Structural identifiability of reaction-diffusion processes in mathematical biology

Three-state logistic FUCCI model of cell migration

In[5]:=
```
(* Define equations*)
sys1 = {
    D[r[x, t], t] -
     (D1 * D[r[x, t], {x, 2}] - λ1 * r[x, t] + 2 λ3 g[x, t] * (1 - n[x, t] / K)),
    D[y[x, t], t] - (D2 * D[y[x, t], {x, 2}] + λ1 * r[x, t] - λ2 y[x, t] ),
    D[g[x, t], t] -
     (D3 * D[g[x, t], {x, 2}] + λ2 y[x, t] - λ3 g[x, t] * (1 - n[x, t] / K))
   } /. n[x, t] → r[x, t] + y[x, t] + g[x, t];
```

In[6]:=
```
(* Obtain parameters in the above expression *)
params = Quiet[Complement[Variables[sys1], Join[{r[x, t], y[x, t], g[x, t]},
    Select[Variables[sys1], #[[0]][[1]] === r || #[[0]][[1]] === y || #[[0]][[1]] === g &]]]]
```

Out[6]= {D1, D2, D3, K, λ1, λ2, λ3}

In[7]:=
```
(* Solve for y *)
```

In[8]:=
```
sol1 = FullSimplify[Solve[sys1[[3]] == 0, y[x, t]][[1]]]
```

Out[8]= $\left\{y[x,t] \to \dfrac{-\lambda 3\, g[x,t]^2 + \lambda 3\, g[x,t]\,(K - r[x,t]) + K\left(g^{(0,1)}[x,t] - D3\, g^{(2,0)}[x,t]\right)}{K\,\lambda 2 + \lambda 3\, g[x,t]}\right\}$

In[9]:=
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(* Substitute into remaining equations *)
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In[10]:=
```
sys2 = Together[Expand[sys1⟦1 ;; 2⟧ /. sol1 /. D[sol1, t] /. D[sol1, {x, 2}]]]];
sys3 = {sys2⟦1⟧⟦2⟧, sys2⟦2⟧⟦2⟧}
```

Out[11]=
```
{-2 K λ2 λ3 g[x, t] + 2 λ2 λ3 g[x, t]^2 +
   K λ1 λ2 r[x, t] + λ1 λ3 g[x, t] × r[x, t] + 2 λ2 λ3 g[x, t] × r[x, t] +
   2 λ3 g[x, t] g^(0,1)[x, t] + K λ2 r^(0,1)[x, t] + λ3 g[x, t] r^(0,1)[x, t] -
   2 D3 λ3 g[x, t] g^(2,0)[x, t] - D1 K λ2 r^(2,0)[x, t] - D1 λ3 g[x, t] r^(2,0)[x, t],
  K^3 λ2^3 λ3 g[x, t] - K^2 λ2^3 λ3 g[x, t]^2 + 2 K^2 λ2^2 λ3^2 g[x, t]^2 - 2 K λ2^2 λ3^2 g[x, t]^3 +
   K λ2 λ3^3 g[x, t]^3 - λ2 λ3^3 g[x, t]^4 - K^3 λ1 λ2^3 r[x, t] - 3 K^2 λ1 λ2^2 λ3 g[x, t] × r[x, t] -
   K^2 λ2^3 λ3 g[x, t] × r[x, t] - 3 K λ1 λ2 λ3^2 g[x, t]^2 r[x, t] -
   2 K λ2^2 λ3^2 g[x, t]^2 r[x, t] - λ1 λ3^3 g[x, t]^3 r[x, t] - λ2 λ3^3 g[x, t]^3 r[x, t] +
   K^3 λ2^3 g^(0,1)[x, t] + K^3 λ2^2 λ3 g^(0,1)[x, t] + K^2 λ2 λ3^2 g[x, t] g^(0,1)[x, t] -
   2 K λ2 λ3^2 g[x, t]^2 g^(0,1)[x, t] - λ3^3 g[x, t]^3 g^(0,1)[x, t] -
   K^2 λ2^2 λ3 r[x, t] g^(0,1)[x, t] - K λ2 λ3^2 g[x, t] × r[x, t] g^(0,1)[x, t] -
   K^2 λ2 λ3 g^(0,1)[x, t]^2 - K λ3^2 g[x, t] g^(0,1)[x, t]^2 - K^2 λ2^2 λ3 g[x, t] r^(0,1)[x, t] -
   2 K λ2 λ3^2 g[x, t]^2 r^(0,1)[x, t] - λ3^3 g[x, t]^3 r^(0,1)[x, t] + K^3 λ2^2 g^(0,2)[x, t] +
   2 K^2 λ2 λ3 g[x, t] g^(0,2)[x, t] + K λ3^2 g[x, t]^2 g^(0,2)[x, t] +
   2 D2 K^2 λ2^2 λ3 g^(1,0)[x, t]^2 + 2 D2 K^2 λ2 λ3^2 g^(1,0)[x, t]^2 -
   2 D2 K λ2 λ3^2 r[x, t] g^(1,0)[x, t]^2 - 2 D2 K λ3^2 g^(0,1)[x, t] g^(1,0)[x, t]^2 +
   2 D2 K^2 λ2^2 λ3 g^(1,0)[x, t] r^(1,0)[x, t] + 2 D2 K λ2 λ3^2 g[x, t] g^(1,0)[x, t] r^(1,0)[x, t] +
   2 D2 K^2 λ2 λ3 g^(1,0)[x, t] g^(1,1)[x, t] + 2 D2 K λ3^2 g[x, t] g^(1,0)[x, t] g^(1,1)[x, t] -
   D3 K^3 λ2^3 g^(2,0)[x, t] - D2 K^3 λ2^2 λ3 g^(2,0)[x, t] +
   2 D2 K^2 λ2^2 λ3 g[x, t] g^(2,0)[x, t] - 2 D3 K^2 λ2^2 λ3 g[x, t] g^(2,0)[x, t] -
   D2 K^2 λ2 λ3^2 g[x, t] g^(2,0)[x, t] + 3 D2 K λ2 λ3^2 g[x, t]^2 g^(2,0)[x, t] -
   D3 K λ2 λ3^2 g[x, t]^2 g^(2,0)[x, t] + D2 λ3^3 g[x, t]^3 g^(2,0)[x, t] +
   D2 K^2 λ2^2 λ3 r[x, t] g^(2,0)[x, t] + D2 K λ2 λ3^2 g[x, t] × r[x, t] g^(2,0)[x, t] +
   D2 K^2 λ2 λ3 g^(0,1)[x, t] g^(2,0)[x, t] + D3 K^2 λ2 λ3 g^(0,1)[x, t] g^(2,0)[x, t] +
   D2 K λ3^2 g[x, t] g^(0,1)[x, t] g^(2,0)[x, t] + D3 K λ3^2 g[x, t] g^(0,1)[x, t] g^(2,0)[x, t] +
   2 D2 D3 K λ3^2 g^(1,0)[x, t]^2 g^(2,0)[x, t] - D2 D3 K^2 λ2 λ3 g^(2,0)[x, t]^2 -
   D2 D3 K λ3^2 g[x, t] g^(2,0)[x, t]^2 + D2 K^2 λ2^2 λ3 g[x, t] r^(2,0)[x, t] +
   2 D2 K λ2 λ3^2 g[x, t]^2 r^(2,0)[x, t] + D2 λ3^3 g[x, t]^3 r^(2,0)[x, t] -
   D2 K^3 λ2^2 g^(2,1)[x, t] - D3 K^3 λ2^2 g^(2,1)[x, t] - 2 D2 K^2 λ2 λ3 g[x, t] g^(2,1)[x, t] -
   2 D3 K^2 λ2 λ3 g[x, t] g^(2,1)[x, t] - D2 K λ3^2 g[x, t]^2 g^(2,1)[x, t] -
   D3 K λ3^2 g[x, t]^2 g^(2,1)[x, t] - 2 D2 D3 K^2 λ2 λ3 g^(1,0)[x, t] g^(3,0)[x, t] -
   2 D2 D3 K λ3^2 g[x, t] g^(1,0)[x, t] g^(3,0)[x, t] + D2 D3 K^3 λ2^2 g^(4,0)[x, t] +
   2 D2 D3 K^2 λ2 λ3 g[x, t] g^(4,0)[x, t] + D2 D3 K λ3^2 g[x, t]^2 g^(4,0)[x, t]}
```

In[12]:=
```
(* Obtain coefficients *)
obsvars = Quiet[Join[{r[x, t], g[x, t]},
   Select[Variables[sys3], #⟦0⟧⟦1⟧ === r || #⟦0⟧⟦1⟧ === g &]]]
```

Out[12]=
```
{r[x, t], g[x, t], g^(0,1)[x, t], r^(0,1)[x, t], g^(0,2)[x, t], g^(1,0)[x, t], r^(1,0)[x, t],
 g^(1,1)[x, t], g^(2,0)[x, t], r^(2,0)[x, t], g^(2,1)[x, t], g^(3,0)[x, t], g^(4,0)[x, t]}
```

In[13]:=

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coef1 = Catenate[Values@CoefficientRules[sys3, obsvars]]
```

Out[13]=

$$\{\lambda1\,\lambda3 + 2\,\lambda2\,\lambda3,\ K\,\lambda1\,\lambda2,\ 2\,\lambda2\,\lambda3,\ 2\,\lambda3,\ \lambda3,\ -2\,D3\,\lambda3,\ -D1\,\lambda3,\ -2\,K\,\lambda2\,\lambda3,$$

$$K\,\lambda2,\ -D1\,K\,\lambda2,\ -\lambda1\,\lambda3^3 - \lambda2\,\lambda3^3,\ -3\,K\,\lambda1\,\lambda2\,\lambda3^2 - 2\,K\,\lambda2^2\,\lambda3^2,\ -K\,\lambda2\,\lambda3^2,$$

$$D2\,K\,\lambda2\,\lambda3^2,\ -3\,K^2\,\lambda1\,\lambda2^2\,\lambda3 - K^2\,\lambda2^3\,\lambda3,\ -K^2\,\lambda2^2\,\lambda3,\ -2\,D2\,K\,\lambda2\,\lambda3^2,\ D2\,K^2\,\lambda2^2\,\lambda3,$$

$$-K^3\,\lambda1\,\lambda2^3,\ -\lambda2\,\lambda3^3,\ -\lambda3^3,\ -\lambda3^3,\ D2\,\lambda3^3,\ D2\,\lambda3^3,\ -2\,K\,\lambda2^2\,\lambda3^2 + K\,\lambda2\,\lambda3^3,$$

$$-2\,K\,\lambda2\,\lambda3^2,\ -2\,K\,\lambda2\,\lambda3^2,\ K\,\lambda3^2,\ 3\,D2\,K\,\lambda2\,\lambda3^2 - D3\,K\,\lambda2\,\lambda3^2,\ 2\,D2\,K\,\lambda2\,\lambda3^2,$$

$$-D2\,K\,\lambda3^2 - D3\,K\,\lambda3^2,\ D2\,D3\,K\,\lambda3^2,\ -K^2\,\lambda2^3\,\lambda3 + 2\,K^2\,\lambda2^2\,\lambda3^2,\ -K\,\lambda3^2,$$

$$D2\,K\,\lambda3^2 + D3\,K\,\lambda3^2,\ K^2\,\lambda2\,\lambda3^2,\ -K^2\,\lambda2^2\,\lambda3,\ 2\,K^2\,\lambda2\,\lambda3,\ 2\,D2\,K\,\lambda2\,\lambda3^2,\ 2\,D2\,K\,\lambda3^2,$$

$$-2\,D2\,D3\,K\,\lambda3^2,\ -D2\,D3\,K\,\lambda3^2,\ 2\,D2\,K^2\,\lambda2^2\,\lambda3 - 2\,D3\,K^2\,\lambda2^2\,\lambda3 - D2\,K^2\,\lambda2\,\lambda3^2,$$

$$D2\,K^2\,\lambda2^2\,\lambda3,\ -2\,D2\,K^2\,\lambda2\,\lambda3 - 2\,D3\,K^2\,\lambda2\,\lambda3,\ 2\,D2\,D3\,K^2\,\lambda2\,\lambda3,\ K^3\,\lambda2^3\,\lambda3,\ -K^2\,\lambda2\,\lambda3,$$

$$-2\,D2\,K\,\lambda3^2,\ D2\,K^2\,\lambda2\,\lambda3 + D3\,K^2\,\lambda2\,\lambda3,\ K^3\,\lambda2^3 + K^3\,\lambda2^2\,\lambda3,\ K^3\,\lambda2^2,\ 2\,D2\,D3\,K\,\lambda3^2,$$

$$2\,D2\,K^2\,\lambda2^2\,\lambda3 + 2\,D2\,K^2\,\lambda2\,\lambda3^2,\ 2\,D2\,K^2\,\lambda2^2\,\lambda3,\ 2\,D2\,K^2\,\lambda2\,\lambda3,\ -2\,D2\,D3\,K^2\,\lambda2\,\lambda3,$$

$$-D2\,D3\,K^2\,\lambda2\,\lambda3,\ -D3\,K^3\,\lambda2^3 - D2\,K^3\,\lambda2^2\,\lambda3,\ -D2\,K^3\,\lambda2^2 - D3\,K^3\,\lambda2^2,\ D2\,D3\,K^3\,\lambda2^2\}$$

In[14]:=

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(* Normalise by a coefficient *)
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In[15]:=

```
coef2 = FullSimplify[coef1 / coef1[[5]]]
```

Out[15]=

$$\left\{\lambda1 + 2\,\lambda2,\ \frac{K\,\lambda1\,\lambda2}{\lambda3},\ 2\,\lambda2,\ 2,\ 1,\ -2\,D3,\ -D1,\ -2\,K\,\lambda2,\ \frac{K\,\lambda2}{\lambda3},\ -\frac{D1\,K\,\lambda2}{\lambda3},\ -\left((\lambda1 + \lambda2)\,\lambda3^2\right),\right.$$

$$-K\,\lambda2\,(3\,\lambda1 + 2\,\lambda2)\,\lambda3,\ -K\,\lambda2\,\lambda3,\ D2\,K\,\lambda2\,\lambda3,\ -K^2\,\lambda2^2\,(3\,\lambda1 + \lambda2),\ -K^2\,\lambda2^2,\ -2\,D2\,K\,\lambda2\,\lambda3,$$

$$D2\,K^2\,\lambda2^2,\ -\frac{K^3\,\lambda1\,\lambda2^3}{\lambda3},\ -\lambda2\,\lambda3^2,\ -\lambda3^2,\ -\lambda3^2,\ D2\,\lambda3^2,\ D2\,\lambda3^2,\ K\,\lambda2\,\lambda3\,(-2\,\lambda2 + \lambda3),$$

$$-2\,K\,\lambda2\,\lambda3,\ -2\,K\,\lambda2\,\lambda3,\ K\,\lambda3,\ (3\,D2 - D3)\,K\,\lambda2\,\lambda3,\ 2\,D2\,K\,\lambda2\,\lambda3,\ -((D2 + D3)\,K\,\lambda3),$$

$$D2\,D3\,K\,\lambda3,\ -K^2\,\lambda2^2\,(\lambda2 - 2\,\lambda3),\ -K\,\lambda3,\ (D2 + D3)\,K\,\lambda3,\ K^2\,\lambda2\,\lambda3,\ -K^2\,\lambda2^2,\ 2\,K^2\,\lambda2,$$

$$2\,D2\,K\,\lambda2\,\lambda3,\ 2\,D2\,K\,\lambda3,\ -2\,D2\,D3\,K\,\lambda3,\ -D2\,D3\,K\,\lambda3,\ K^2\,\lambda2\,(2\,D2\,\lambda2 - 2\,D3\,\lambda2 - D2\,\lambda3),$$

$$D2\,K^2\,\lambda2^2,\ -2\,(D2 + D3)\,K^2\,\lambda2,\ 2\,D2\,D3\,K^2\,\lambda2,\ K^3\,\lambda2^3,\ -K^2\,\lambda2,\ -2\,D2\,K\,\lambda3,\ (D2 + D3)\,K^2\,\lambda2,$$

$$\frac{K^3\,\lambda2^2\,(\lambda2 + \lambda3)}{\lambda3},\ \frac{K^3\,\lambda2^2}{\lambda3},\ 2\,D2\,D3\,K\,\lambda3,\ 2\,D2\,K^2\,\lambda2\,(\lambda2 + \lambda3),\ 2\,D2\,K^2\,\lambda2^2,\ 2\,D2\,K^2\,\lambda2,$$

$$\left.-2\,D2\,D3\,K^2\,\lambda2,\ -D2\,D3\,K^2\,\lambda2,\ -\frac{K^3\,\lambda2^2\,(D3\,\lambda2 + D2\,\lambda3)}{\lambda3},\ -\frac{(D2 + D3)\,K^3\,\lambda2^2}{\lambda3},\ \frac{D2\,D3\,K^3\,\lambda2^2}{\lambda3}\right\}$$