Localisation and Reconstruction of Structural Model Errors in Dynamic Systems

Can we infer the cause from effect?

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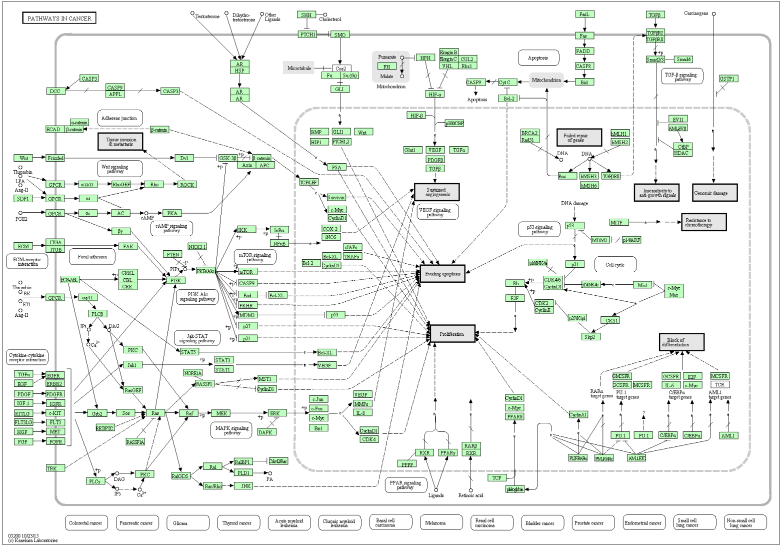
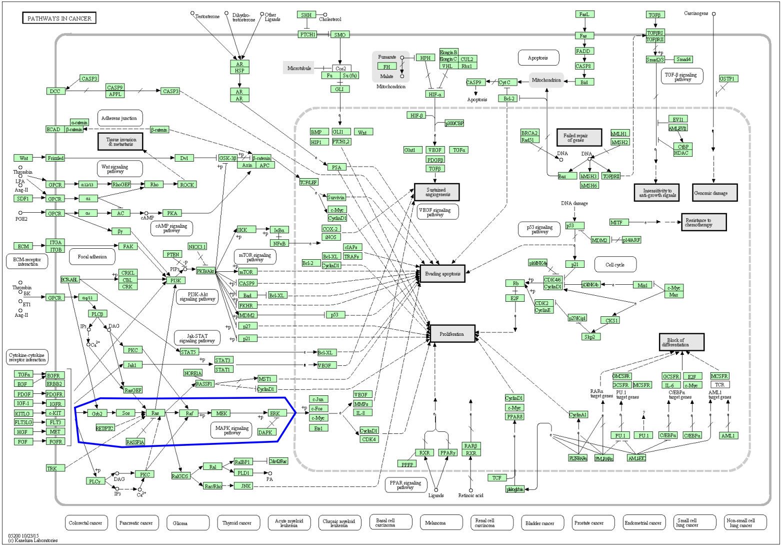
How to model a complex dynamical system?

Pathways in Cancer (KEGG hsa05200, 10/23/25, Kaneshisa Lab)

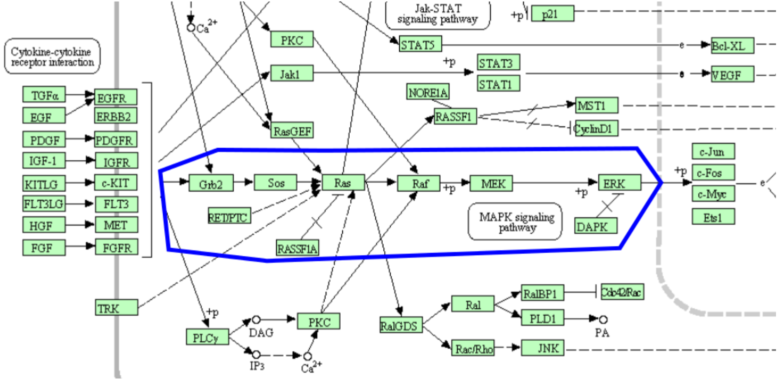


Modelling subnetworks

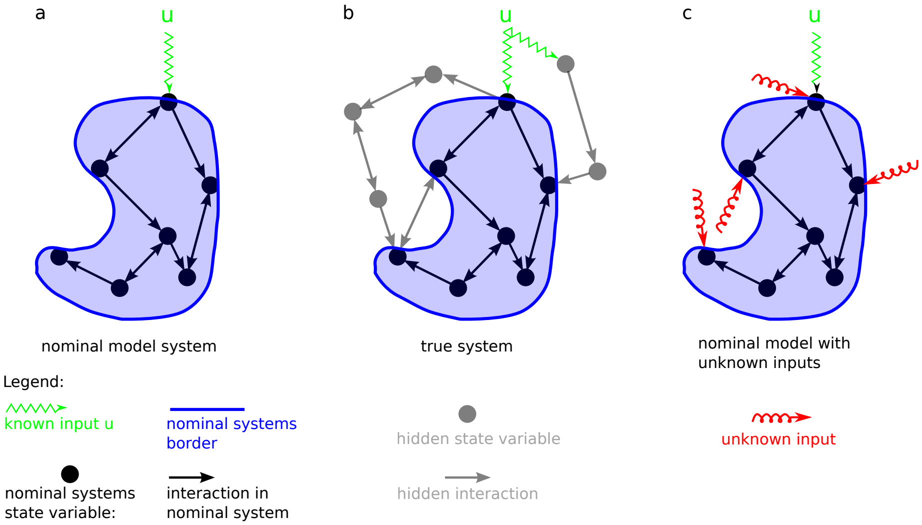
Pathways in Cancer (KEGG hsa05200, 10/23/25, Kaneshisa Lab)



Open systems



The nominal model and the true system



Reconstructing the input from the output

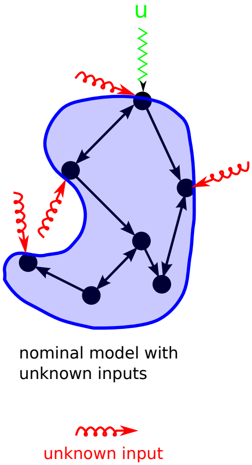
System:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w}\\ \mathbf{y} &= \mathbf{h}(\mathbf{x})\end{aligned}$$

The unknown input $\mathbf{w}(t)$ represents either

- structural model errors or
- hidden inputs from the exterior

When is it possible to reconstruct the unknown input $\mathbf{w}(t)$ from the measured output $\mathbf{y}(t)$?



Invertibility

Mathematical definition

System:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w} \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}) \end{aligned}$$

Definition

The system is invertible, if two different inputs $\mathbf{w}^{(1)}(t) \neq \mathbf{w}^{(2)}(t)$ generate different outputs $\mathbf{y}^{(1)}(t) \neq \mathbf{y}^{(2)}(t)$.

Unknown input reconstruction

Basic principle

Data: $\mathbf{y}^{data}(t_k)$ at discrete time points t_k, $k = 1, \ldots, N$

Optimal control problem:

$$\min_{\mathbf{w}(t)} \sum_{k=1}^{N} \|\mathbf{y}^{data}(t_k) - \mathbf{y}(t_k)\|_2^2 + \mathcal{R}(\mathbf{w})$$

subject to

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{w}$$

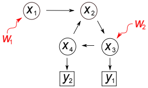
$$\mathbf{y} = \mathbf{h}(\mathbf{x})$$

See a large amount of literature, e.g.

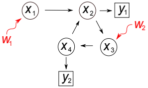
- Chen et al. (2007). Int. J. Control. 63. 85-105.
- Schelker et al. (2012) Bioinformatics 28, i529-i534.
- Engelhardt, B. et al. (2016) Sci. Rep. 6, 20772.
- Engelhardt, B. et al. (2017) J. Royal Soc. Interface 14, 20170332.
- Tsiantis et al. (2018) Bioinformatics 34, 2433–2440.

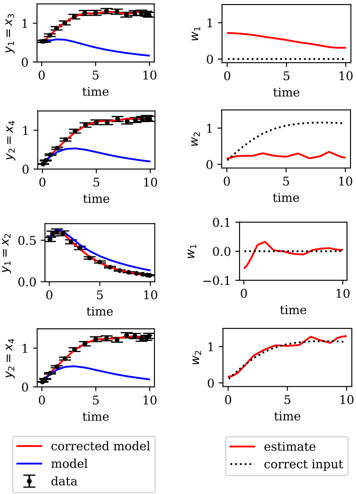
Example for unknown input reconstruction

not invertible



invertible





Invertibility

Algebraic criteria

Linear Systems: $\mathbf{f}(\mathbf{x}) = A\mathbf{x}$

- M. Sain and J. Massey, 1969, 14, 141 IEEE Transactions on Automatic Control
- Silverman, 1969, 14, 270 IEEE Transactions on Automatic Control
- Kahl et al., Phys. Rev. X, 2019

Nonlinear Systems

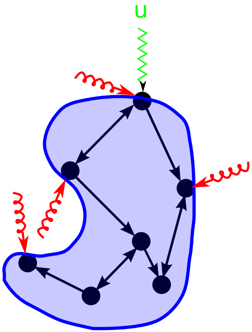
- R. M. Hirschorn, 1997, SIAM Journal on Control and Optimization 17, 289.
- M. Fliess, 1986, A note on the invertibility of nonlinear input-output differential systems, Systems and Control Letters 8, 147.
- T. Wey, 1998, IFAC Proceedings Volumes 31, 257.

Problem: Very difficult to apply to real systems.

Influence graph

System:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w}\\ \mathbf{y} &= \mathbf{h}(\mathbf{x})\end{aligned}$$



nominal model with unknown inputs

unknown input

Influence graph g:

Nodes $\mathcal{N}$: $\{x_1, \ldots, x_n\}$
Edges $\mathcal{E}$: $x_i \longrightarrow x_j$ if $\frac{\partial f_j}{\partial x_i} \not\equiv 0$

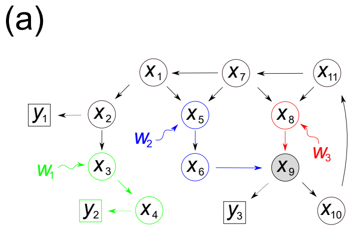
Input and output node sets:

Input Nodes: $S = \{k \in \{1, \ldots n\} | w_k(t) \not\equiv 0\}$
Output nodes: $Z = \{j \in \{1, \ldots n\} | \frac{\partial \mathbf{h}}{\partial x_j} \not\equiv 0\}$

Structural Invertibility

The graph structure is enough

Wey, T. IFAC Proceedings 31, 257 (1998); Kahl et al., Phys. Rev. X, 2019



- S, Z and g denote the input nodes, output nodes and the graph

Structural Invertibility

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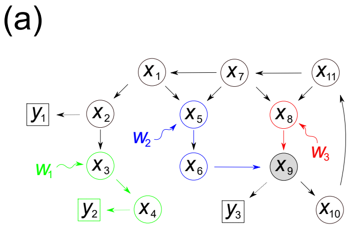
Wey, T. IFAC Proceedings 31, 257 (1998); Kahl et al., Phys. Rev. X, 2019



- S, Z and g denote the input nodes, output nodes and the graph
- Invertibility depends only on (S, g, Z)

Structural Invertibility

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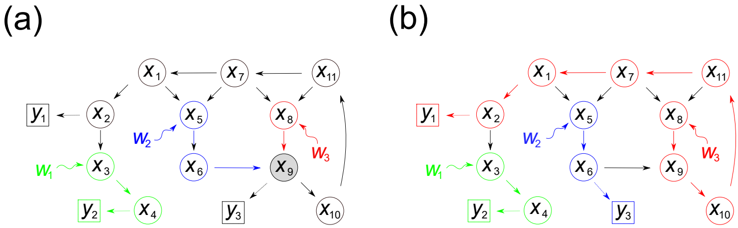
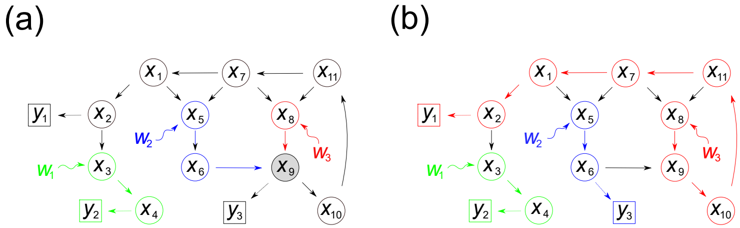


- S, Z and g denote the input nodes, output nodes and the graph
- Invertibility depends only on (S, g, Z)
- Invertibility criterion:

Structural Invertibility

The graph structure is enough

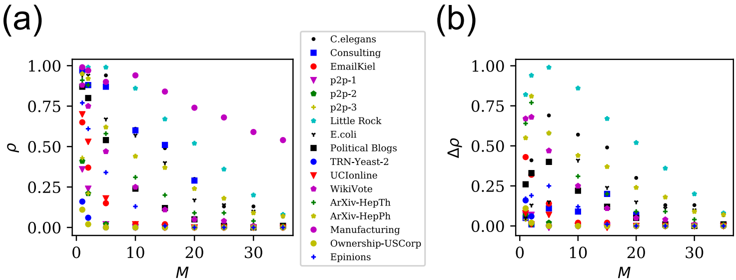
Wey, T. IFAC Proceedings 31, 257 (1998); Kahl et al., Phys. Rev. X, 2019



- S, Z and g denote the input nodes, output nodes and the graph
- Invertibility depends only on (S, g, Z)
- Invertibility criterion:
  1. There is a directed path connecting each input node in S with one output node Z
  2. These path are node disjoint (don't intersect)

Invertibility of real networks

Sample M input nodes S and select outputs randomly or optimally



(a) real with random outputs and (b) improvement with optimal output set S^*.

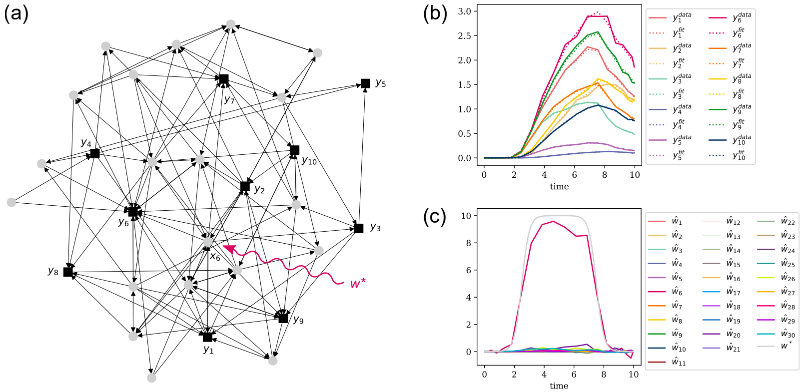
- ρ gives the probability of invertibility

Optimal sensor node selection provides drastic improvements (see Kahm et al., 2019, Phys. Rev. X)

What if the location of the model errors is unknown?

Localisation of unknown inputs (Kahl, Weber and Kschischo, IEEE TCNS 2021)

Example: A model error $\mathbf{w}$ with $w_6(t) \neq 0$ and $w_k(t) = 0$ for $k \in \{1, \ldots, 30\} \setminus \{6\}$



(a) Influence graph (b) Output (c) True and reconstructed ($\hat{\mathbf{w}}$) model error.

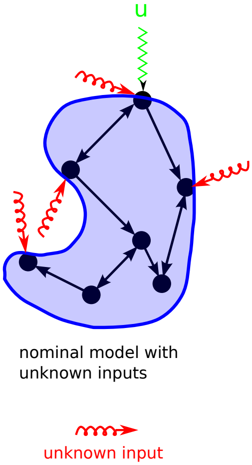
Localisability

When is it possible to identify S (i.e. the nonzero components of $\mathbf{w}(t)$)?

System:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w} \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}) \end{aligned}$$

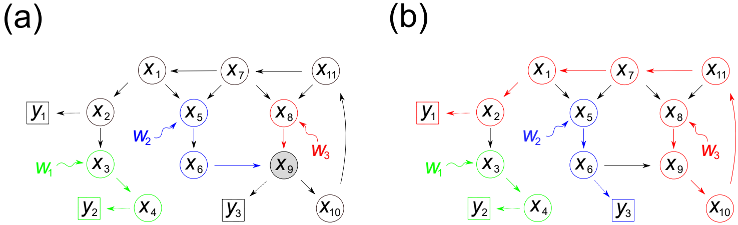
Given: $\mathbf{f}, \mathbf{h}$ and $\mathbf{y}^{data}(t)$



Gammoid structure

Definition

- $\Gamma = (\mathcal{N}, g, Z)$ is a **gammoid**.
- If there is a set of node disjoint paths from the input set $S \subset \mathcal{N}$ to the output set Z, we say S is **independent in** Γ



(a) $S = (3, 5, 8)$ is not independent in Γ. (b) $S = (3, 5, 8)$ is independent in Γ'.

Rank, Nullity (Kernel) and Spark

Definition

Let $\Gamma = (\mathcal{N}, g, Z)$ be a gammoid.

- The cardinality of the largest independent input set $\tilde{S} \subset S$ is the **rank of** S
- **Nullity**: $\mathrm{null} S := \mathrm{card} S - \mathrm{rank} S$
- **Spark of** Γ: The cardinality of the smallest dependent input set $S \subset \mathcal{N}$.

Sparse error localisation (Kahm, Weber and Kschischo 2021)

Theorem

Let $\Gamma = (\mathcal{N}, g, Z)$ *be the gammoid corresponding to the system*

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w} \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}) \end{aligned}$$

and $\Phi : \mathbf{w} \mapsto \mathbf{y}$ *be the corresponding input-output map. The number of nonzero components of* $\mathbf{w}$ *is denoted by* $\|\mathbf{w}\|_0$*. For an observed output* $\mathbf{y}^{data}(t)$ *the solution of*

$$\Phi(\mathbf{w}) = \mathbf{y}^{data}$$

is unique if

$$\|\mathbf{w}\|_0 < \frac{spark\Gamma}{2}.$$

Sparse error localisation (Kahm, Weber and Kschischo 2021)

Example

- $\|\mathbf{w}\|_0 = 1$ model error requires *spark* $\Gamma \geq 3$
- $\|\mathbf{w}\|_0 = 2$ model errors (e.g. misspecified reaction rate) requires *spark* $\Gamma \geq 5$

Remarks

1. The spark depends on the graph g and output set Z or measured states.
2. The spark is difficult to compute for large networks
3. For linear systems, a feasible approximation of the spark is possible.

Simultaneous error localisation and reconstruction

Linear nominal model $\mathbf{f} = A\mathbf{x}$

Let again be $\Phi : \mathbf{w} \mapsto \mathbf{y}$ be the input output map defined by

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{w} \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}) \end{aligned}$$

and $\mathbf{y}^{data}$ be an observed output function.

Reconstruction problem: minimise $\|\mathbf{w}\|_0$ subject to $\|\Phi(w) - \mathbf{y}^{data}\|_2 \leq \epsilon$

Theorem

The solutions of the reconstruction problem and the relaxed problem

$$\mathit{minimise} \|\mathbf{w}\|_1 \;\mathit{subject\ to}\; \|\Phi(w) - \mathbf{y}^{data}\|_2 \leq \epsilon$$

coincide with a certain accuracy (Kahm, Weber and Kschischo, IEEE TCNS 2021) and the relaxed problem is convex.

Simultaneous error localisation and reconstruction

Remarks

1. The theorem applies for a specific norm definition for $\mathbf{w}(t) = (w_1(t), \ldots, w_n(t))^T$.
   Let $\|w_k\|_p = \sqrt[p]{\int_0^T |w_k(t)|^p dt}$, Then we use the norm

$$\|\mathbf{w}\|_q = \sqrt[q]{\sum_{k=1}^{n} \|w_k\|_p^q}$$

   for $p, q \geq 1$.
2. Empirical observation: Works also for nonlinear nominal models $\mathbf{f}$.

Example: Errors of the linearised Lorenz system

Lorenz system (True)

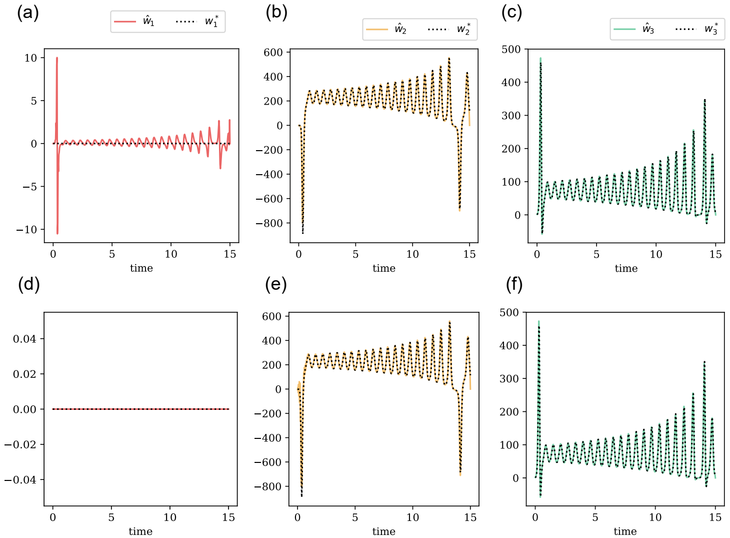
$$\begin{aligned}
\dot{x}(t) &= \sigma y(t) - \sigma x(t) \\
\dot{y}(t) &= -x(t)y(t) + \rho x(t) - y(t) \\
\dot{z}(t) &= x(t)y(t) - \beta z(t) \\
y_1^{data}(t) &= x(t) \\
y_2^{data}(t) &= z(t)
\end{aligned}$$

Linearised system and unknown errors

$$\begin{aligned}
\dot{x}(t) &= \sigma y(t) - \sigma x(t) + w_1(t) \\
\dot{y}(t) &= \rho x(t) - y(t) + w_2(t) \\
\dot{z}(t) &= -\beta z(t) + w_3(t) \\
y_1^(t) &= x(t) \\
y_2^(t) &= z(t)
\end{aligned}$$

Example: Errors of the linearised Lorenz system

Different regularisation parameters



Summary and Outlook

Summary

- Model error
  (see also Engelhardt et al., Sci Rep (2016), J. R. Soc. Interface (2017))
- Invertibility
  (Kahl et al. ,Phys Rev X (2019))
- Localisation and Reconstruction
  (Kahl, Weber and Kschischo, IEE TCNS (2021), Kahl and Kschischo, Frontiers in Physiology (2021))
- Numerical Implementation
  (Newmiwaka et al. Bioinformatics (2021))

Outlook

- Extension of all results to nonlinear systems
- Automatic model extension (model for the error)