

Structural identifiability of reaction-diffusion processes in mathematicabiology

Generic two-state reaction-diffusion-advection equations

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In[*]:= (* Define equations*)
sys1 = {
  D[u[x, t], t] -
    (Du * D[u[x, t], {x, 2}] +  $\alpha u$  * D[u[x, t], x] + p1 * u[x, t] + p2 * v[x, t] + p3),
  D[v[x, t], t] -
    (Dv * D[v[x, t], {x, 2}] +  $\alpha v$  * D[v[x, t], x] + p4 * u[x, t] + p5 * v[x, t] + p6)
};

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

Out[*]=
{Du, Dv, p1, p2, p3, p4, p5, p6,  $\alpha u$ ,  $\alpha v$ }

In[*]:= (* Define observation function *)
obsrep1 = u[x, t]  $\rightarrow$  n[x, t] - v[x, t]

Out[*]=
u[x, t]  $\rightarrow$  n[x, t] - v[x, t]

In[*]:= (* Substitute *)
sys2 = sys1 /.
  Table[D[obsrep1, {t, i[[1]]}, {x, i[[2]]}], {i, {{0, 0}, {1, 0}, {0, 1}, {0, 2}}}]

Out[*]=

$$\left\{ \begin{aligned} & -p3 - p1 (n[x, t] - v[x, t]) - p2 v[x, t] + n^{(0,1)}[x, t] - v^{(0,1)}[x, t] - \\ & \alpha u (n^{(1,0)}[x, t] - v^{(1,0)}[x, t]) - Du (n^{(2,0)}[x, t] - v^{(2,0)}[x, t]), \\ & -p6 - p4 (n[x, t] - v[x, t]) - p5 v[x, t] + v^{(0,1)}[x, t] - \alpha v v^{(1,0)}[x, t] - Dv v^{(2,0)}[x, t] \end{aligned} \right\}$$


In[*]:= (* Solve sys1 for  $v_{xx}$  and  $v_t$  *)
sol1 = Solve[Table[expr == 0, {expr, sys2}], {D[v[x, t], {x, 2}], D[v[x, t], t]}][[1]]

Out[*]=

$$\left\{ \begin{aligned} & v^{(2,0)}[x, t] \rightarrow -\frac{1}{Du - Dv} \\ & \left( -p3 - p6 - p1 n[x, t] - p4 n[x, t] + p1 v[x, t] - p2 v[x, t] + p4 v[x, t] - p5 v[x, t] + \right. \\ & \quad \left. n^{(0,1)}[x, t] - \alpha u n^{(1,0)}[x, t] + \alpha u v^{(1,0)}[x, t] - \alpha v v^{(1,0)}[x, t] - Du n^{(2,0)}[x, t] \right), \\ & v^{(0,1)}[x, t] \rightarrow -\frac{1}{Du - Dv} \left( -Dv p3 - Du p6 - Dv p1 n[x, t] - Du p4 n[x, t] + \right. \\ & \quad \left. Dv p1 v[x, t] - Dv p2 v[x, t] + Du p4 v[x, t] - Du p5 v[x, t] + Dv n^{(0,1)}[x, t] - \right. \\ & \quad \left. Dv \alpha u n^{(1,0)}[x, t] + Dv \alpha u v^{(1,0)}[x, t] - Du \alpha v v^{(1,0)}[x, t] - Du Dv n^{(2,0)}[x, t] \right) \end{aligned} \right\}$$


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In[*]:= (* Write out new expressions *)

```
sys3 = {
  D[v[x, t], {x, 2}] - (D[v[x, t], {x, 2}] /. sol1),
  D[v[x, t], t] - (D[v[x, t], t] /. sol1)
}
```

Out[*]:=

$$\left\{ \frac{1}{Du - Dv} \left(-p3 - p6 - p1 n[x, t] - p4 n[x, t] + p1 v[x, t] - p2 v[x, t] + p4 v[x, t] - p5 v[x, t] + n^{(0,1)}[x, t] - \alpha u n^{(1,0)}[x, t] + \alpha u v^{(1,0)}[x, t] - \alpha v v^{(1,0)}[x, t] - Du n^{(2,0)}[x, t] \right) + v^{(2,0)}[x, t], v^{(0,1)}[x, t] + \frac{1}{Du - Dv} \left(-Dv p3 - Du p6 - Dv p1 n[x, t] - Du p4 n[x, t] + Dv p1 v[x, t] - Dv p2 v[x, t] + Du p4 v[x, t] - Du p5 v[x, t] + Dv n^{(0,1)}[x, t] - Dv \alpha u n^{(1,0)}[x, t] + Dv \alpha u v^{(1,0)}[x, t] - Du \alpha v v^{(1,0)}[x, t] - Du Dv n^{(2,0)}[x, t] \right) \right\}$$

In[*]:= (* Expand sys12 to make it appropriately determined *)

```
sys4 = Join[sys3, {
  D[sys3[[1]], x],
  D[sys3[[1]], t],
  D[sys3[[2]], x],
  D[sys3[[2]], {x, 2}]
}];
```

In[*]:= (* Variables we wish to keep and eliminate *)

```
nvars = Join[{n[x, t]}, Quiet[Select[Variables[sys4], #[[0]][[1]] === n &]]]
vvars = Join[{v[x, t]}, Quiet[Select[Variables[sys4], #[[0]][[1]] === v &]]]
```

Out[*]:=

```
{n[x, t], n^{(0,1)}[x, t], n^{(0,2)}[x, t], n^{(1,0)}[x, t],
 n^{(1,1)}[x, t], n^{(2,0)}[x, t], n^{(2,1)}[x, t], n^{(3,0)}[x, t], n^{(4,0)}[x, t]}
```

Out[*]:=

```
{v[x, t], v^{(0,1)}[x, t], v^{(1,0)}[x, t], v^{(1,1)}[x, t], v^{(2,0)}[x, t], v^{(2,1)}[x, t], v^{(3,0)}[x, t]}
```

In[*]:= (* Convert system to matrix form *)

```
A1 = Table[Coefficient[Expand[expr], var], {expr, sys4}, {var, vvars}];
B1 = Table[{0, 0, 0, 0, 0, 0, 0} /. CoefficientRules[expr, vvars], {expr, sys4}];
```

```
In[*]:= (* Row reduction (automatic) *)
op = RowReduce[Join[A1, IdentityMatrix[6], 2]] [[;;, -6 ;;]];
FullSimplify[op.A1] // MatrixForm
```

Out[*] // MatrixForm =

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & -\frac{(Du-Dv) \left((Du-Dv) (p1-p2+p4-p5) - (\alpha u - \alpha v)^2 \right)}{(Dv (p1-p2) + Du (p4-p5)) (p1-p2+p4-p5)^2} & -\frac{((Du-Dv) (2 Dv p1-2 Dv p2+Du p4+Dv p4-(Du+Dv) p5) \alpha u)+}{(} \\ 0 & 1 & 0 & 0 & 0 & \frac{(Du-Dv) \left(p1-p2+p4-p5 - \frac{(\alpha u - \alpha v) (p4 \alpha u - p5 \alpha u + (p1-p2) \alpha v)}{Dv (p1-p2) + Du (p4-p5)} \right)}{(p1-p2+p4-p5)^2} & \frac{(\alpha u - \alpha v) (Dv^2 (p1-p2)^2 + Dv (p4-p5) (2 Du (} \\ 0 & 0 & 1 & 0 & 0 & -\frac{(Du-Dv) (\alpha u - \alpha v)}{(Dv (p1-p2) + Du (p4-p5)) (p1-p2+p4-p5)} & \frac{Dv^2 (-p1+p2) + Du^2 (p} \\ 0 & 0 & 0 & 1 & 0 & \frac{(Du-Dv) (p4 \alpha u - p5 \alpha u + (p1-p2) \alpha v)}{(Dv (p1-p2) + Du (p4-p5)) (p1-p2+p4-p5)} & -Dv p1+ \\ 0 & 0 & 0 & 0 & 1 & \frac{Du-Dv}{Dv p1-Dv p2+Du p4-Du p5} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

```
In[*]:= op // MatrixForm
```

Out[*] // MatrixForm =

$$\begin{pmatrix} 0 & \frac{Du-Dv}{Dv p1-Dv p2+Du p4-Du p5} & \frac{(Du-Dv) (-2 Dv p1 \alpha u+2 Dv p2 \alpha u-Du p4 \alpha u-Dv p4 \alpha u+Du p5 \alpha u+Dv p5 \alpha u+Du)}{(p1-p2+p4-p5)^2 (Dv p1-Dv p2+} \\ 0 & 0 & \frac{(Dv p1-Dv p2+Du p4-Du p5)}{(p1-p2+p4-p5)^2} \\ 0 & 0 & \frac{Du-Dv}{p1-p2+p4-p5} \\ 0 & 0 & \frac{-Dv p1+Dv p2-Du p4+D} {p1-p2+p4-p5} \\ 0 & 0 & 0 \\ 1 & \frac{-p1+p2-p4+p5}{Dv p1-Dv p2+Du p4-Du p5} & \frac{\left(\frac{p1}{Du-Dv} - \frac{p2}{Du-Dv} + \frac{p4}{Du-Dv} - \frac{p5}{Du-Dv} \right)^2 \left(-\frac{Dv p1}{Du-Dv} + \frac{Dv p2}{Du-Dv} - \frac{Du p4}{Du-Dv} + \frac{Du p5}{Du-Dv} \right) \left(\frac{\alpha u}{Du-Dv} - \frac{\alpha v}{Du-Dv} \right) - \left(\frac{p1}{Du-Dv} - \frac{p2}{Du-Dv} + \frac{p4}{Du-Dv} - \frac{p5}{Du-Dv} \right)^2 \left(-\left(\frac{p1}{Du-Dv} - \frac{p2}{Du-Dv} + \frac{p4}{Du-Dv} - \frac{p5}{Du-Dv} \right)^3 \left(-\frac{Dv p1}{Du-Dv} + \right.} \end{pmatrix}$$

```
In[*]:= (* Polynomial equation in n *)
expr1 = Expand[FullSimplify[op.B1] [[-1]]]
```

Out[*] =

$$\begin{aligned} & -\frac{p3 p4}{Dv (p1-p2) + Du (p4-p5)} + \frac{p3 p5}{Dv (p1-p2) + Du (p4-p5)} + \frac{p1 p6}{Dv (p1-p2) + Du (p4-p5)} - \\ & \frac{p2 p6}{Dv (p1-p2) + Du (p4-p5)} - \frac{p2 p4 n[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{p1 p5 n[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \\ & \frac{p1 n^{(0,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{p5 n^{(0,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{n^{(0,2)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \\ & \frac{p5 \alpha u n^{(1,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{p1 \alpha v n^{(1,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{\alpha u n^{(1,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \\ & \frac{\alpha v n^{(1,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{Dv p1 n^{(2,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{Du p5 n^{(2,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \\ & \frac{\alpha u \alpha v n^{(2,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{Du n^{(2,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{Dv n^{(2,1)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \\ & \frac{Dv \alpha u n^{(3,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{Du \alpha v n^{(3,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} - \frac{Du Dv n^{(4,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \\ & \frac{Dv \alpha u n^{(3,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{Du \alpha v n^{(3,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} + \frac{Du Dv n^{(4,0)}[x, t]}{Dv (p1-p2) + Du (p4-p5)} \end{aligned}$$

```

In[ ]:= (* Get coefficients *)
coef1 = Values@CoefficientRules[expr1, nvars]

Out[ ]:=

$$\left\{ -\frac{p_2 p_4}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{p_1 p_5}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5}, \right.$$


$$-\frac{p_1}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} - \frac{p_5}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$\frac{1}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5}, \frac{p_5 \alpha u}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{p_1 \alpha v}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$-\frac{\alpha u}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} - \frac{\alpha v}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$\frac{Dv\ p1}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{Du\ p5}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{\alpha u \alpha v}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$-\frac{Du}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} - \frac{Dv}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$\frac{Dv\ \alpha u}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{Du\ \alpha v}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5},$$


$$\frac{Du\ Dv}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5}, -\frac{p_3 p_4}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} +$$


$$\frac{p_3 p_5}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} + \frac{p_1 p_6}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} - \frac{p_2 p_6}{Dv\ p1 - Dv\ p2 + Du\ p4 - Du\ p5} \Big\}$$


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```

In[ ]:= (* Normalise so one coefficient is unity *)
coef3 = FullSimplify[coef1 / coef1[[3]]]

Out[ ]:=
{-p2 p4 + p1 p5, -p1 - p5, 1, p5 \alpha u + p1 \alpha v, -\alpha u - \alpha v, Dv p1 + Du p5 + \alpha u \alpha v,
-Du - Dv, Dv \alpha u + Du \alpha v, Du Dv, p3 (-p4 + p5) + (p1 - p2) p6}

```

Verify that a single polynomial expression is expected

```

In[ ]:= sys5 = Join[
  Catenate[Table[Table[D[sys3[[1]], {x, i}], {t, k - i}], {i, 0, k}], {k, 0, 2}],
  Catenate[Table[Table[D[sys3[[2]], {x, i}], {t, k - i}], {i, 0, k}], {k, 0, 3}]
];

In[ ]:= vvarsexp = Join[{v[x, t]}, Quiet[Select[Variables[sys5], #[[0]][[1]] === v &]]];

In[ ]:= (* Convert system to matrix form *)
A2 = Table[Coefficient[Expand[expr], var], {expr, sys5}, {var, vvarsexp}];
B2 = Table[{0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0} /.
  CoefficientRules[expr, vvarsexp], {expr, sys5}];
M2 = Transpose[Insert[Transpose[A2], B2, Length[vvarsexp] + 1]];

In[ ]:= MatrixRank[M2] - MatrixRank[A2]

Out[ ]:=
1

```