EINDHOVEN UNIVERSITY OF TECHNOLOGY

Data-driven model learning in interconnected systems

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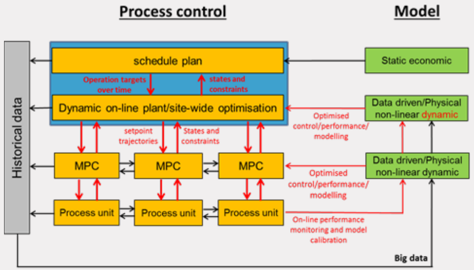
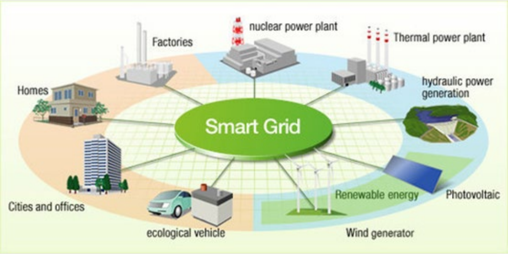
Introduction – dynamic networks

Decentralized process control



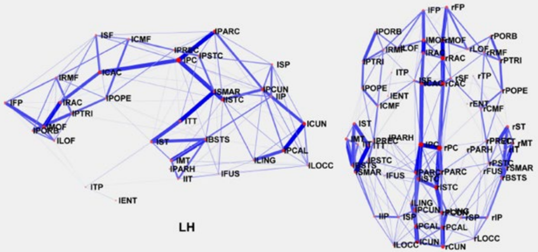


Smart power grid

Pierre et al. (2012)

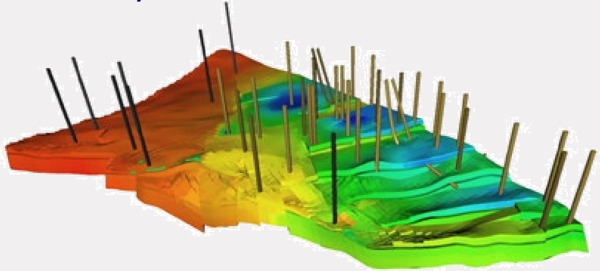
Complex machines

Brain network



P. Hagmann et al. (2008)

Hydrocarbon reservoirs

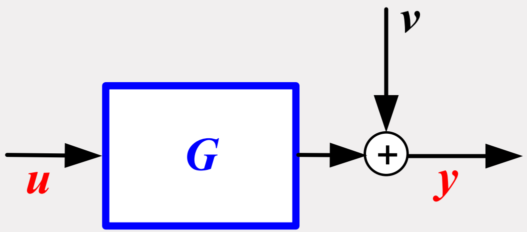


Mansoori (2014)

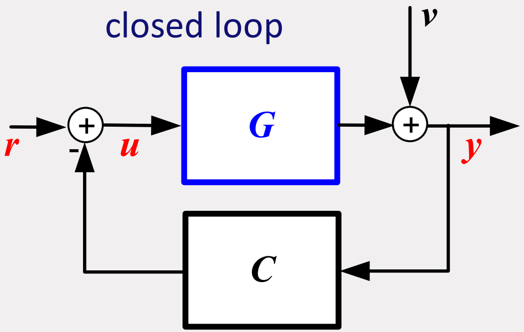
Introduction

The classical (multivariable) data-driven modeling problems[1] :

open loop



closed loop



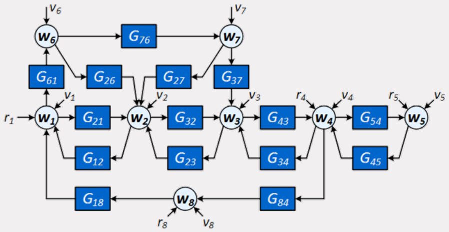
Identify a model of G on the basis of measured signals u, y (and possibly r), focusing on *continuous LTI dynamics*.

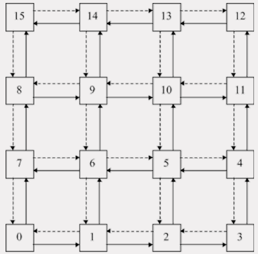
In interconnected systems (networks) the **structure / topology** becomes important to include

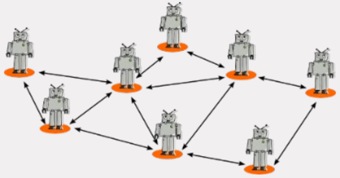
[1] Ljung (1999), Söderström and Stoica (1989), Pintelon and Schoukens (2012)

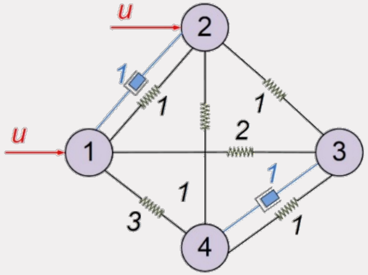
Network models

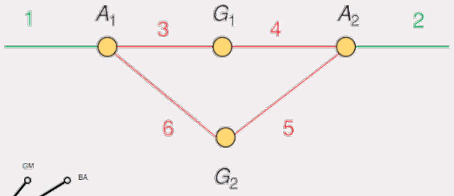
- scalable, describing the physics
- dynamic elements with cause-effect
- handling feedback loops (cycles)
- combining physical and cyber components
- centered around measured signals
- allow disturbances and probing signals

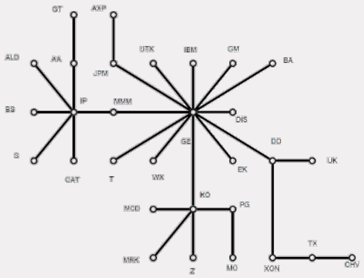


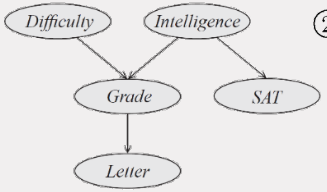


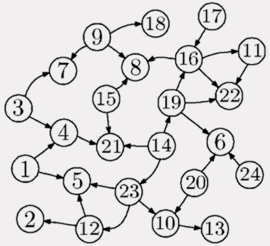


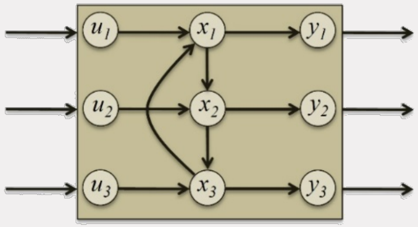


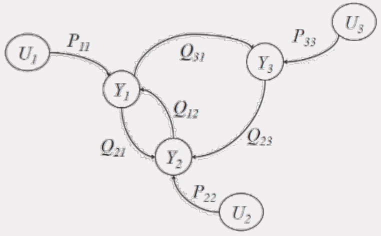






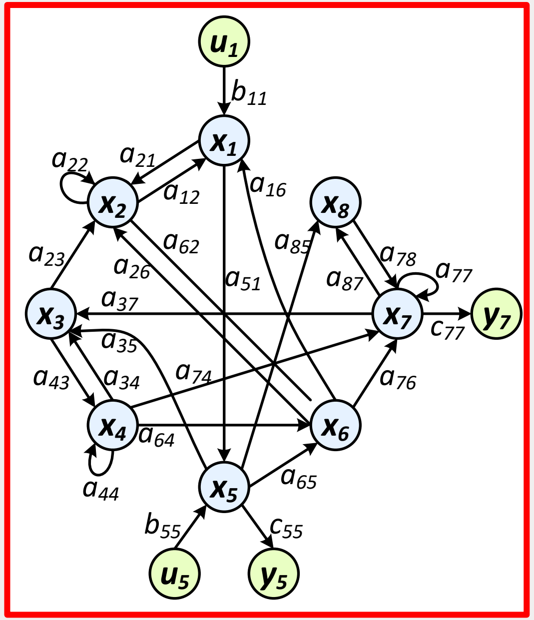






D. Materassi and M.V. Salapaka (2012)
www.momo.cs.okayama-u.ac.jp
E.A. Carara and F.G. Moraes (2008)
P.M.J. Van den Hof et al (2013)
J.C. Willems (2007)
X.Cheng (2019)
R.N. Mantegna (1999)
D. Koller and N. Friedman (2009)
P.E. Paré et al (2013)
E. Yeung et al (2010)

Network models



State space representation

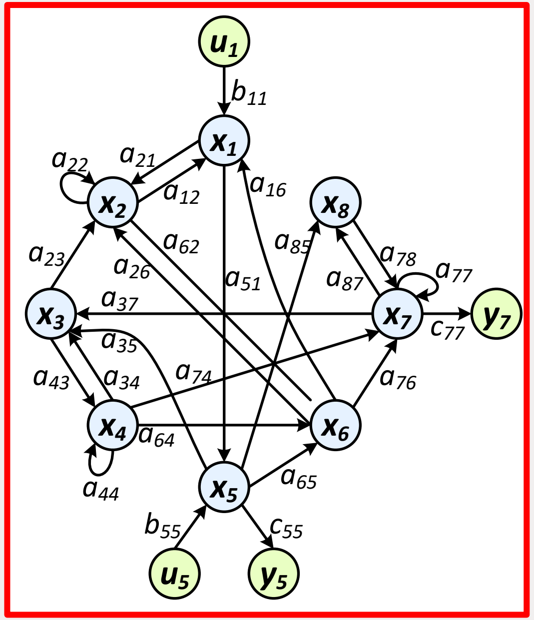
$$
\begin{aligned}
x(k+1) &= Ax(k) + Bu(k) \\
y(k) &= Cx(k) + Du(k)
\end{aligned}
$$

- States as **nodes** in a (directed) graph
- State transitions (1 step in time) reflected by a_{ij}
- Transitions are encoded in links
- Ultimate break-down of system structure
- Actuation (u) and sensing (y) reflected by separate links

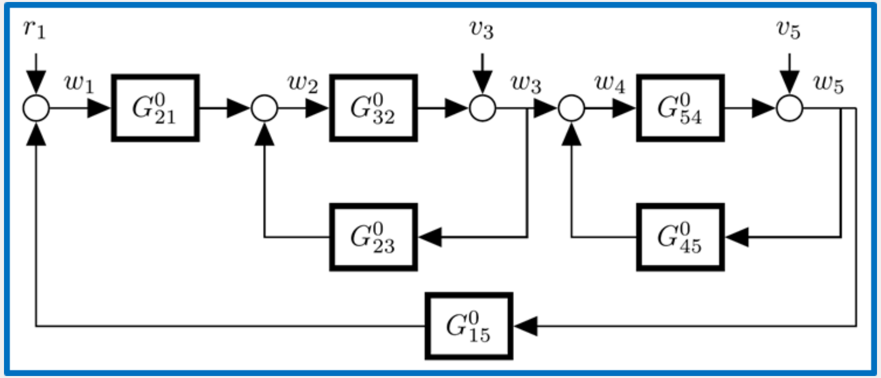
For data-driven modeling problems:

- Lump unmeasured states in dynamic **modules**

Network models



State space representation [1]

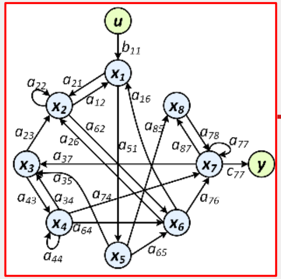


Module representation [2]

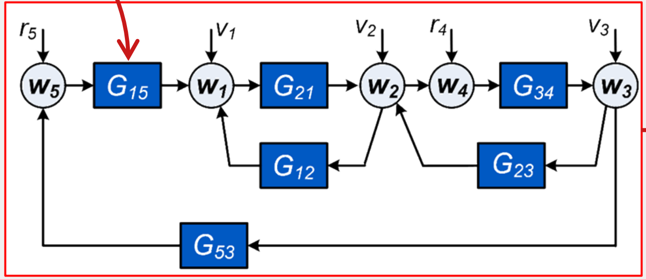
[1] Goncalves, Warnick, Sandberg, Yeung, Yuan, Scherpen,…

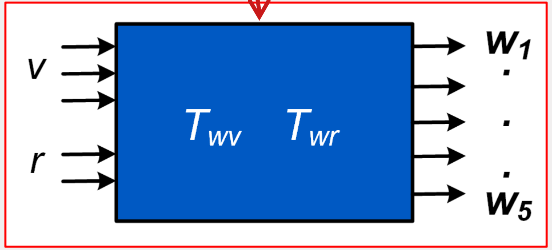
[2] VdH, Dankers, Goncalves, Warnick, Gevers, Bazanella, Hendrickx, Materassi, Weerts,…

Dynamic network models - zooming



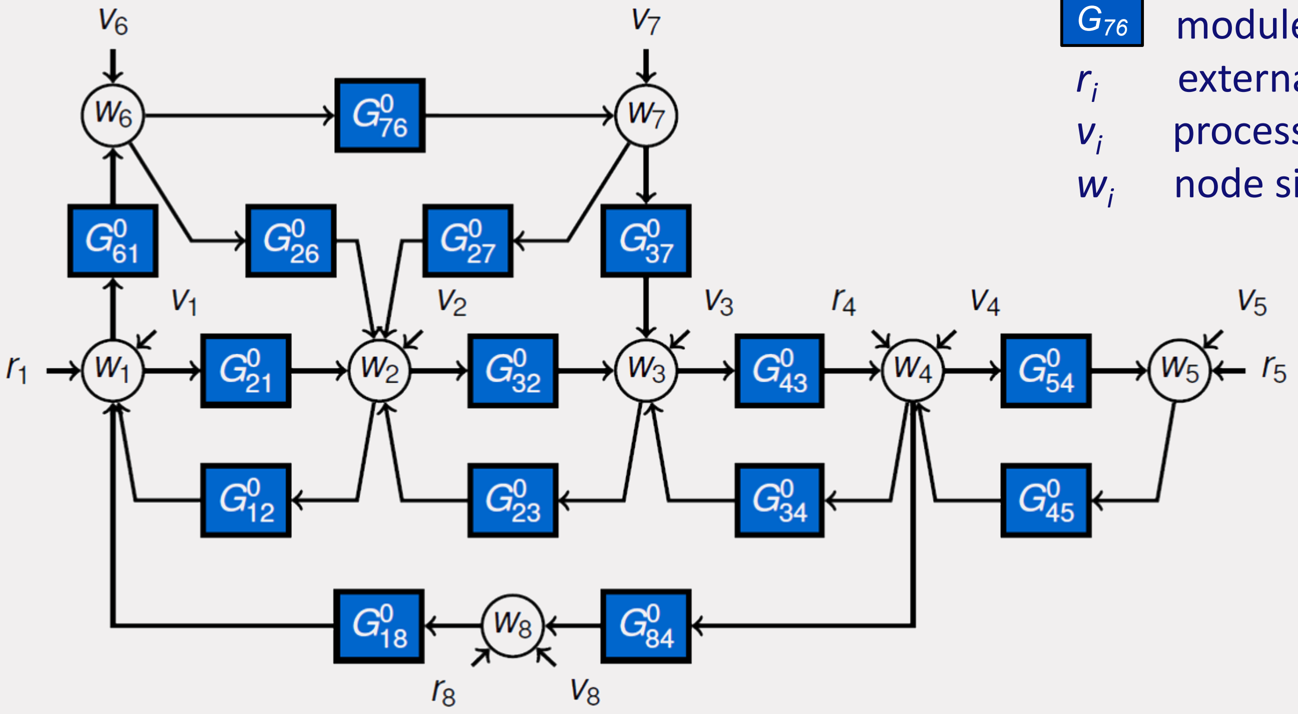
Increasing level of detail





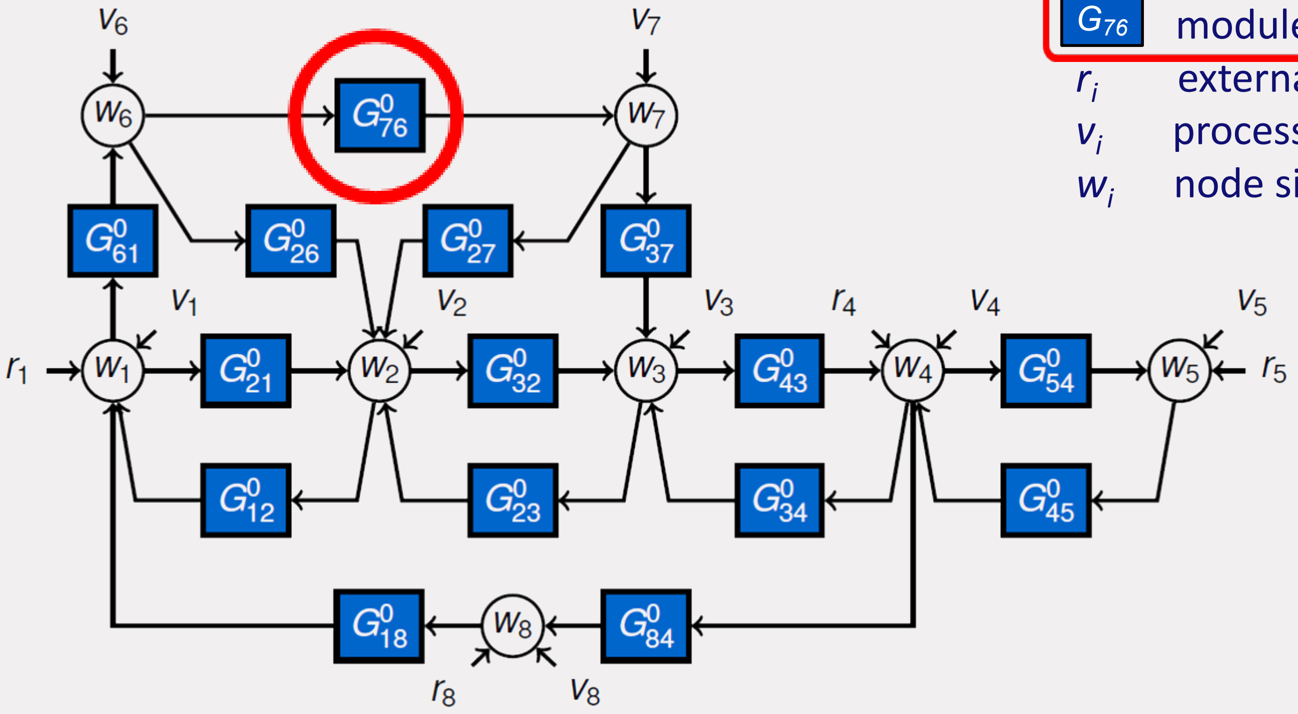
Decreasing structural information

Dynamic network setup



G_{76} module
r_i external excitation
v_i process noise
w_i node signal

Dynamic network setup



G_{76} module
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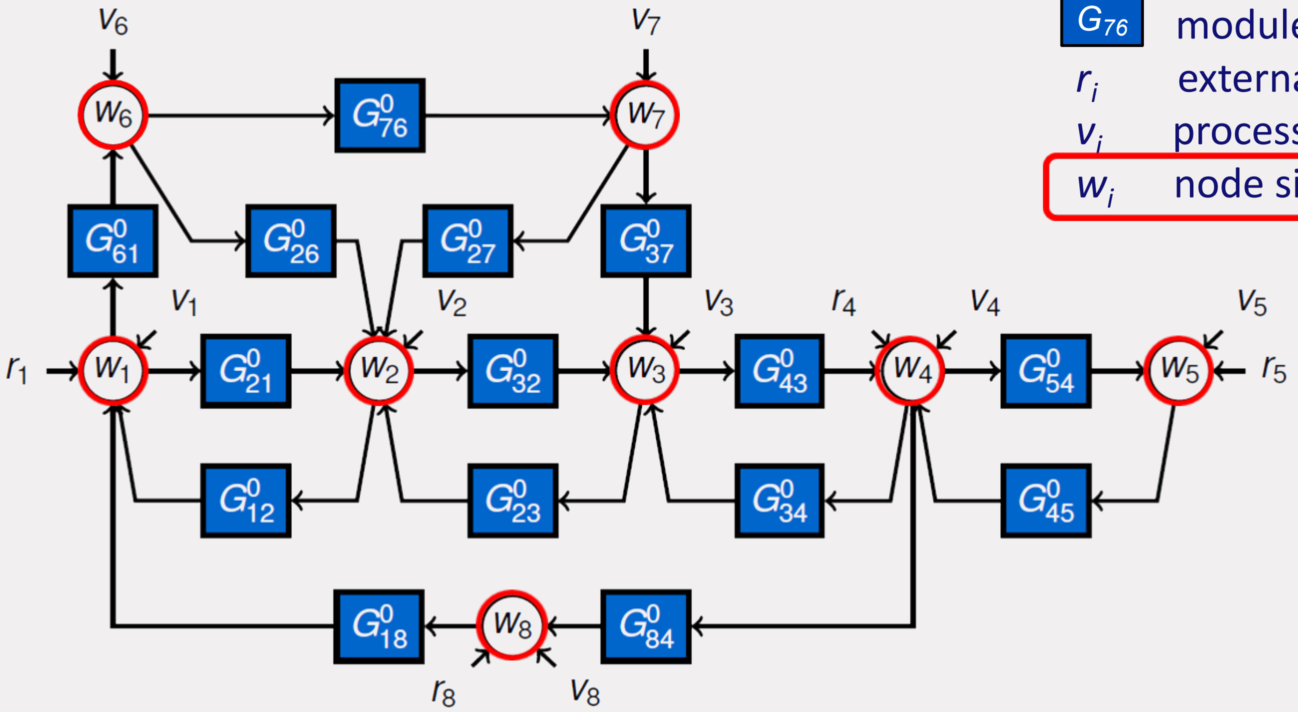
Dynamic network setup



G_{76} module

r_i external excitation

v_i process noise

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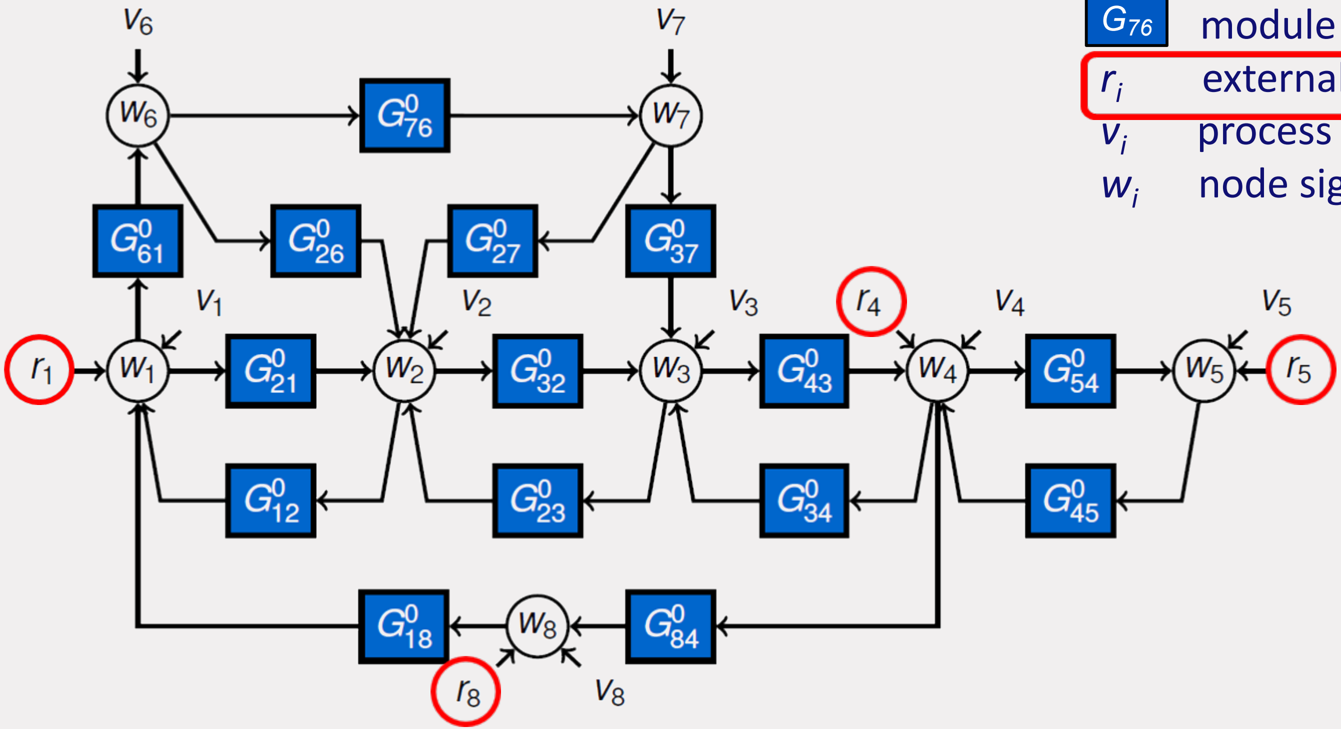
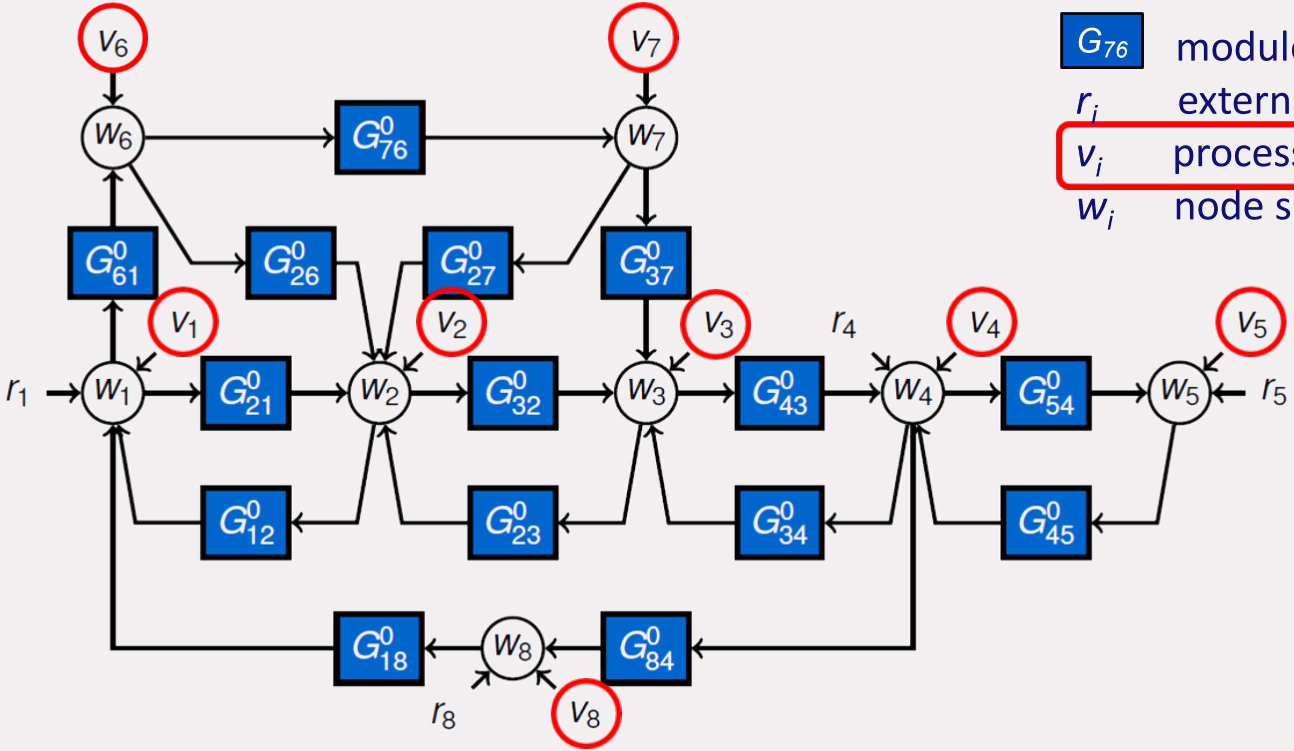
Dynamic network setup



G_{76}	module
r_i	external excitation
v_i	process noise
w_i	node signal

Dynamic network setup



G_{76}	module
r_i	external excitation
v_i	process noise
w_i	node signal

Dynamic network setup

Collecting all equations:

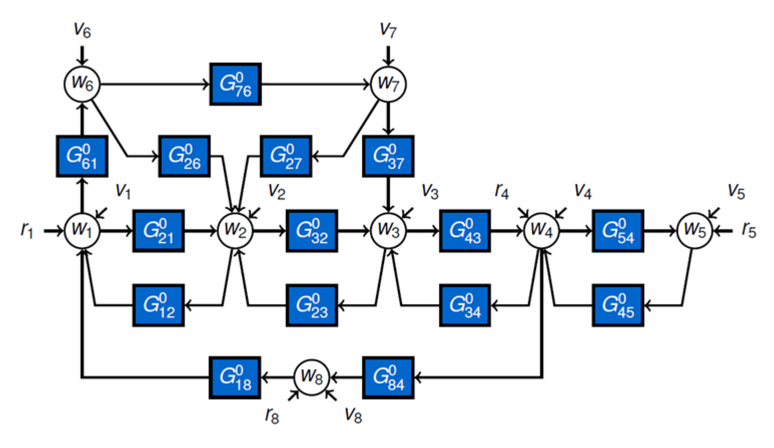
$$\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_L \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & G^0_{12} & \cdots & G^0_{1L} \\ G^0_{21} & 0 & \ddots & G^0_{2L} \\ \vdots & \ddots & \ddots & \vdots \\ G^0_{L1} & G^0_{L2} & \cdots & 0 \end{bmatrix}}_{\text{Network matrix } G^0(q)} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_L \end{bmatrix} + R^0 \begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_K \end{bmatrix} + H^0 \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_p \end{bmatrix}$$

$$w(t) = G^0(q)w(t) + \underbrace{R^0(q)r(t)}_{u(t)} + v(t); \qquad v(t) = H^0(q)e(t); \quad cov(e) = \Lambda$$

- Typically R^0 is just a (static) selection matrix, indicating which nodes have an excitation signal.
- The topology of the network is encoded in the structure (non-zero entries) of G^0.
- r and e are called external signals.

J. Gonçalves and S. Warnick, IEEE TAC, 2008.
PVdH et al., Automatica, 2013.

Dynamic network setup



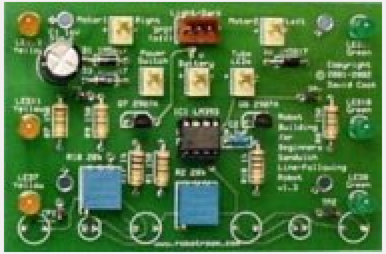
Measured time series:

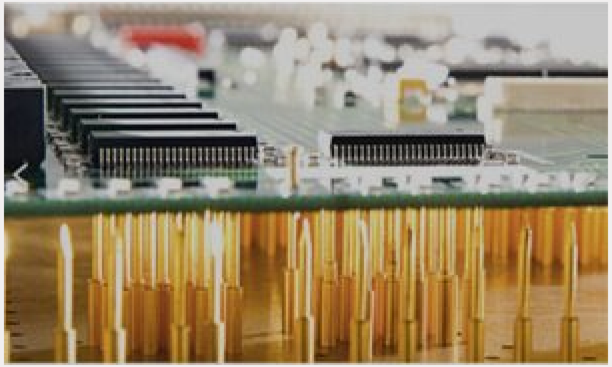
$$\{w_i(t)\}_{i=1,\cdots L};\ \ \{r_j(t)\}_{j=1,\cdots K}$$

Many challenging data-driven modeling and diagnostics challenges appear

- Identification of a local module (known topology)
- Identification of the full network
- Topology estimation
- Identifiability
- Sensor and excitation allocation
- Diagnostics and fault detection
- User prior knowledge of modules
- Distributed identification
- Scalable algorithms

Application: Printed Circuit Board (PCB) Testing

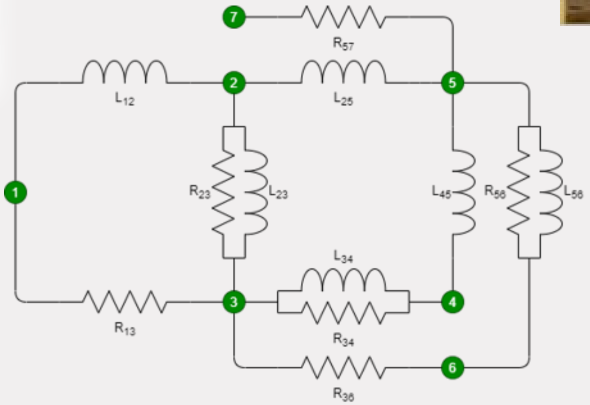


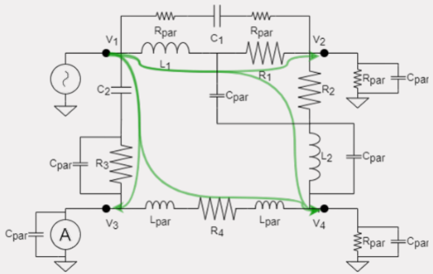


Source: Altium

Detection of

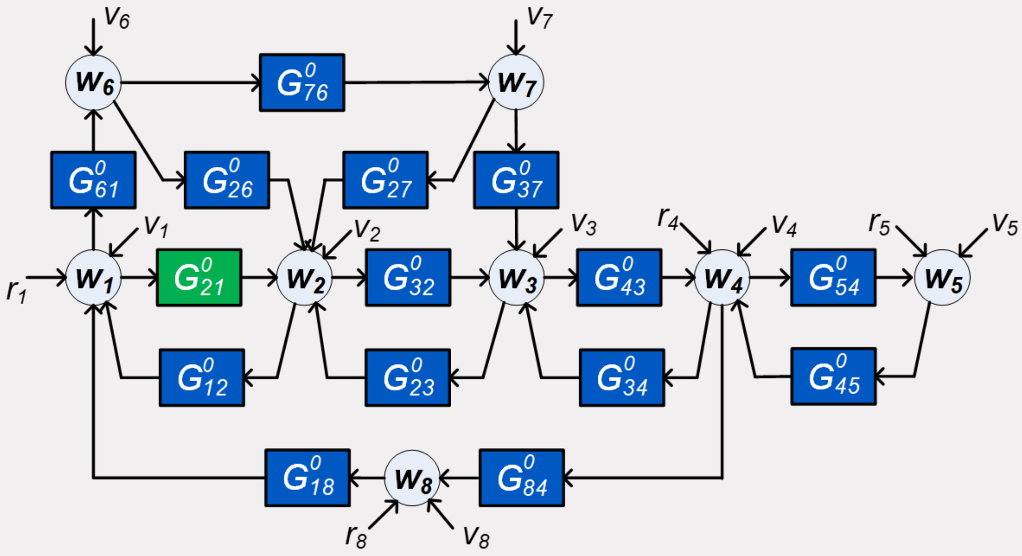
- component failures
- parasitic effects





Single module identification

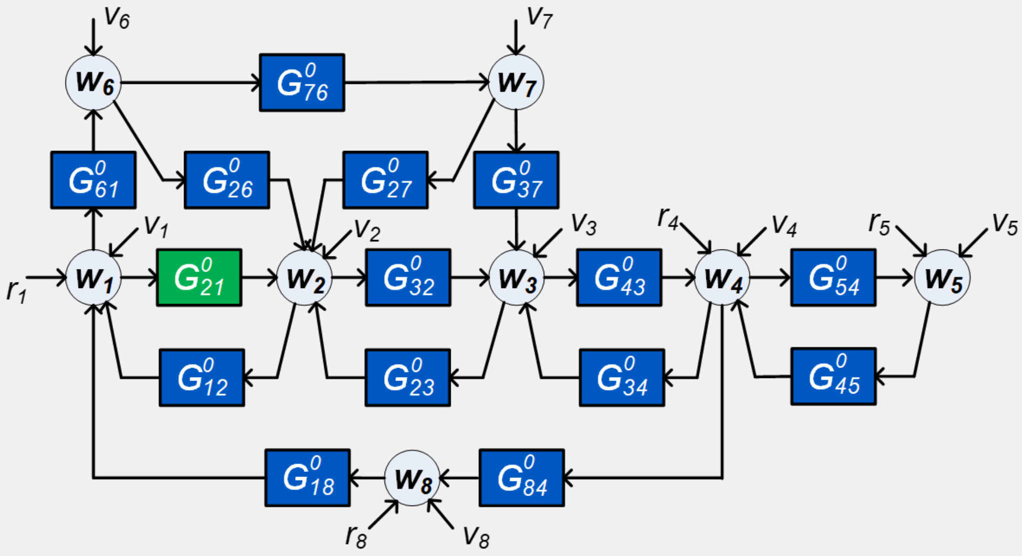
Single module identification



For a network with
known topology:

- Identify G^0_{21} on the basis of measured signals
- Which signals to measure? Preference for local measurements
- When is there enough excitation / data informativity?

Single module identification



Different types of methods:

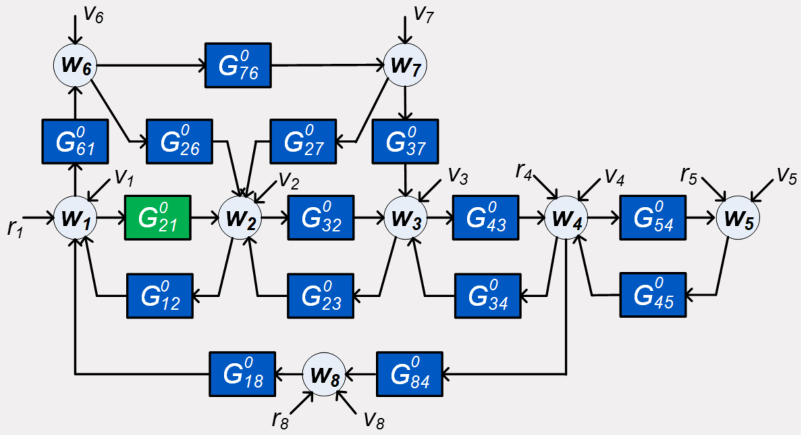
Indirect methods:

- Rely on mappings $r \to w$ and on sufficient excitation signals r

Direct methods:

- Rely on mappings $w \to w$ and use excitation from both r and v signals

Single module identification



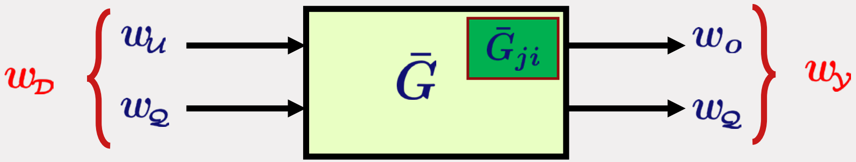
Local direct method:

(consistency and minimum variance properties)

Select a subnetwork:

- Predicted outputs: $w_{\mathcal{Y}}$
- Predictor inputs: $w_{\mathcal{D}}$

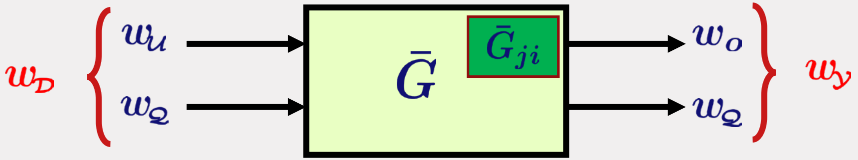
such that prediction error minimization leads to an accurate estimate of G^0_{21}



Note: same node signals can appear in input and output

TU/e

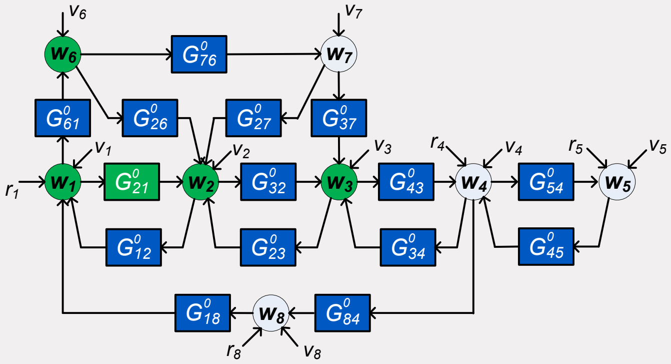
Single module identification

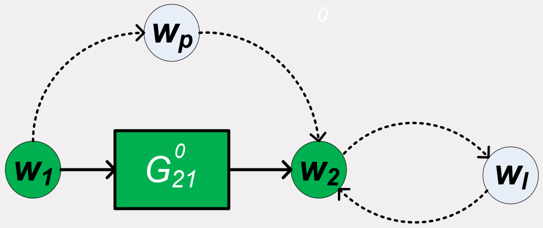


Conditions for arriving at an accurate (consistent) model:

1. Module invariance: $\bar{G}_{ji} = G^0_{ji}$ when removing discarded nodes (immersion)
2. Handling of confounding variables
3. Data-informativity
4. *Technical condition on presence of delays*

Single module identification - module invariance





A sufficient condition for module invariance:

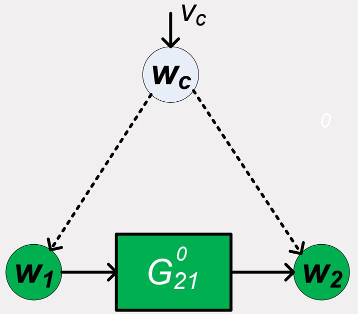
All parallel paths, and loops around the output,
should be "blocked" by a measured node that is present in $w_{\mathcal{D}}$

All other signals can be removed/immersed from the network[2]

Alternative graph-based formulation in terms of disconnecting sets in [3]

[1] Dankers et al., TAC 2016
[3] Shi et al., Automatica 2022
[2] Generalizations available in Linder&Enqvist (2017), Weerts et al, (2020)

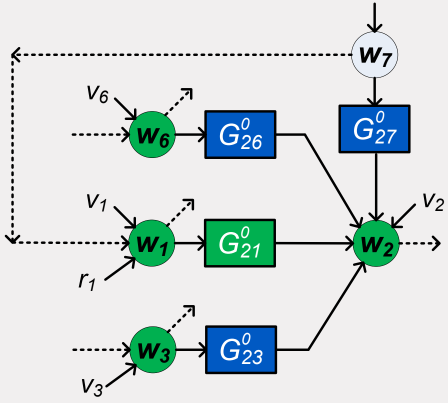
Single module identification - confounding variables



Confounding variable [1][2]:

Unmeasured signal that has (unmeasured paths) to both the input and output of an estimation problem.

In networks they can appear in two different ways:



Direct:

- If disturbances on inputs and outputs are correlated.

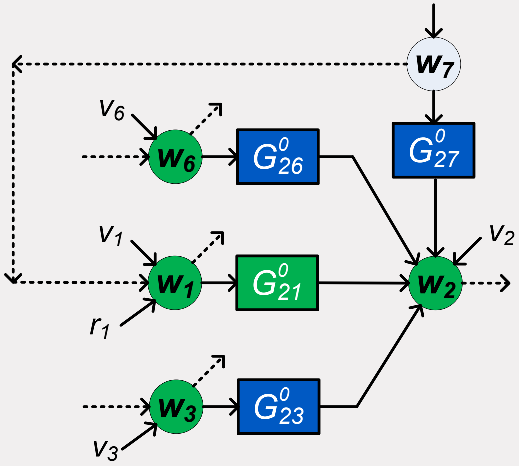
Indirect:

- If non-measured in-neighbors of an output affect signals in the inputs.

[1] J. Pearl, *Stat. Surveys, 3,* 96-146, 2009
[2] A.G. Dankers et al., *Proc. IFAC World Congress*, 2017.

Confounding variables

- **Direct** confounding variables



e.g., v_1 is correlated with v_2

In identification we know how to handle correlated disturbances: we model them!

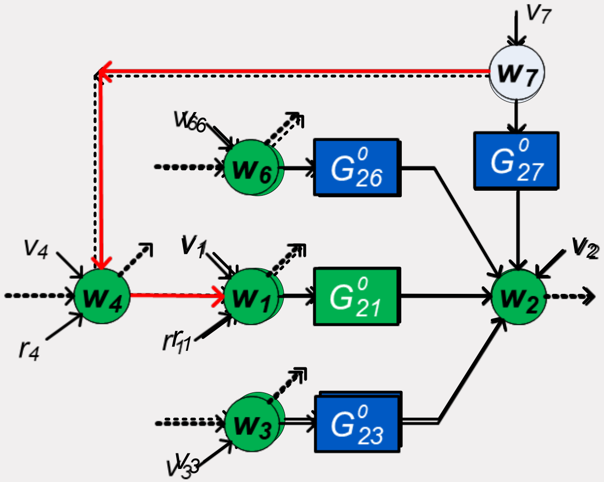
Solution:

Include w_1 as output and use a multivariate noise model

$$w_{\mathcal{D}} = \{w_1, w_3, w_6\} \quad w_{\mathcal{Y}} = \{w_1, w_2\}$$

Confounding variables

- **Indirect** confounding variable:



Non-measurable w_7 is a confounding variable

Two possible solutions:

1. Include w_4 ➡ add predictor input

$$w_{\mathcal{D}} = \{w_1, w_3, w_4, w_6\} \quad w_{\mathcal{Y}} = \{w_2\}$$

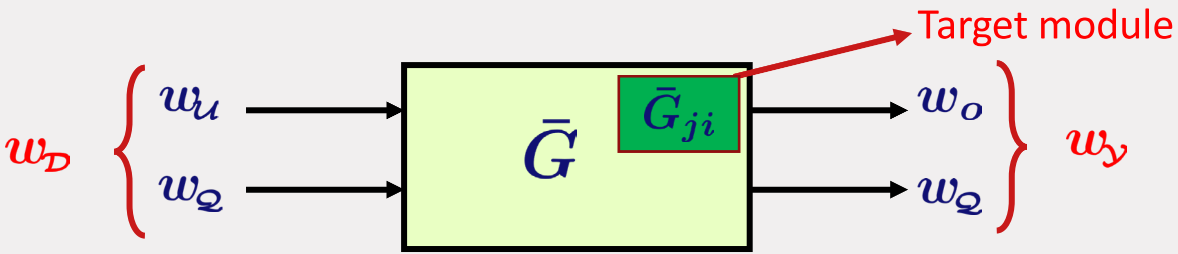
2. Predict w_1 too ➡ add predictor output

$$w_{\mathcal{D}} = \{w_1, w_3, w_6\} \quad w_{\mathcal{Y}} = \{w_1, w_2\}$$

- There are degrees of freedom in choosing the predictor model

Direct method

General setup:

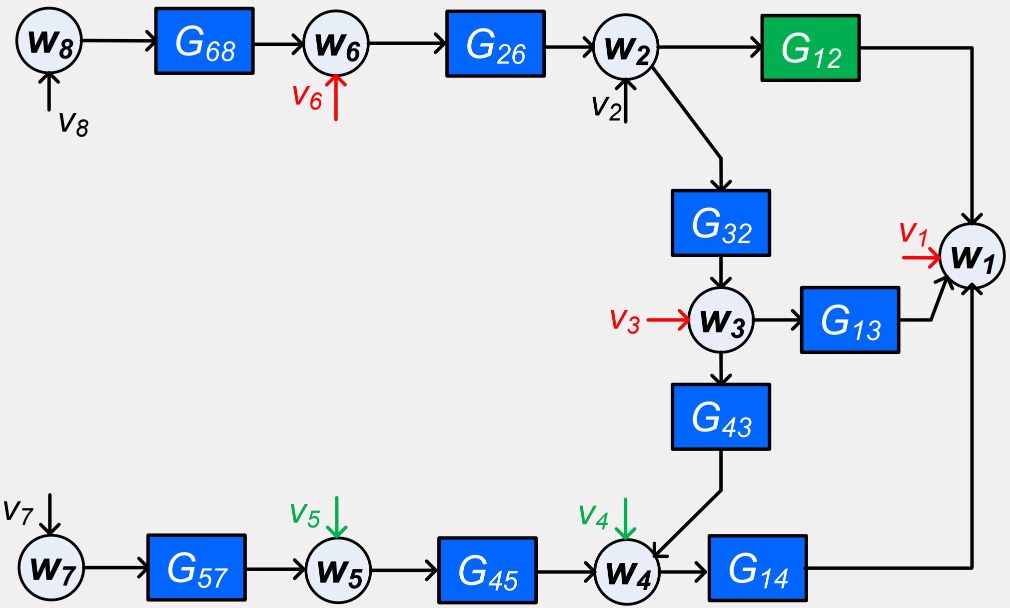


Different algorithms for arriving at predictor models:

- Full input case: include all in-neighbors of $w_{\mathcal{Y}}$
- Minimum node signals case : maximize number of outputs
- User selection case : dedicated choice based on measurable nodes

Different strategies – direct method

- Full input case
- User selection case
- Minimum measurements case



Network with v_1 correlated with v_3 and v_6.
v_4 correlated with v_5.

Full input case

We include all in-neighbors of the predicted outputs as predictor inputs

Maximum use of information in signals

$$w_{\mathcal{D}} = \{2,3,4\} \quad w_{\mathcal{Y}} = \{1\}$$

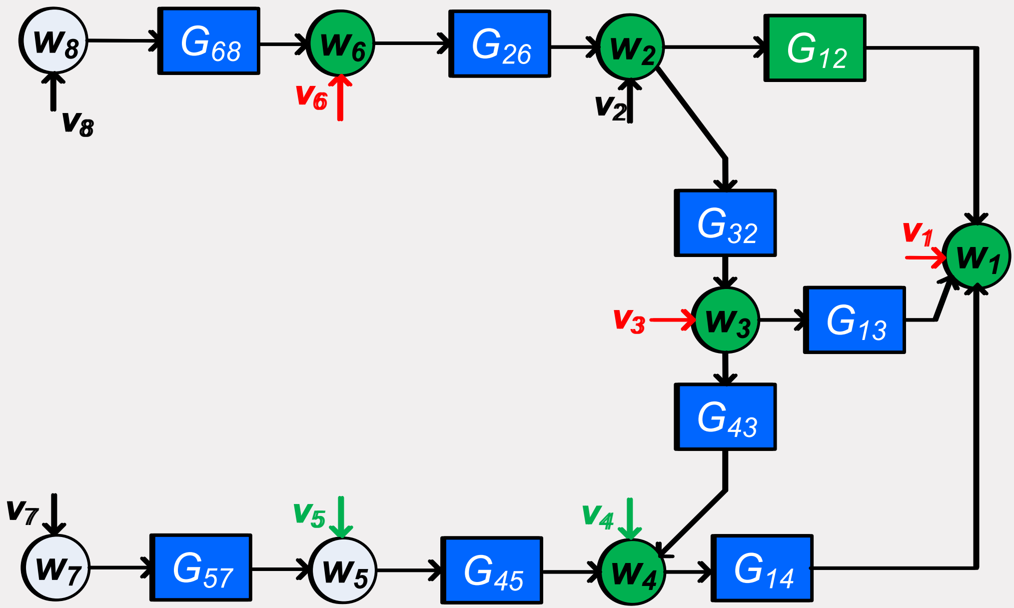
Handling direct confounding variable:

$$w_{\mathcal{D}} = \{2,3,4\} \quad w_{\mathcal{Y}} = \{1,3\}$$

Handling indirect confounding variable:

$$w_{\mathcal{D}} = \{2,3,4,6\} \quad w_{\mathcal{Y}} = \{1,3\}$$

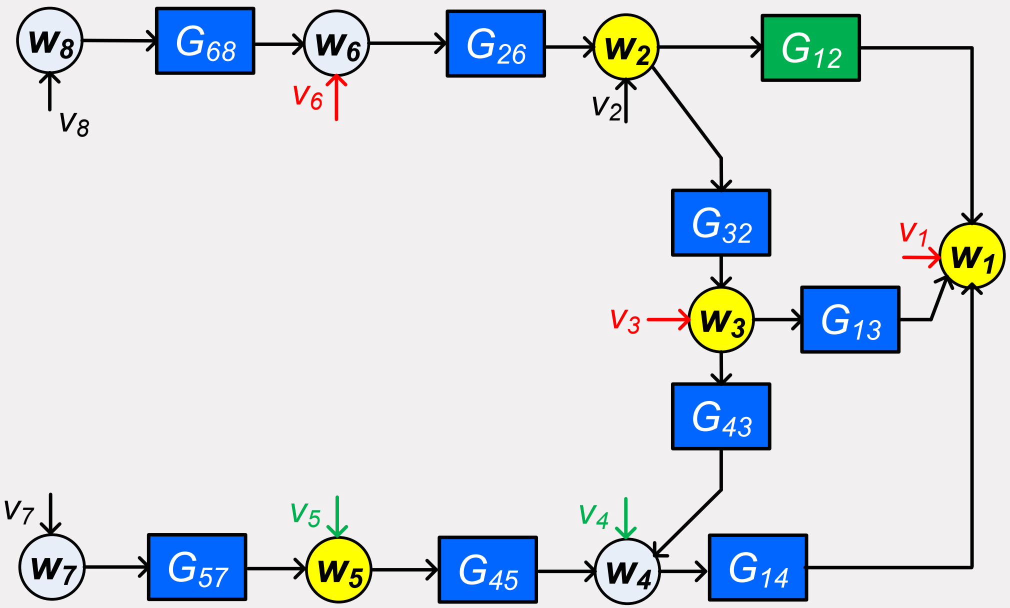
Direct identification $w_{\mathcal{D}} \rightarrow w_{\mathcal{Y}}$



User selection case

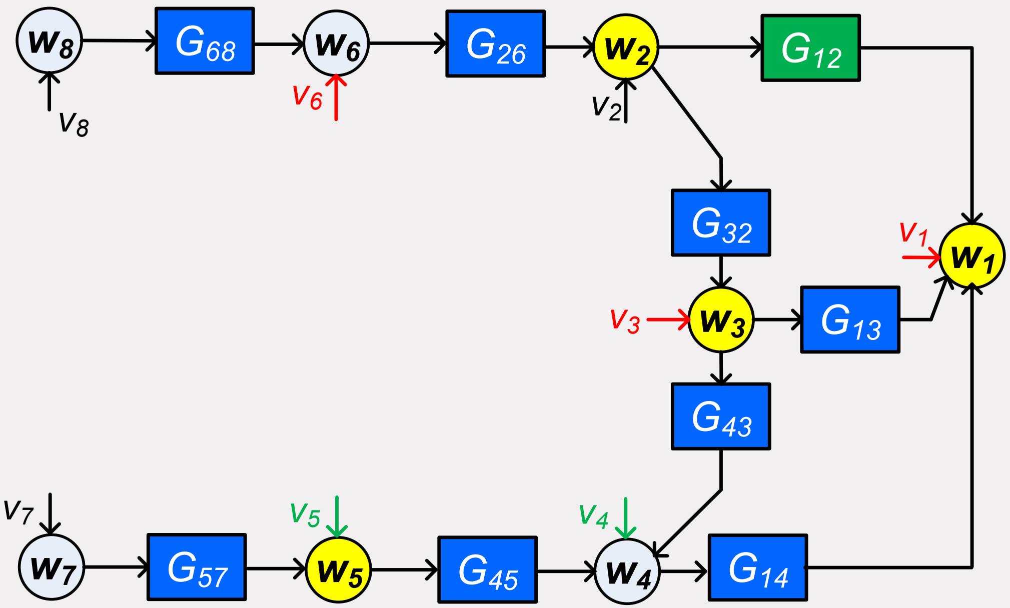
- The user does not have access to all node signals
- Four node signals can be measured
- Parallel path and loop condition is satisfied
- Start with:

$$w_{\mathcal{D}} = \{2, 3\} \quad w_{\mathcal{Y}} = \{1\}$$



User selection case

$$w_{\mathcal{D}} = \{2,3\} \quad w_{\mathcal{Y}} = \{1\}$$



Handling direct confounding variable:

$$w_{\mathcal{D}} = \{2,3\} \quad w_{\mathcal{Y}} = \{1,3\}$$

Indirect confounding variables:

(v_4, v_5):

$$w_{\mathcal{D}} = \{2,3,5\} \quad w_{\mathcal{Y}} = \{1,3,5\}$$

v_6:

$$w_{\mathcal{D}} = \{2,3,5\} \quad w_{\mathcal{Y}} = \{1,2,3,5\}$$

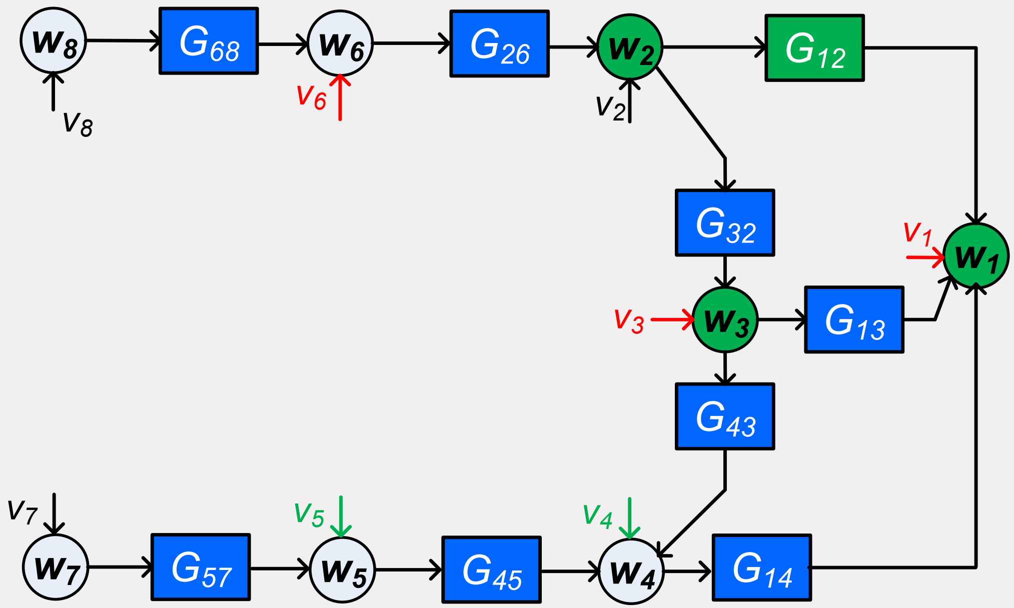
Direct identification $w_{\mathcal{D}} \rightarrow w_{\mathcal{Y}}$

Minimum measurements case

- Select signals to satisfy the parallel path and loop condition
- Handle all confounding variables by including signals in output

$$w_{\mathcal{D}} = \{2, 3\} \quad w_{\mathcal{Y}} = \{1, 2, 3\}$$

Direct identification $w_{\mathcal{D}} \rightarrow w_{\mathcal{Y}}$



Different strategies for same network and target module

Same network with different identification setups that lead to **consistent estimate of the target module** with **Maximum likelihood properties** based on the strategy used.

Full input case	User selection case	Minimum measurements case
$\begin{bmatrix} w_2 \\ w_3 \\ w_4 \\ w_6 \end{bmatrix} \rightarrow \begin{bmatrix} w_1 \\ w_3 \end{bmatrix}$	$\begin{bmatrix} w_2 \\ w_3 \\ w_5 \end{bmatrix} \rightarrow \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_5 \end{bmatrix}$	$\begin{bmatrix} w_2 \\ w_3 \end{bmatrix} \rightarrow \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$

Data informativity conditions: $dim(r) \geq dim(w_{\mathcal{Q}})$ (see later)

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Single module identification

Serious degrees of freedom in selecting the predictor model to satisfy the first two conditions:

1. Module invariance – PPL test
2. Handling confounding variables

While presuming that data-informativity can always be satisfied by adding sufficient # of r-signals.

WRONG!

Single module identification – data-informativity

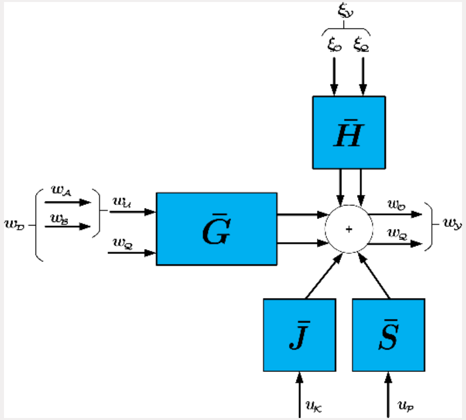
Predictor model equation:

$$w_{\mathcal{Y}}(t) = \bar{G}(q,\theta)w_{\mathcal{D}}(t) + \bar{H}(q,\theta)\xi_{\mathcal{Y}}(t) + \bar{J}(q,\theta)u_{\mathcal{K}}(t) + \bar{S}u_{\mathcal{P}}(t)$$

Typical data-informativity condition:

κ persistently exciting $\boxed{\Phi_{\kappa}(\omega) > 0 \text{ for almost all } \omega}$

$$\kappa(t) := \begin{bmatrix} w_{\mathcal{D}}(t) \\ \xi_{\mathcal{Y}}(t) \\ u_{\mathcal{K}}(t) \end{bmatrix}$$ inputs of the predictor model



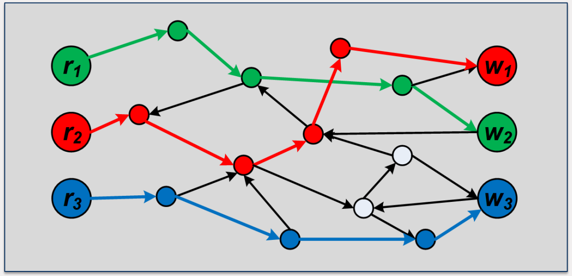
Rank-based condition can generically be satisfied based on a graph-based condition

[1] K.R. Ramaswamy et al., IEEE-TAC, 2021.

Data informativity (path-based condition)

A signal $y(t) = F(q)x(t)$ with x persistently exciting, is persistently exciting iff F has **full row rank**.

This condition can be verified in a generic sense, by considering the **generic rank** of F [1],[2]



$b_{\mathcal{R}\to\mathcal{W}} = 3$

linking to the maximum number of **vertex disjoint paths** between inputs and outputs

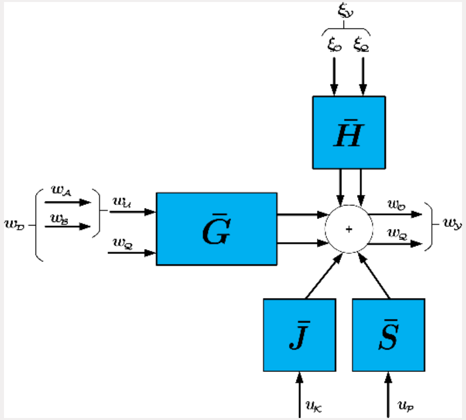
κ persistently exciting holds **generically** if there are $dim(\kappa)$ **vertex disjoint paths** between external signals $\{u, e\}$and $\kappa = \begin{bmatrix} w_{\mathcal{D}} \\ \xi_{\mathcal{Y}} \\ u_{\mathcal{K}} \end{bmatrix}$

Equivalently:

$dim(w_{\mathcal{D}})$ vertex disjoint paths between $\{u, e\} \backslash \{\xi_{\mathcal{Y}}, u_{\mathcal{K}}\}$ and $w_{\mathcal{D}}$

[1] Van der Woude, 1991
[2] Hendrickx, Gevers & Bazanella, CDC 2017, TAC 2019.
[3] VdH et al., CDC 2020.

Data informativity (path-based condition)



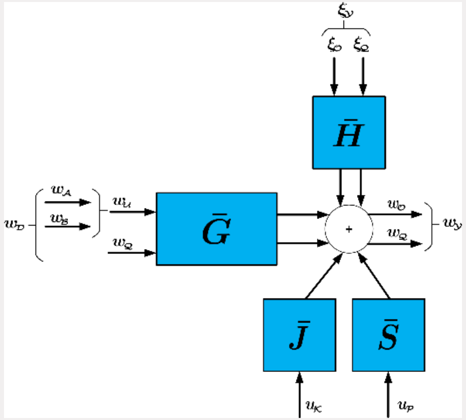
Specific result for networks with **full rank disturbances**:

Every node signal in $w_{\mathcal{Q}}$ requires an excitation in $u_{\mathcal{P}}$ having a 1-transfer to $w_{\mathcal{Y}}$

$$w_{\mathcal{Y}}(t) = \bar{G}(q,\theta)w_{\mathcal{D}}(t) + \bar{H}(q,\theta)\xi_{\mathcal{Y}}(t) + \bar{J}(q,\theta)u_{\mathcal{K}}(t) + \bar{S}u_{\mathcal{P}}(t)$$

- For every node in $w_{\mathcal{Q}}$ we need a *u*-excitation
- More expensive experiments with growing # outputs
- A node $w_{\mathcal{Q}}$ whose excitation appears in $u_{\mathcal{K}}$ can never be sufficiently excited

Data informativity (path-based condition)



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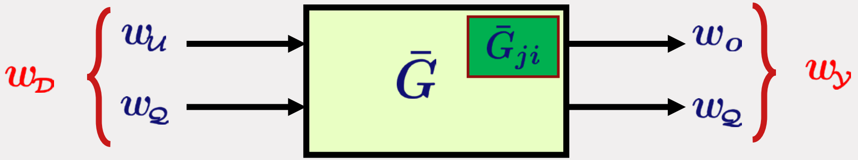
Additional condition for a node $w_{\mathcal{Q}}$ to be effectively ``excitable'':

Every loop around a node in $w_{\mathcal{Q}}$ should be blocked by a node in $w_{\mathcal{D}}$.

This additional graph-based condition needs to be integrated in the predictor model algorithm

[1] VdH et al., IFAC 2023 submitted.

Single module identification



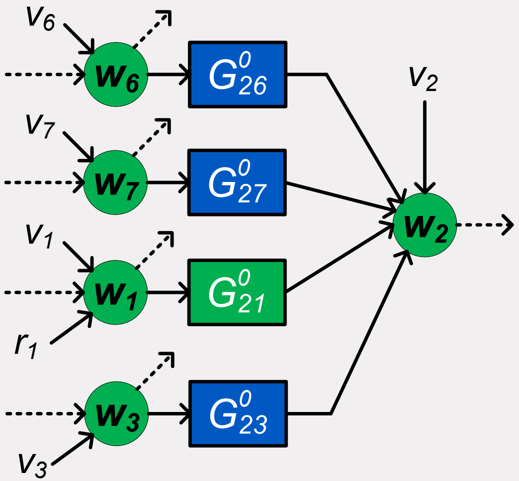
Conditions for arriving at an accurate model:

1. Module invariance: $\bar{G}_{ji} = G^0_{ji}$
2. Handling of confounding variables
3. Data-informativity
4. *Technical conditions on presence of delays*

Path-based conditions on the network graph

Single module identification

Typical solution:



- MISO (sometimes MIMO) estimation problem
- to be solved by your favorite estimation algorithm

Machine learning in local module identification

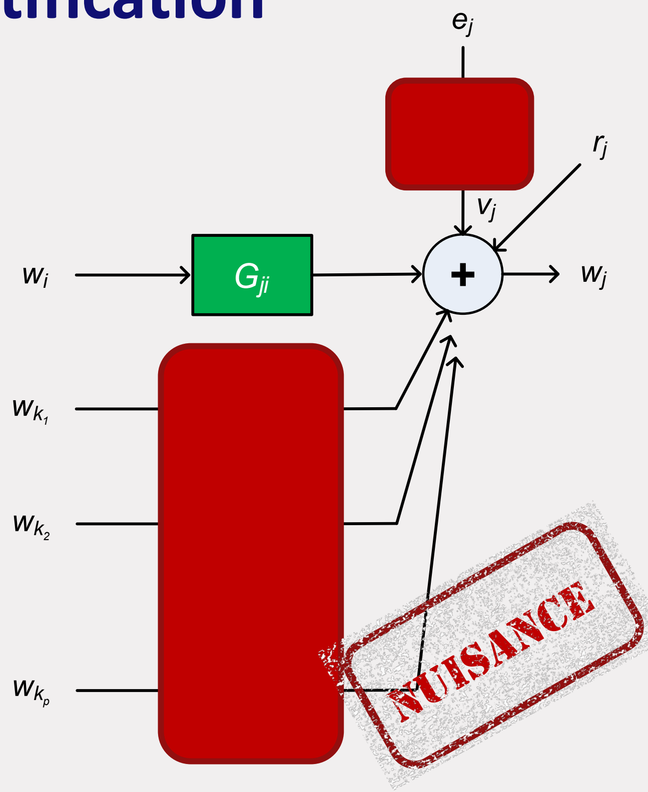
- MISO identification with all modules parameterized
- Brings in two major problems :
  - Large number of parameters to estimate
  - Model order selection step for each module (CV, AIC, BIC)

- For 5 modules, combinations = 244,140,625

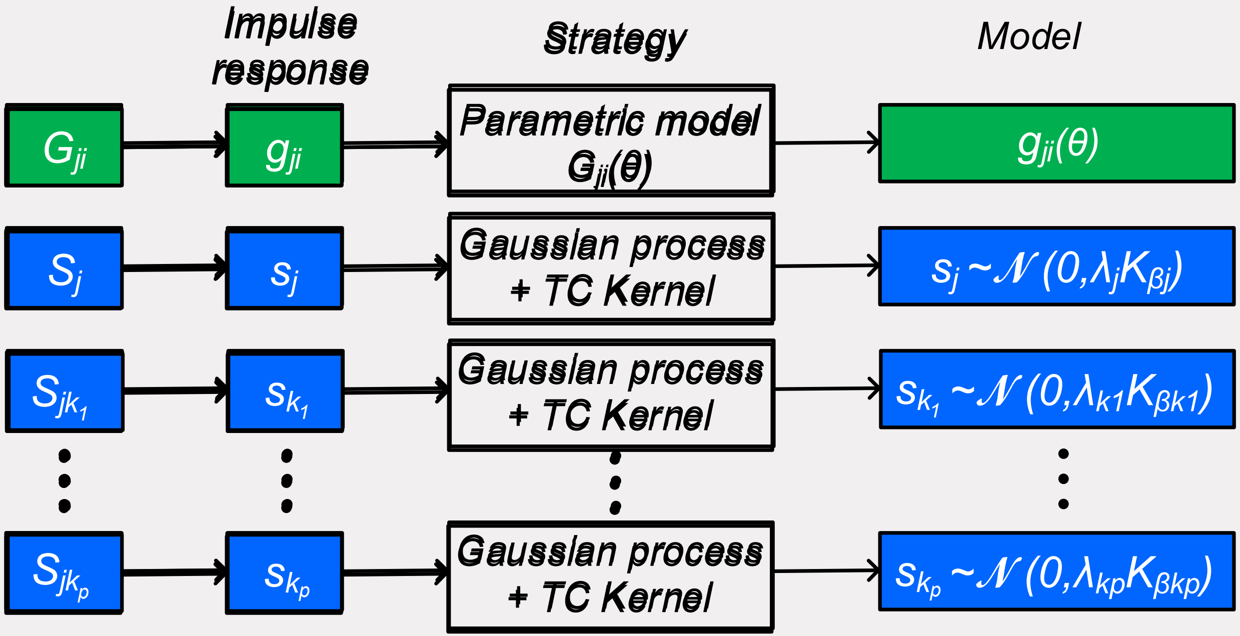
Increases variance

Computationally challenging

- We need only the target module. No NUISANCE!



Machine learning in local module identification



- smaller no. of parameters
- simpler model order selection step
- scalable to large dynamic networks
- simpler optimization problems to estimate parameters

Maximize marginal likelihood of output data: $\hat{\eta} = \underset{\eta}{\operatorname{argmax}}\, p(w_j; \eta)$

$$\eta := \begin{bmatrix} \theta & \lambda_j & \lambda_{k_1} & \dots & \lambda_{k_p} & \beta_j & \beta_{k_1} & \dots & \beta_{k_p} & \sigma_j^2 \end{bmatrix}^{\top}$$

[1] Everitt et al., *Automatica* 2017.
[2] K.R. Ramaswamy et al., *Automatica*, 2021.

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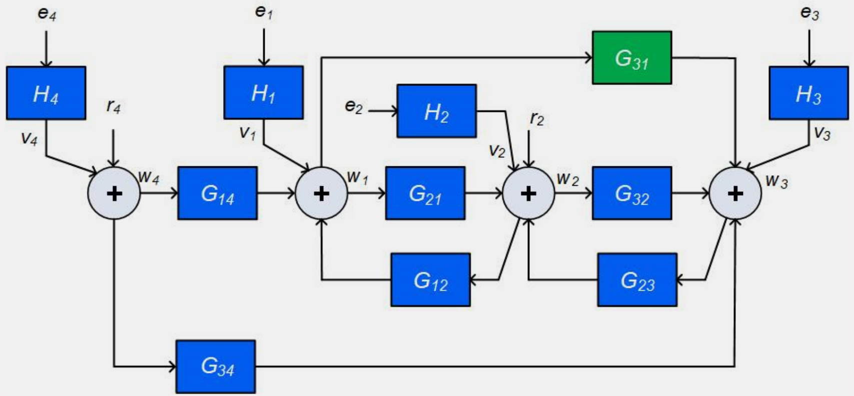
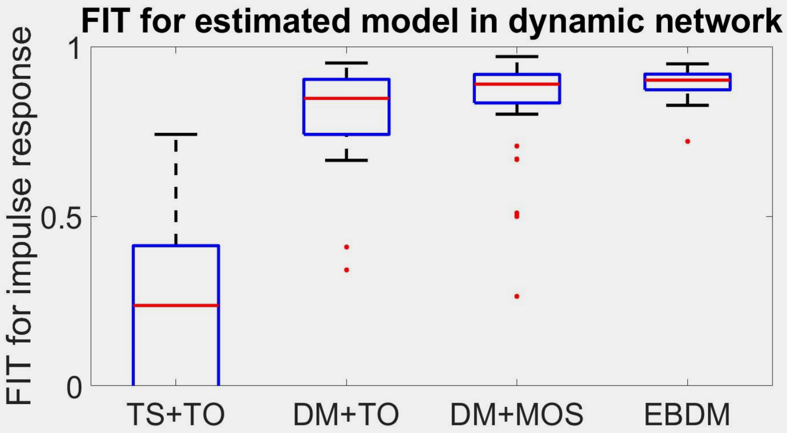
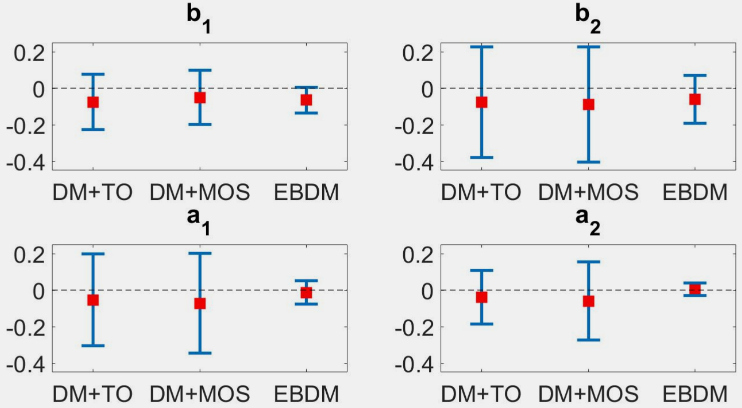
Numerical simulation

- Identify G_{31} given data
- 50 independent MC simulation
- Data = 500







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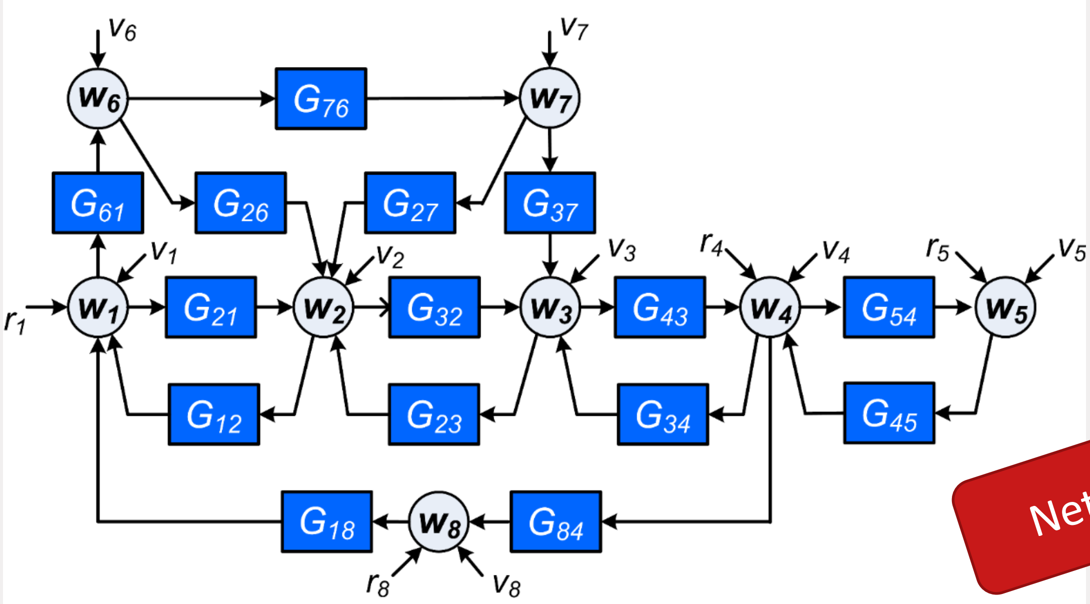
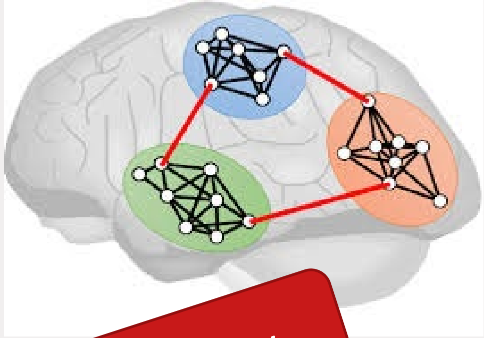
Summary single module identification

- Path-based conditions that the predictor model should satisfy
- Different algorithms for synthesizing predictor model
- Degrees of freedom in sensor / actuator placement
- Methods for **consistent** and **minimum variance** module estimation, and effective (scalable) algorithms

Generic network identifiability

Full network identification





Network identifiability

Under which conditions can we estimate the topology and/or dynamics of the full network?

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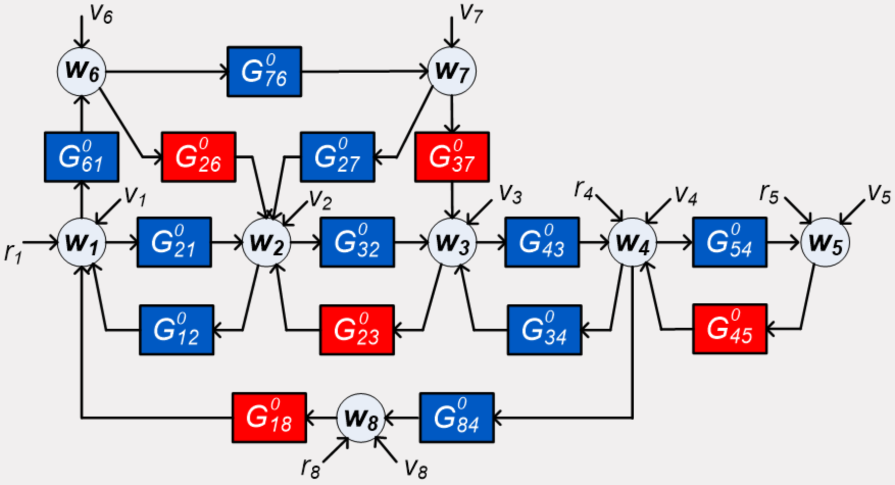
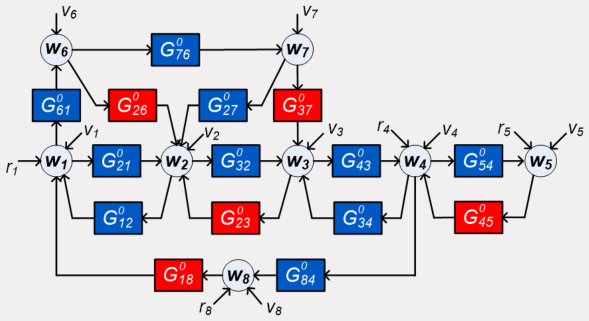
Network identifiability



blue = unknown
red = known

Question: Can different dynamic networks be *distinguished* from each other from measured signals w, r ?

Network identifiability



The identifiability problem:

The network **model**:

$$w(t) = G(q)w(t) + R(q)r(t) + \underbrace{H(q)e(t)}_{v(t)}$$

can be transformed with any rational $P(q)$:

$$P(q)w(t) = P(q)\{G(q)w(t)+R(q)r(t)+H(q)e(t)\}$$

to an **equivalent model**:

$$w(t) = \tilde{G}(q)w(t) + \tilde{R}(q)r(t) + \tilde{H}(q)e(t)$$

→ **Nonuniqueness,** unless there are structural constraints on G, R, H.

[1] Weerts, Linder et al., Automatica, 2019.
[2] Bottegal et al., SYSID 2017

Network identifiability

Consider a **network model set**:

$$\mathcal{M} = \{(G(\theta), R(\theta), H(\theta))\}_{\theta \in \Theta}$$

representing structural constraints on the considered models:

- modules that are fixed and/or zero (topology)
- locations of excitation signals
- disturbance correlation

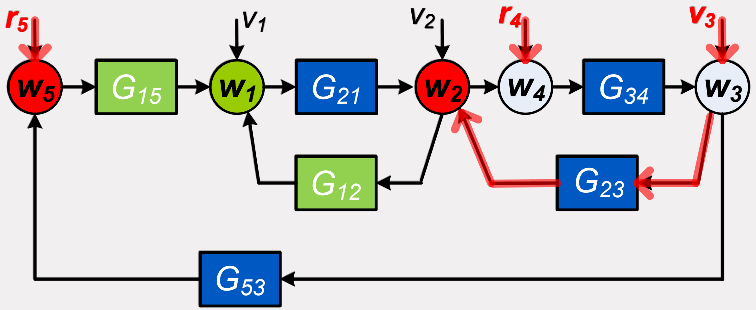
Generic identifiability of $\mathcal{M}$:

- There do not exist distinct equivalent models (generating the same data)
- for almost all models in the set.

[1] Weerts et al., SYSID2015; Weerts et al., Automatica, March 2018;
[2] Bazanella, CDC2017; Hendrickx et al., IEEE-TAC, 2019.

Example 5-node network

Conditions for identifiability → rank conditions on transfer function



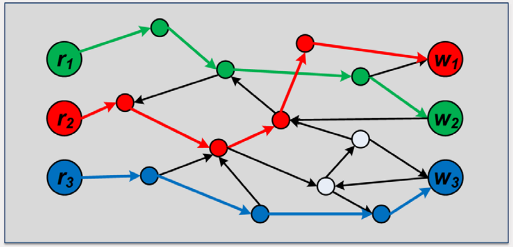
Full row rank of

$$\begin{bmatrix} v_3 \\ r_4 \\ r_5 \end{bmatrix} \longrightarrow \begin{bmatrix} w_2 \\ w_5 \end{bmatrix}$$

For the **generic case**, the rank can be calculated by a graph-based condition[1],[2] :

Generic rank = number of vertex-disjoint paths

2 vertex-disjoint paths → full row rank 2



The rank condition has to be checked for all nodes.

[1] Van der Woude, 1991
[2] Hendrickx, Gevers & Bazanella, CDC 2017, TAC 2019

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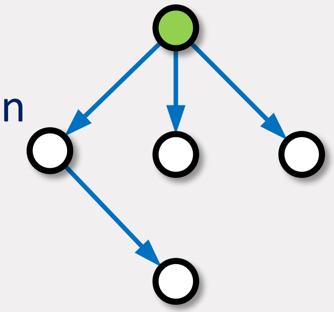
Synthesis solution for network identifiability

Allocating external signals for generic identifiability:

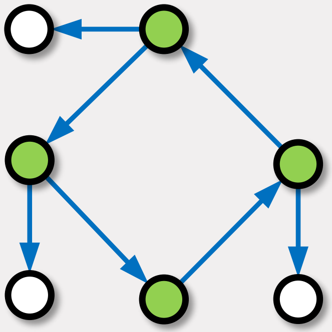
1. Cover the graph of the network model set by a set of **disjoint pseudo-trees**

   Pseudo-trees:

   Tree with root in green



   Cycle with outgoing trees;
   Any node in cycle is root



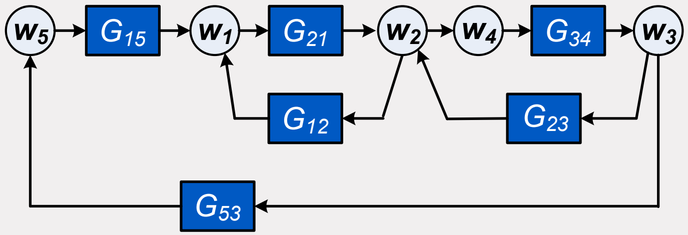
   Edges are **disjoint** and all out-neighbours of a node are in the same pseudo-tree

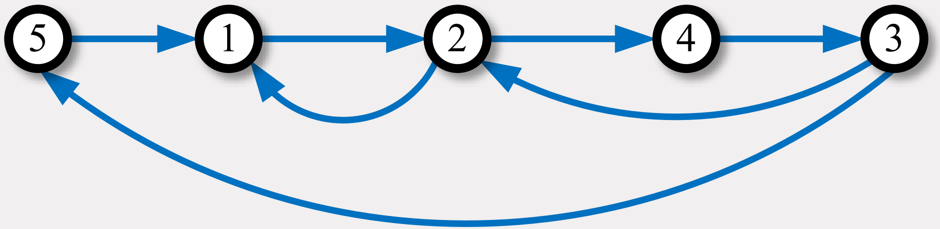
2. Assign an independent external signal (r or e) at a root of each pseudo-tree.

   This guarantees generic identifiability of the model set.

[1] X. Cheng, S. Shi and PVdH, TAC, February 2022.

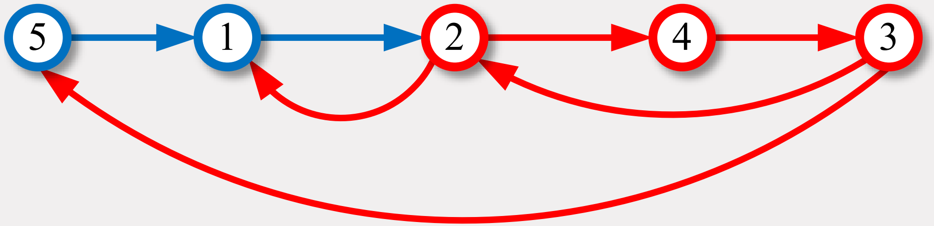
Where to allocate external excitations for network identifiability?





All indicated modules are parametrized

Two disjoint pseudo-trees



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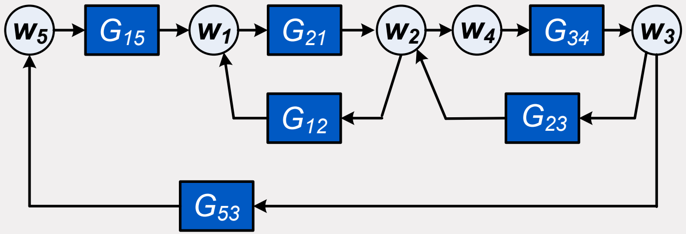
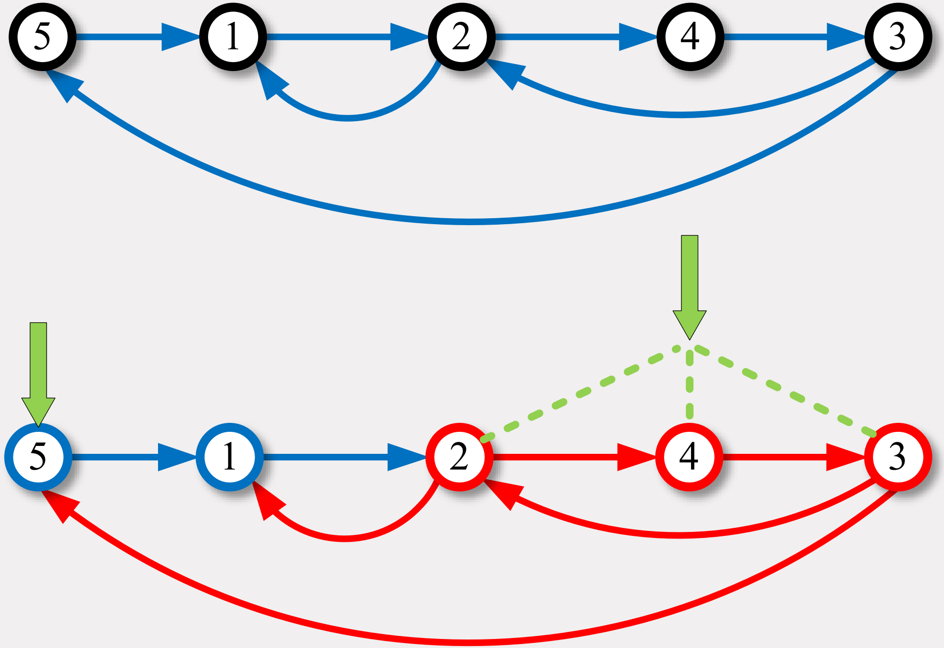
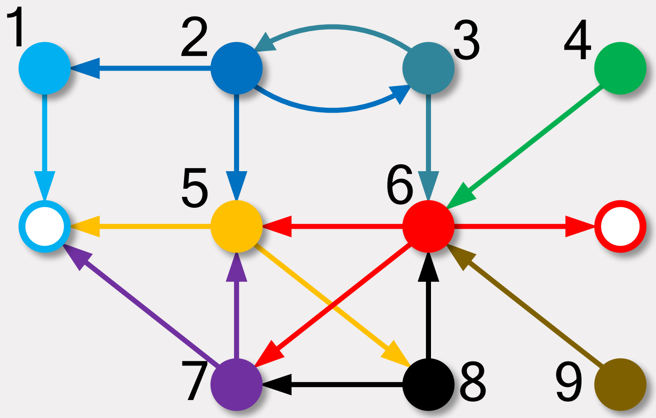




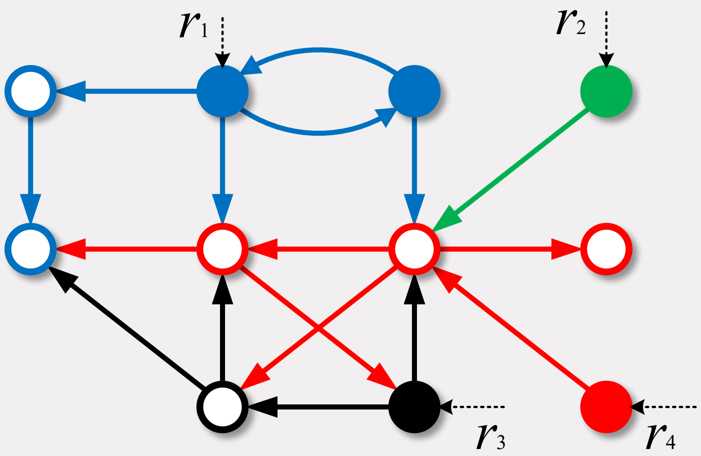
Two independent excitations
guarantee
generic network identifiability

[1] X. Cheng, S. Shi and PVdH, CDC 2019.

Where to allocate external excitations for network identifiability?



Pseudo-tree merging algorithm [1]



- Nodes are signals $\boldsymbol{w}$ and external signals $(\boldsymbol{r}, \boldsymbol{e})$ that are input to parametrized link
- Known (nonparametrized) links do not need to be covered

[1] X. Cheng, S. Shi and PVdH, TAC, February 2022.

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Summary identifiability of full network

Identifiability of network model sets is determined by

- Presence and location of external signals, and
- Correlation of disturbances
- Topology of parametrized modules

- Graphic-based tool for synthesizing allocation of external signals

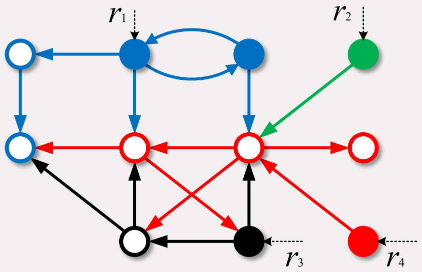
Extensions:

- Situations where not all node signals are measured [1]

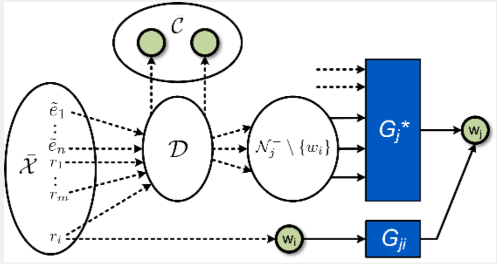
[1] Bazanella, CDC 2019.

Related topics...

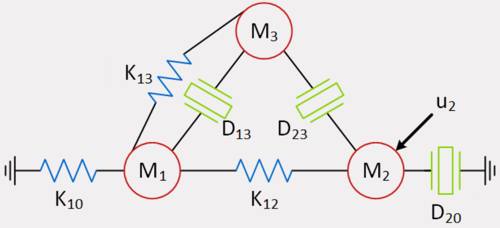
- Excitation allocation for full network identifiability[1]



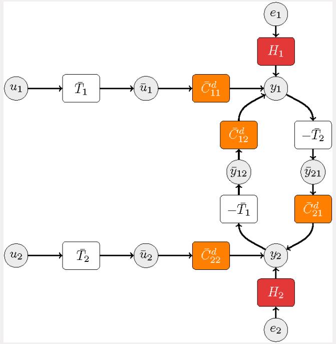
- Subnetwork identifiability[3]



- Diffusively coupled networks [2]



- Distributed controller identification[4]



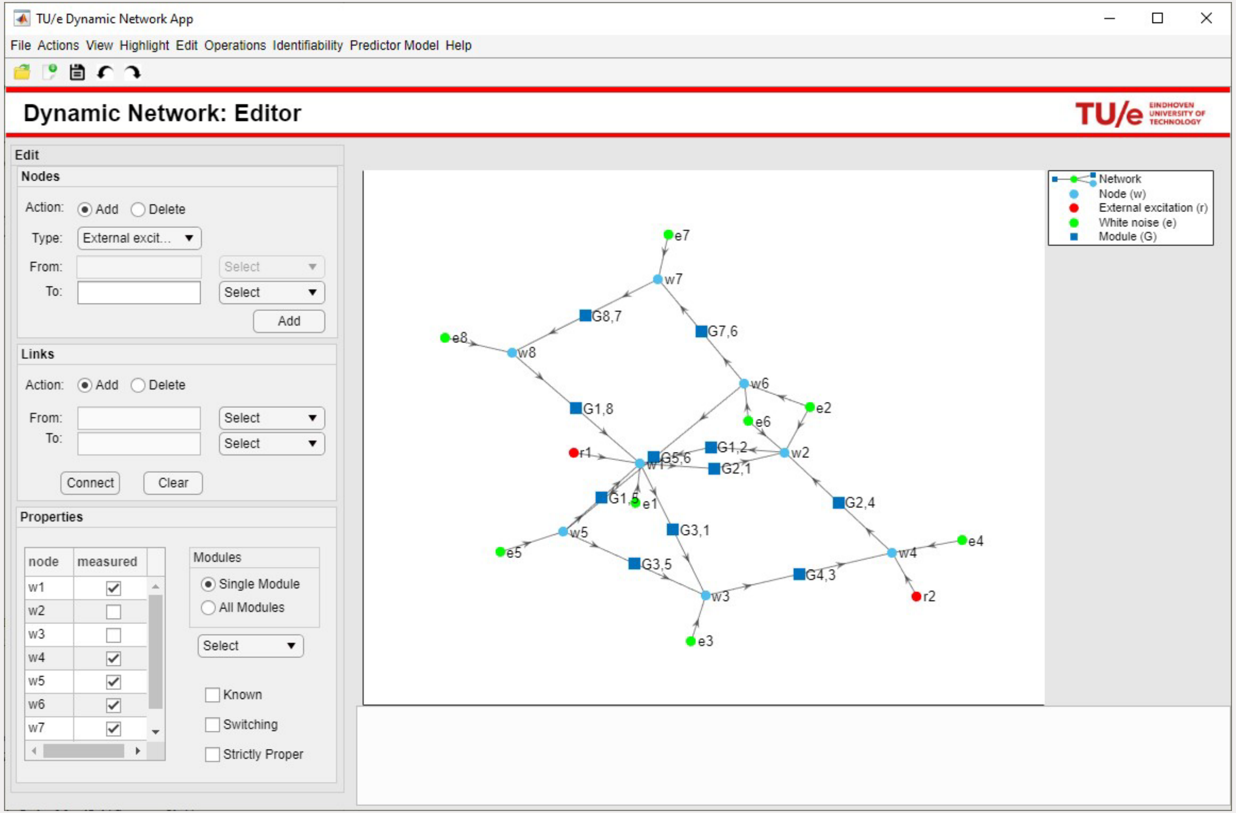
[1] Cheng et al., IEEE-TAC, February 2022.

[3] Shi et al., IEEE-TAC, January 2023.

[2] Kivits et al., IEEE- TAC, June 2023.

[4] Steentjes, PhD thesis, June 2022.

Algorithms implemented in SYSDYNET Toolbox



Structural analysis and operations on dynamic networks

- Edit and manipulate
- Assign properties to nodes and modules
- Immersion of nodes, PPL test
- Generic identifiability analysis and synthesis
- Predictor model selection for single module ID

to be complemented with

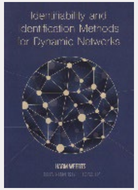
- estimation algorithms for single module and full network ID;
- topology estimation

Beta-version as of mid February 2023 to be downloaded from www.sysdynet.net

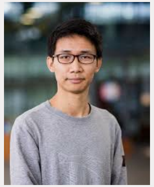
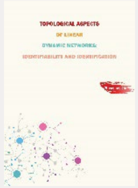
ERC SYSDYNET Team: data-driven modeling in dynamic networks

Research team:

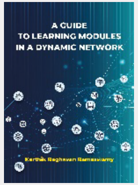

Arne Dankers

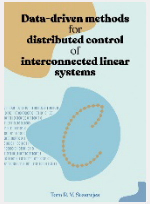
Harm Weerts

Shengling Shi

Karthik Ramaswamy

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European Research Council

Further reading

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