Structural identifiability of reaction-diffusion processes in mathematical biology

# Two-state linear cell cycle model

In[•]:=
```
(* Define equations*)
sys0 = {
   D[r[x, t], t] - (D1 * D[r[x, t], {x, 2}] - k1 * r[x, t] + 2 * k2 * g[x, t]),
   D[g[x, t], t] - (D2 * D[g[x, t], {x, 2}] + k1 * r[x, t] - k2 * g[x, t])
  };
```

In[•]:=
```
(* Obtain parameters in the above expression *)
params = Quiet[Complement[Variables[sys0], Join[{r[x, t], g[x, t]},
    Select[Variables[sys0], #[[0]][[1]] === r || #[[0]][[1]] === g &]]]]
```

Out[•]=

{D1, D2, k1, k2}

## Observations of a sum of state variables

In[•]:=
```
(* Define observation function *)
obs = r[x, t] → n[x, t] - g[x, t]
```

Out[•]=

$r[x, t] \to -g[x, t] + n[x, t]$

In[•]:=
```
(* Substitute *)
sys1 =
 sys /. Table[D[obs, {t, i[[1]]}, {x, i[[2]]}], {i, {{0, 0}, {1, 0}, {0, 1}, {0, 2}}}]
```

Out[•]=

$$\{-2\, k2\, g[x, t] + k1\, (-g[x, t] + n[x, t]) - g^{(0,1)}[x, t] + n^{(0,1)}[x, t] - D1\, \left(-g^{(2,0)}[x, t] + n^{(2,0)}[x, t]\right),$$
$$k2\, g[x, t] - k1\, (-g[x, t] + n[x, t]) + g^{(0,1)}[x, t] - D2\, g^{(2,0)}[x, t]\}$$

In[•]:=
```
(* Solve sys1 for v_xx and v_t *)
sol1 = Solve[Table[expr == 0, {expr, sys1}], {D[g[x, t], {x, 2}], D[g[x, t], t]}][[1]]
```

Out[•]=

$$\left\{g^{(2,0)}[x, t] \to -\frac{-k2\, g[x, t] + n^{(0,1)}[x, t] - D1\, n^{(2,0)}[x, t]}{D1 - D2},\right.$$
$$g^{(0,1)}[x, t] \to -\frac{1}{D1 - D2}\left(D1\, k1\, g[x, t] - D2\, k1\, g[x, t] + D1\, k2\, g[x, t] - 2\, D2\, k2\, g[x, t] - \right.$$
$$\left.\left. D1\, k1\, n[x, t] + D2\, k1\, n[x, t] + D2\, n^{(0,1)}[x, t] - D1\, D2\, n^{(2,0)}[x, t]\right)\right\}$$

In[ ]:=
```
(* Expression in terms of only n *)
expr1 = ((D[g[x, t], {x, 2}, t] /. D[sol1, {x, 2}]) -
      (D[g[x, t], {x, 2}, t] /. D[sol1, t])) /. sol1
```

Out[ ]=

$$\frac{1}{D1-D2}\Bigg(n^{(0,2)}[x,t]+\frac{1}{D1-D2}\,k2\,\big(D1\,k1\,g[x,t]-D2\,k1\,g[x,t]+D1\,k2\,g[x,t]-2\,D2\,k2\,g[x,t]-D1\,k1\,n[x,t]+D2\,k1\,n[x,t]+D2\,n^{(0,1)}[x,t]-D1\,D2\,n^{(2,0)}[x,t]\big)-D1\,n^{(2,1)}[x,t]\Bigg)-\frac{1}{D1-D2}\Bigg(-D1\,k1\,n^{(2,0)}[x,t]+D2\,k1\,n^{(2,0)}[x,t]-\frac{D1\,k1\,\big(-k2\,g[x,t]+n^{(0,1)}[x,t]-D1\,n^{(2,0)}[x,t]\big)}{D1-D2}+\frac{D2\,k1\,\big(-k2\,g[x,t]+n^{(0,1)}[x,t]-D1\,n^{(2,0)}[x,t]\big)}{D1-D2}-\frac{D1\,k2\,\big(-k2\,g[x,t]+n^{(0,1)}[x,t]-D1\,n^{(2,0)}[x,t]\big)}{D1-D2}+\frac{2\,D2\,k2\,\big(-k2\,g[x,t]+n^{(0,1)}[x,t]-D1\,n^{(2,0)}[x,t]\big)}{D1-D2}+D2\,n^{(2,1)}[x,t]-D1\,D2\,n^{(4,0)}[x,t]\Bigg)$$

In[ ]:=
```
(* Expand and collect coefficients *)
expr2 = FullSimplify[expr1 * (D1 - D2)]
```

Out[ ]=

$$-k1\,k2\,n[x,t]+(k1+k2)\,n^{(0,1)}[x,t]+n^{(0,2)}[x,t]-D2\,k1\,n^{(2,0)}[x,t]-D1\,k2\,n^{(2,0)}[x,t]-D1\,n^{(2,1)}[x,t]-D2\,n^{(2,1)}[x,t]+D1\,D2\,n^{(4,0)}[x,t]$$

In[ ]:=
```
(* Normalise so one coefficient is unity *)
expr2 = FullSimplify[expr2 / Coefficient[expr2, D[n[x, t], {t, 2}]]]
```

Out[ ]=

$$-k1\,k2\,n[x,t]+(k1+k2)\,n^{(0,1)}[x,t]+n^{(0,2)}[x,t]-D2\,k1\,n^{(2,0)}[x,t]-D1\,k2\,n^{(2,0)}[x,t]-D1\,n^{(2,1)}[x,t]-D2\,n^{(2,1)}[x,t]+D1\,D2\,n^{(4,0)}[x,t]$$

```
(* Extract coefficients *)
```

In[ ]:=
```
nvars = Join[{n[x, t]}, Quiet[Select[Variables[expr2], #[[0]][[1]] === n &]]]
```

Out[ ]=

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

In[ ]:=
```
Values@CoefficientRules[expr2, nvars]
```

Out[ ]=

$$\{-k1\,k2,\ k1+k2,\ 1,\ -D2\,k1-D1\,k2,\ -D1-D2,\ D1\,D2\}$$