ]=

$$\{\mathrm{Dc},\ \mathrm{D}\rho,\ k,\ \alpha,\ \chi\}$$

In[ ]:=
```
(* Eliminate second derivatives from second equation *)
```

In[ ]:=
```
sys2 = {
   sys1[[1]],
   Expand[sys1[[1]] * Coefficient[sys1[[2]], D[c[x, t], {x, 2}]] -
     sys1[[2]] * Coefficient[sys1[[1]], D[c[x, t], {x, 2}]]]
  }
```

Out[ ]=

$$\left\{\rho^{(0,1)}[x,t]+\chi\, c^{(1,0)}[x,t]\, \rho^{(1,0)}[x,t]+\chi\, \rho[x,t]\, c^{(2,0)}[x,t]-\mathrm{D}\rho\, \rho^{(2,0)}[x,t],\right.$$
$$-k\,\chi\, c[x,t]\times\rho[x,t]+\alpha\,\chi\,\rho[x,t]^2-\chi\,\rho[x,t]\, c^{(0,1)}[x,t]-$$
$$\left.\mathrm{Dc}\,\rho^{(0,1)}[x,t]-\mathrm{Dc}\,\chi\, c^{(1,0)}[x,t]\,\rho^{(1,0)}[x,t]+\mathrm{Dc}\,\mathrm{D}\rho\,\rho^{(2,0)}[x,t]\right\}$$

In[ ]:=
```
(* Expand the system to the appropriate order *)
sys3 = Join[
    Catenate[Table[Table[D[sys2[[1]], {x, i}, {t, m - i}], {i, 0, m}], {m, 0, 2}]],
    Catenate[Table[Table[D[sys2[[2]], {x, i}, {t, m - i}], {i, 0, m}], {m, 0, 3}]]
   ];
cvars = Join[{c[x, t]}, Quiet[Select[Variables[sys3], #[[0]][[1]] === c &]]]
```

Out[ ]=

$$\{c[x,t],\ c^{(0,1)}[x,t],\ c^{(0,2)}[x,t],\ c^{(0,3)}[x,t],\ c^{(0,4)}[x,t],$$
$$c^{(1,0)}[x,t],\ c^{(1,1)}[x,t],\ c^{(1,2)}[x,t],\ c^{(1,3)}[x,t],\ c^{(2,0)}[x,t],$$
$$c^{(2,1)}[x,t],\ c^{(2,2)}[x,t],\ c^{(3,0)}[x,t],\ c^{(3,1)}[x,t],\ c^{(4,0)}[x,t]\}$$

In[ ]:=
```
(* Convert the system to matrix form *)
A1 = Table[Coefficient[Expand[expr], var], {expr, sys3}, {var, cvars}];
B1 = Table[Table[0, {i, 1, Length[cvars]}] /.
     CoefficientRules[expr, cvars], {expr, sys3}];
M1 = Transpose[Insert[Transpose[A1], B1, Length[cvars] + 1]];
```

In[ ]:=
```
(* Number of polynomial expressions that we expected *)
MatrixRank[M1] - MatrixRank[A1]
```

Out[ ]=
```
1
```

In[ ]:=
```
(* Obtain expression *)
```

In[ ]:=
```
R1 = Quiet[UpperTriangularize[LUDecomposition[M1]〚1〛]];
expr1 = R1〚-1, -1〛
```

Out[ ]=

$$4\,\alpha\,\chi\,\rho^{(1,0)}[x,t]\,\rho^{(1,1)}[x,t] + 2\,\alpha\,\chi\,\rho^{(0,1)}[x,t]\,\rho^{(2,0)}[x,t] + \cdots 20 \cdots + \frac{\left(3\,\chi\,\rho^{\cdots 1 \cdots}[x,t] - \cdots 1 \cdots\right)\left(\cdots 1 \cdots\right)\left(\cdots 1 \cdots\right)}{\chi \cdots 1 \cdots \left(\cdots 1 \cdots + \cdots 1 \cdots - \frac{\cdots 1 \cdots}{\cdots 1 \cdots}\right)} + \mathrm{Dc}\,\mathrm{D}\rho\,\rho^{(4,1)}[x,t] - \frac{\mathrm{Dc}\,\rho^{(1,0)}[x,t]\left(6\,\alpha\,\chi\,\rho^{(1,0)}[x,t]\,\rho^{(2,0)}[x,t] + \cdots 14 \cdots + \mathrm{Dc}\,\mathrm{D}\rho\,\rho^{(5,0)}[x,t]\right)}{\rho[x,t]}$$

Full expression not available (original memory size: 0.3 MB)

In[ ]:=
```
expr2 = Numerator[Together[expr1]];
```

In[ ]:=
```
(* Obtain coefficients *)
ρvars = Join[{ρ[x, t]}, Quiet[Select[Variables[sys3], #〚0〛〚1〛 === ρ &]]];
coef1 = Values@CoefficientRules[expr2, ρvars];
```

In[ ]:=
```
(* Normalise to ensure uniqueness *)
```

In[ ]:=
```
coef2 = coef1 / coef1〚17〛
```

Out[ ]=

$$\{-k\,\alpha\chi,\ -\alpha\chi,\ \alpha\chi,\ Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ Dc\,\alpha\chi,\ k\,\alpha\chi,\ \alpha\chi,\ -2\,\alpha\chi,\ -k^2,\ k,\ Dc\,\alpha\chi,\ Dc\,k^2,$$
$$-Dc\,k,\ -\alpha\chi,\ -2\,k,\ 1,\ 2\,Dc\,k,\ -Dc,\ -1,\ Dc,\ -k\,\alpha\chi,\ \alpha\chi,\ Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ -3\,\alpha\chi,$$
$$5\,Dc\,\alpha\chi,\ -5\,Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ Dc^2\,\alpha\chi,\ -2\,Dc^2\,\alpha\chi,\ 4\,Dc\,\alpha\chi,\ D\rho\,k^2,\ Dc\,k+2\,D\rho\,k,\ Dc+D\rho,$$
$$-Dc\,D\rho\,k,\ -Dc\,D\rho,\ -D\rho\,k,\ -Dc-D\rho,\ Dc\,D\rho,\ Dc^2\,\alpha\chi,\ -Dc\,D\rho\,k^2,\ Dc\,D\rho\,k,\ -Dc^2\,k-2\,Dc\,D\rho\,k,$$
$$Dc^2+Dc\,D\rho,\ -Dc^2-Dc\,D\rho,\ Dc^2\,D\rho\,k,\ Dc^2\,D\rho,\ -Dc^2\,D\rho,\ 2\,\alpha\chi,\ k^2,\ -1,\ -Dc\,k,\ Dc,\ k,\ 1,$$
$$-2\,Dc,\ 1,\ k\,\alpha\chi,\ 3\,\alpha\chi,\ -3\,Dc\,\alpha\chi,\ -8\,Dc\,\alpha\chi,\ -5\,Dc\,k^2-D\rho\,k^2,\ 3\,Dc\,k-2\,D\rho\,k,\ -Dc-D\rho,$$
$$Dc^2\,k+Dc\,D\rho\,k,\ Dc\,D\rho,\ Dc\,k,\ -2\,Dc,\ -Dc\,D\rho,\ 3\,Dc+D\rho,\ 4\,Dc^2\,k+Dc\,D\rho\,k,\ -3\,Dc^2-Dc\,D\rho,$$
$$3\,Dc^2+Dc\,D\rho,\ -1,\ -\alpha\chi,\ -10\,Dc\,k+D\rho\,k,\ 5\,Dc+D\rho,\ Dc^2-Dc\,D\rho,\ Dc-D\rho,\ 4\,Dc^2+Dc\,D\rho,$$
$$-5\,Dc,\ -Dc\,k\,\alpha\chi,\ 8\,Dc\,\alpha\chi,\ Dc^2\,\alpha\chi,\ -21\,Dc\,\alpha\chi,\ 5\,Dc^2\,\alpha\chi,\ -Dc\,k,\ Dc,\ Dc^2\,k+Dc\,D\rho\,k,$$
$$-3\,Dc^2+Dc\,D\rho,\ Dc^2\,D\rho,\ Dc^2-2\,Dc\,D\rho,\ -10\,Dc^2\,\alpha\chi,\ 5\,Dc\,D\rho\,k^2,\ 5\,Dc^2\,k+6\,Dc\,D\rho\,k,$$
$$5\,Dc^2+5\,Dc\,D\rho,\ -6\,Dc^2\,D\rho\,k,\ -5\,Dc^2\,D\rho,\ -4\,Dc^2-4\,Dc\,D\rho,\ -Dc^3+3\,Dc^2\,D\rho,\ -Dc^2\,D\rho\,k,$$
$$Dc^3+Dc^2\,D\rho,\ -Dc^3\,D\rho,\ Dc^3\,D\rho,\ -Dc,\ Dc\,D\rho,\ -Dc\,D\rho\,k,\ -4\,Dc^2+2\,Dc\,D\rho,\ 4\,Dc^2\,D\rho,$$
$$Dc^3,\ -3\,Dc\,D\rho,\ -4\,Dc^2\,D\rho\,k,\ 3\,Dc^2\,D\rho,\ -Dc^3-7\,Dc^2\,D\rho,\ Dc^3\,D\rho,\ -Dc^3\,D\rho,\ Dc,\ 5\,Dc\,k,$$
$$-2\,Dc,\ -Dc^2+Dc\,D\rho,\ -4\,Dc,\ -4\,Dc^2-Dc\,D\rho,\ 7\,Dc,\ 12\,Dc\,\alpha\chi,\ 4\,Dc\,k^2,\ -3\,Dc\,k,\ -3\,Dc,$$
$$-12\,Dc^2\,k-Dc\,D\rho\,k,\ 5\,Dc^2-Dc\,D\rho,\ -Dc^2\,D\rho,\ 3\,Dc,\ 3\,Dc^2+Dc\,D\rho,\ -25\,Dc^2\,k-5\,Dc\,D\rho\,k,$$
$$-4\,Dc\,D\rho,\ 3\,Dc^3-2\,Dc^2\,D\rho,\ -6\,Dc^3-Dc^2\,D\rho,\ 12\,Dc^2+4\,Dc\,D\rho,\ 3\,Dc^3+4\,Dc^2\,D\rho,$$
$$8\,Dc\,k,\ -6\,Dc,\ -12\,Dc^2+2\,Dc\,D\rho,\ -25\,Dc^2-2\,Dc\,D\rho,\ 4\,Dc,\ 4\,Dc\,k\,\alpha\chi,\ 8\,Dc\,\alpha\chi,$$
$$-20\,Dc^2\,\alpha\chi,\ 16\,Dc^2\,\alpha\chi,\ -4\,Dc\,D\rho\,k^2,\ -4\,Dc^2\,k-8\,Dc\,D\rho\,k,\ -4\,Dc^2-4\,Dc\,D\rho,\ 4\,Dc^2\,D\rho\,k,$$
$$4\,Dc^2\,D\rho,\ -5\,Dc^2\,k+4\,Dc\,D\rho\,k,\ 18\,Dc^2+4\,Dc\,D\rho,\ 2\,Dc^3-10\,Dc^2\,D\rho,\ -5\,Dc^2+4\,Dc\,D\rho,$$
$$17\,Dc^2\,D\rho\,k,\ -5\,Dc^3+Dc^2\,D\rho,\ 5\,Dc^3\,D\rho,\ 6\,Dc^3+4\,Dc^2\,D\rho,\ -8\,Dc^3\,D\rho,\ 13\,Dc^2-4\,Dc\,D\rho,$$
$$-13\,Dc^3-15\,Dc^2\,D\rho,\ 25\,Dc^2\,D\rho\,k,\ 10\,Dc^3+28\,Dc^2\,D\rho,\ -13\,Dc^3\,D\rho,\ 19\,Dc^3\,D\rho,$$
$$-12\,Dc^2\,D\rho,\ -3\,Dc^3\,D\rho,\ -2\,Dc,\ -4\,Dc\,k,\ 6\,Dc,\ 6\,Dc^2-2\,Dc\,D\rho,\ 16\,Dc^2+2\,Dc\,D\rho,\ -4\,Dc,$$
$$-4\,Dc\,\alpha\chi,\ 68\,Dc^2\,k+4\,Dc\,D\rho\,k,\ -10\,Dc^2+4\,Dc\,D\rho,\ -4\,Dc^3+6\,Dc^2\,D\rho,\ -62\,Dc^2-4\,Dc\,D\rho,$$
$$28\,Dc^3+10\,Dc^2\,D\rho,\ -30\,Dc^3-16\,Dc^2\,D\rho,\ 68\,Dc^2,\ 44\,Dc^2\,\alpha\chi,\ 4\,Dc^2\,k,\ 4\,Dc^2,\ -4\,Dc^2\,D\rho\,k,$$
$$4\,Dc^3-4\,Dc^2\,D\rho,\ -4\,Dc^3\,D\rho,\ -22\,Dc^2,\ -2\,Dc^3+22\,Dc^2\,D\rho,\ -68\,Dc^2\,D\rho\,k,\ -26\,Dc^3-64\,Dc^2\,D\rho,$$
$$30\,Dc^3\,D\rho,\ 2\,Dc^3\,D\rho,\ 30\,Dc^3+46\,Dc^2\,D\rho,\ -58\,Dc^3\,D\rho,\ 30\,Dc^3\,D\rho,\ -18\,Dc^2,\ -36\,Dc^2\,k,$$
$$54\,Dc^2,\ -12\,Dc^3-18\,Dc^2\,D\rho,\ 18\,Dc^3+18\,Dc^2\,D\rho,\ -36\,Dc^2,\ -36\,Dc^2\,\alpha\chi,\ 36\,Dc^2\,D\rho\,k,$$
$$12\,Dc^3+36\,Dc^2\,D\rho,\ -12\,Dc^3\,D\rho,\ -18\,Dc^3-36\,Dc^2\,D\rho,\ 30\,Dc^3\,D\rho,\ -18\,Dc^3\,D\rho\}$$

In[ ]:=
```
(* CLearly, Dρ, Dc, and k are identifiable. Check expresions involving α *)
coef3 = Select[coef2, MemberQ[Variables[#], α] &]
```

Out[ ]=

$$\{-k\,\alpha\chi,\ -\alpha\chi,\ \alpha\chi,\ Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ Dc\,\alpha\chi,\ k\,\alpha\chi,\ \alpha\chi,\ -2\,\alpha\chi,\ Dc\,\alpha\chi,\ -\alpha\chi,$$
$$-k\,\alpha\chi,\ \alpha\chi,\ Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ -3\,\alpha\chi,\ 5\,Dc\,\alpha\chi,\ -5\,Dc\,k\,\alpha\chi,\ -Dc\,\alpha\chi,\ Dc^2\,\alpha\chi,$$
$$-2\,Dc^2\,\alpha\chi,\ 4\,Dc\,\alpha\chi,\ Dc^2\,\alpha\chi,\ 2\,\alpha\chi,\ k\,\alpha\chi,\ 3\,\alpha\chi,\ -3\,Dc\,\alpha\chi,\ -8\,Dc\,\alpha\chi,\ -\alpha\chi,$$
$$-Dc\,k\,\alpha\chi,\ 8\,Dc\,\alpha\chi,\ Dc^2\,\alpha\chi,\ -21\,Dc\,\alpha\chi,\ 5\,Dc^2\,\alpha\chi,\ -10\,Dc^2\,\alpha\chi,\ 12\,Dc\,\alpha\chi,$$
$$4\,Dc\,k\,\alpha\chi,\ 8\,Dc\,\alpha\chi,\ -20\,Dc^2\,\alpha\chi,\ 16\,Dc^2\,\alpha\chi,\ -4\,Dc\,\alpha\chi,\ 44\,Dc^2\,\alpha\chi,\ -36\,Dc^2\,\alpha\chi\}$$

In[ ]:=
```
Variables[coef3 / (α χ)]
```

Out[ ]=

$$\{Dc,\ k\}$$

In[ ]:=
```
(* Therefore, combination αχ is identifiable,
but individually parameters are not *)
```