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Network reconstruction using dynamical structure functions

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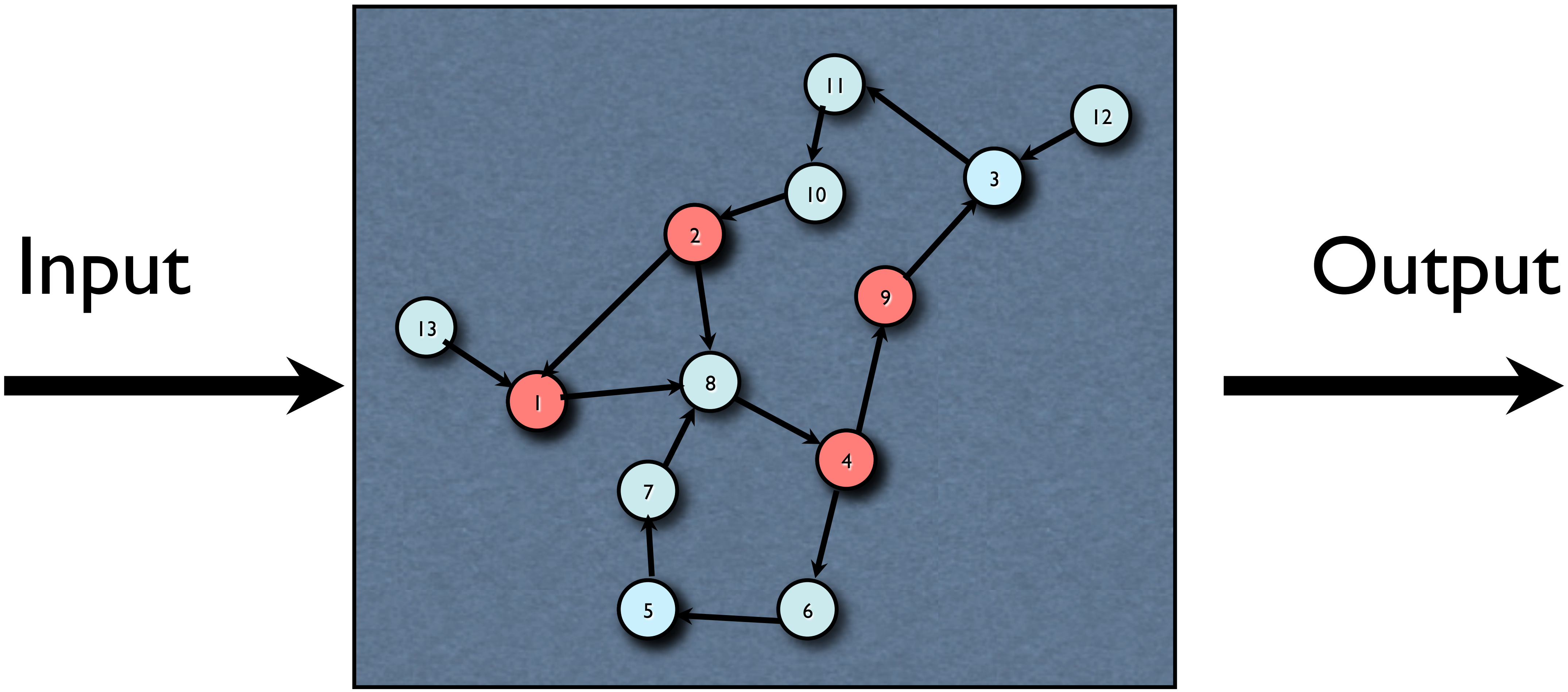
Focus Period, LCCC, Lund
10/2012

Network reconstruction



Modelling chemical reaction networks:
States: concentrations of distinct chemical species in the system.
Dynamics: chemical kinetics governing reaction rates.
Boolean structure: encodes which species react with each other to produce or regulate the production of other species in the system.
Example: gene regulatory networks in cellular biology.

1. Sontag, Essay in Biochemistry 2008.
2. Cantone, et. al. Cell, 2009.

Motivation:
Structure implies functionality:

1. Structural controllability.
2. Structure in MAS.
3. Network motif.

Incomplete knowledge about network
=> incorrect conclusion

1. Silverman and Glover IEEE TAC, 1977, Liu et al. Nature, 2011
2. Olfati-Saber and Murray IEEE TAC 2004.
3. Ma et. al. Cell, 2009. Milo et. al. Science 2002.

Till year 2008, x% of the molecular interactions in cells of Yeast and y% of human are still **unknown**?

x=80
y=99.7

1. Yu et. al. Science, 2008
2. Stumpf et. al. PNAS, 2008.

Current Status

Cell

Resource

A Yeast Synthetic Network for In Vivo Assessment of Reverse-Engineering and Modeling Approaches

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SUMMARY

Systems biology approaches are extensively used to model and reverse engineer gene regulatory networks from experimental data. Conversely, synthetic biology allows "de novo" construction of a regulatory network to seed new functions in the cell. At present, the usefulness and predictive ability of modeling and reverse engineering cannot be assessed and compared rigorously. We built in the yeast *Saccharomyces cerevisiae* a synthetic network, IRMA, for in vivo "benchmarking" of reverse-engineering and modeling approaches. The network is composed of five genes regulating each other through a variety of regulatory interactions; it is negligibly affected by endogenous genes, and it is responsive to small molecules. We measured time series and steady-state expression data after multiple perturbations. These data were used to assess state-of-the-art modeling and reverse-engineering techniques. A semiquantitative model was able to capture and predict the behavior of the network. Reverse engineering based on differential equations and Bayesian networks correctly inferred regulatory interactions from the experimental data.

describe changes in concentration of each gene transcript and protein in a network, as a function of their regulatory interactions (gene regulatory network).

The usefulness of a model lies in its ability to formalize the knowledge about the biological process at hand, to identify inconsistencies between hypotheses and observations, and to predict the behavior of the biological process in yet untested conditions. There are a variety of mathematical formalisms proposed in literature (Di Ventura et al., 2006; Szallasi et al., 2006) to model biological circuits, with ordinary differential equations being the most common.

Synthetic biology aims to use such models to design unique biological "circuits" (synthetic networks) in the cell able to perform specific tasks (e.g., periodic expression of a gene of interest) or to change a biological process in a desired way (e.g., modify metabolism to produce a specific compound of interest) (Gardner et al., 2000; Khosla and Keasling, 2003; Ro et al., 2006).

Interactions among genes, when unknown, can be identified from gene expression data using reverse-engineering methods. Typically, the data consist of measurements at steady state after multiple perturbations (i.e., gene overexpression, knockdown, or drug treatment) or at multiple time points after one perturbation (i.e., time series data). Successful applications of these approaches have been demonstrated in bacteria, yeast, and, recently, in mammalian systems (Basso et al., 2005; Della Gatta et al., 2008; di Bernardo et al., 2005; Faith et al., 2007; Gardner et al., 2003). A plethora of reverse-engineering approaches

network. Reverse engineering based on differential equations and Bayesian networks correctly inferred regulatory interactions from the experimental data.

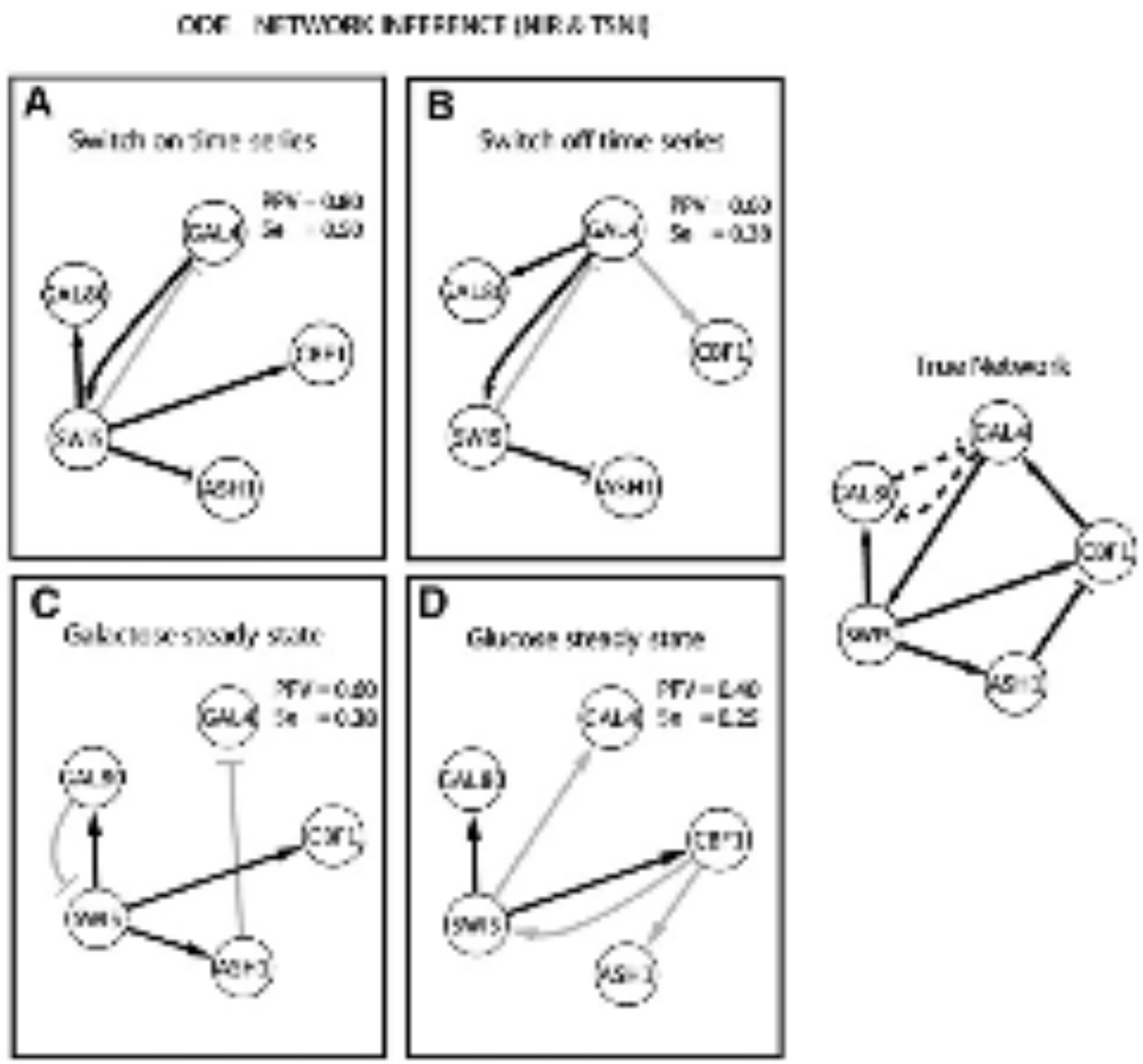


Figure 5. Reverse Engineering of the IRMA Gene Network from Steady-State and Time Series Experimental Data Using the ODE-Based Approach

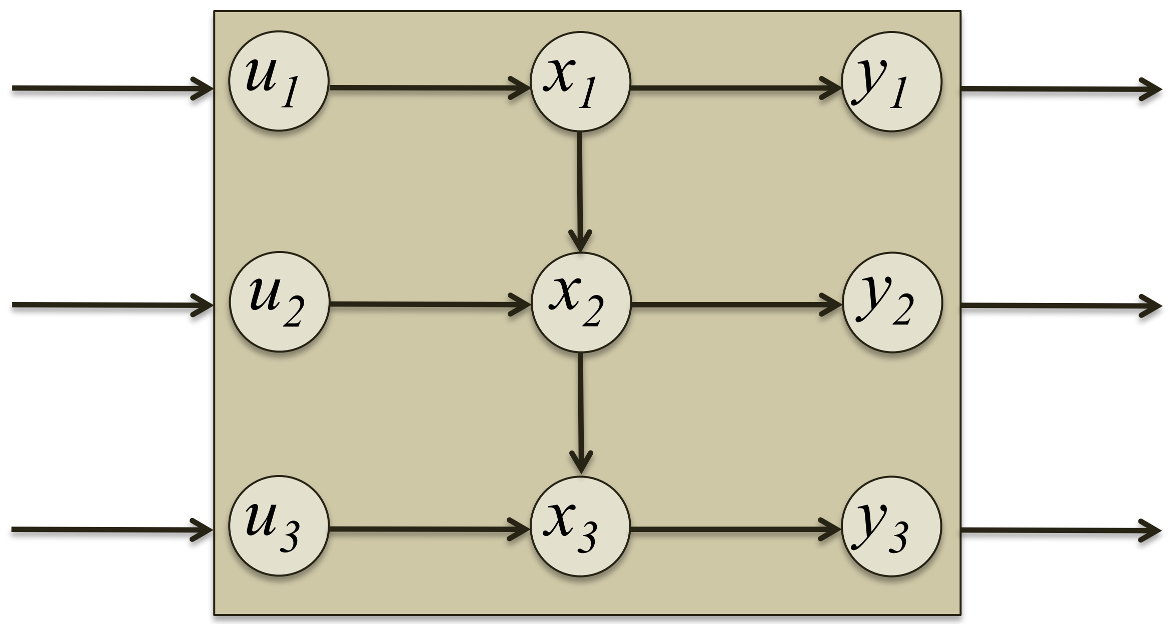
The true network shows the regulatory interactions among genes in IRMA. Dashed lines represent protein-protein interactions. Directed edges with an arrow end represent activation, whereas a dash end represents inhibition.

mance of an algorithm that randomly assigns edges between pair of genes. For example, for a fully connected network, the random algorithm would have a 100% accuracy (PPV = 1) for all the levels of sensitivity (as any pair of genes is connected in the real network). In our network, the expected PPV for a random guess of directed interactions among genes is PPV = 0.40 (40%), so any value higher than 0.4 will be significant. In the case of undirected interactions, the random PPV = 0.70 (70%).

On time series data, the best performance both in terms of PPV and of Se was achieved by the ODE approach (TSNI) on the switch-on data with a PPV = 0.80 and a Se = 0.50 (Figure 5A). ODE performed better than random (PPV = 0.60, Se = 0.38) also on the switch-off data, in Figure 5B, albeit with a lower precision.

Dynamic Bayesian networks (BANJO) performed better than random (PPV = 0.60, Se = 0.38) only on the switch-off experiment, with the same performance as TSNI for this data set (Figure S8B). Bayesian networks failed to perform better than random on the switch-on data (Figure S8A) probably because of the lower number of points (16) as compared to the switch-off time series (21 points).

By comparison of the inferred networks from BANJO and TSNI in the switch-on and switch-off experiments, it is clear that both methods are extracting similar information, albeit with less precision in the case of BANJO. If we consider only the interactions inferred by both methods on the same data set (compare Figure 5A with Figure S8A, and Figures 5B and S8B), we obtained only two interactions, both correct (PPV = 1). This result


u_1
x_1
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u_3
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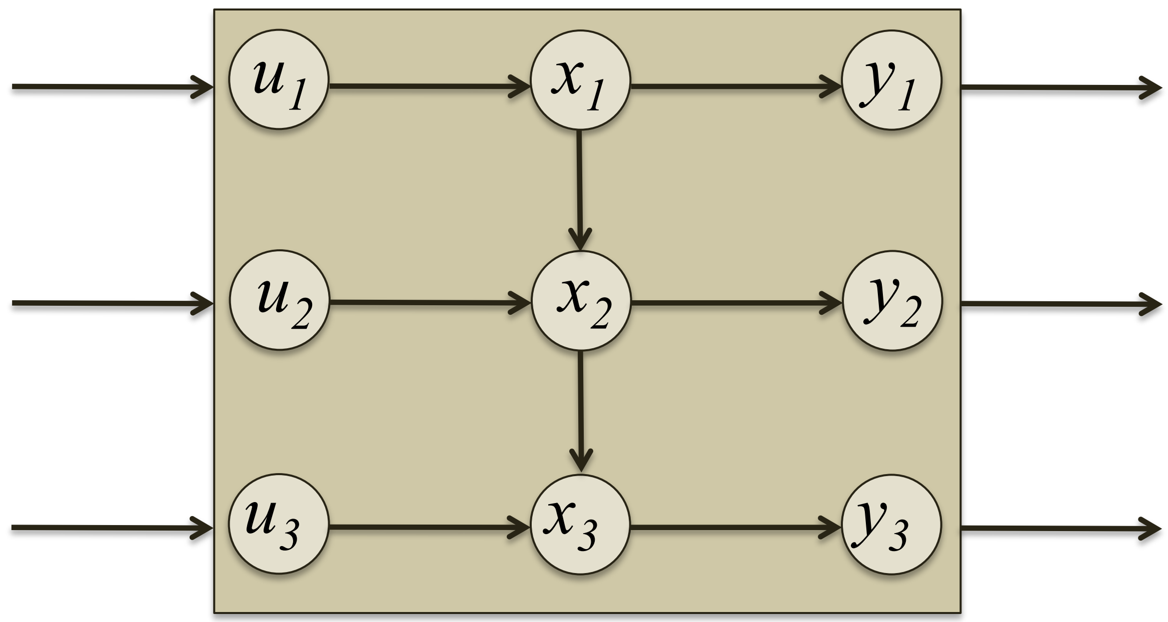

State Space Realisation

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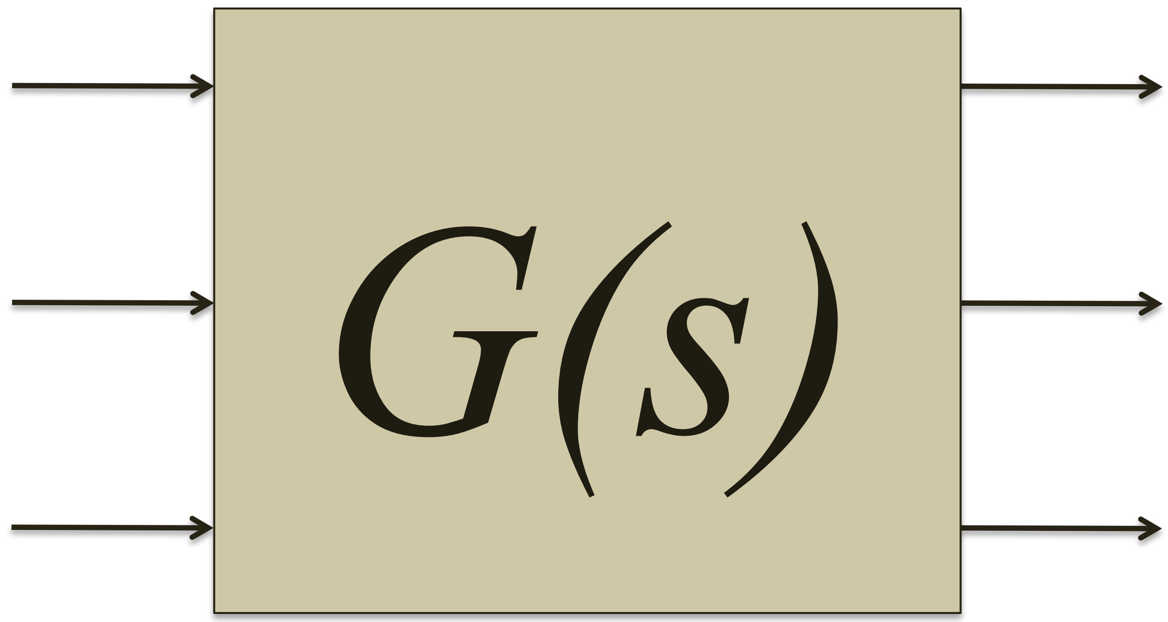

Transfer Function

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What is System Structure?

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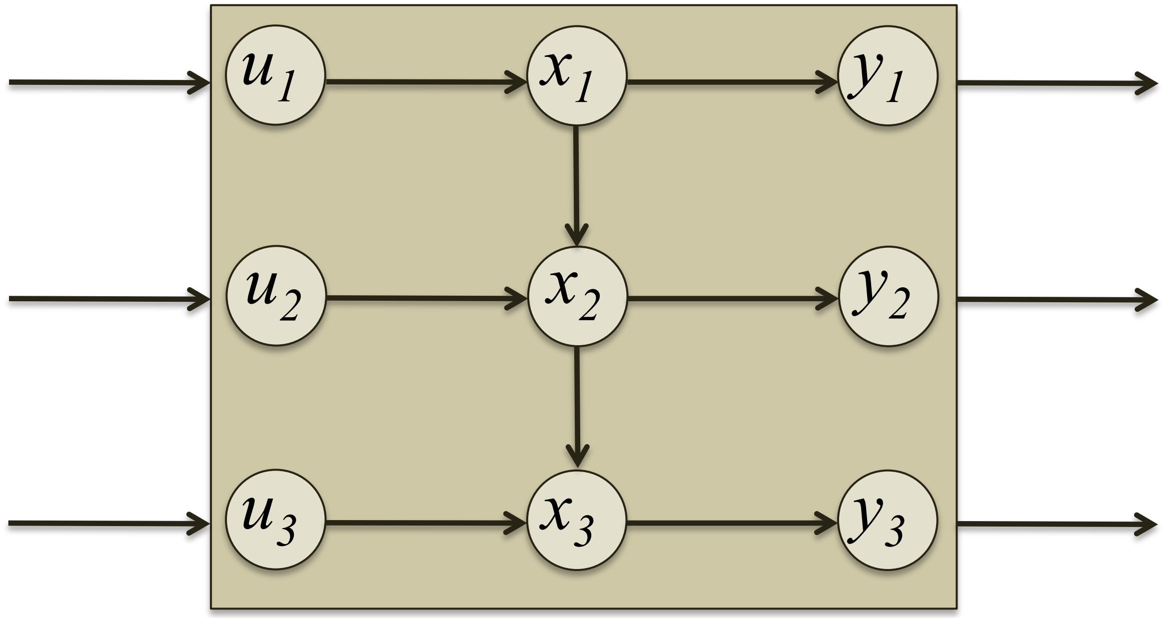
What is System Structure?

Complete Computational Structure



(physical interconnection)

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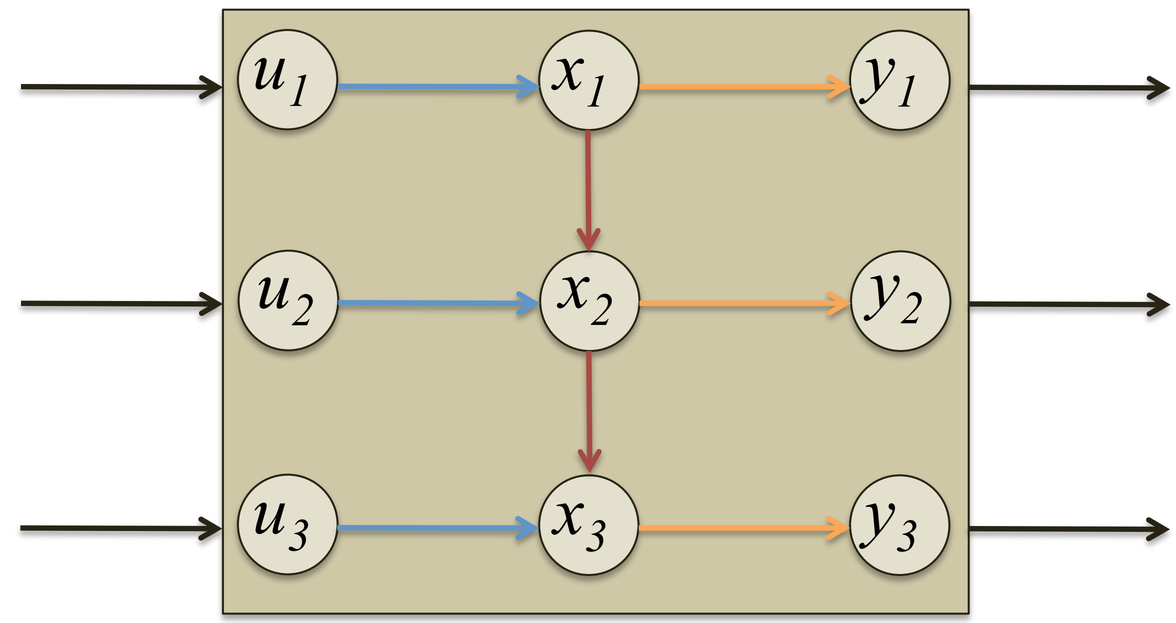

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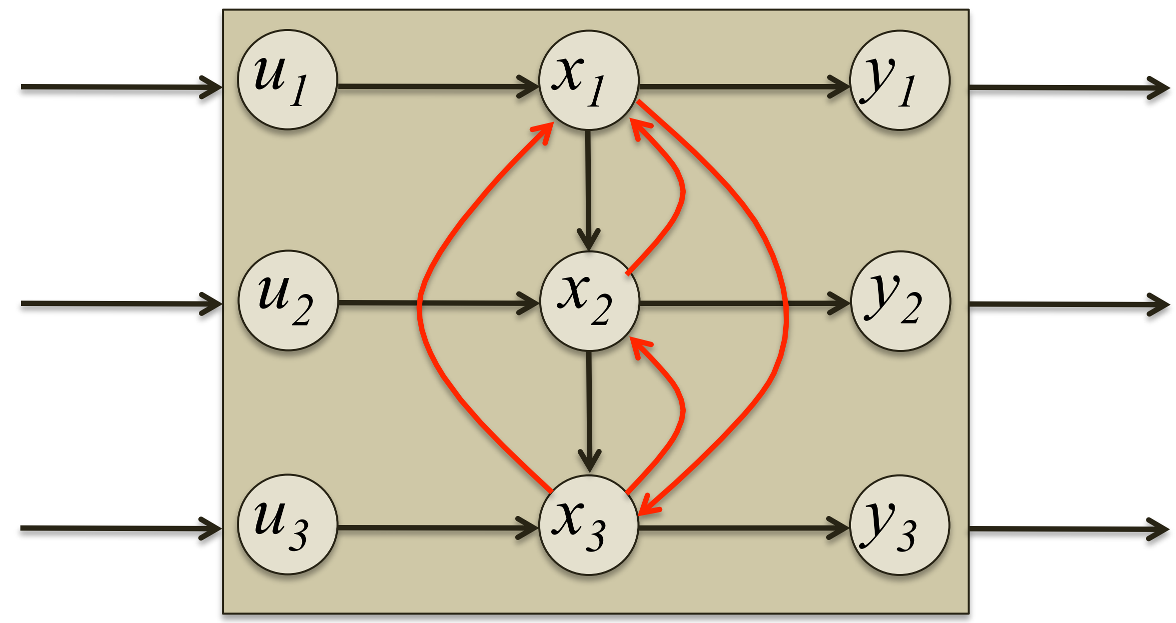

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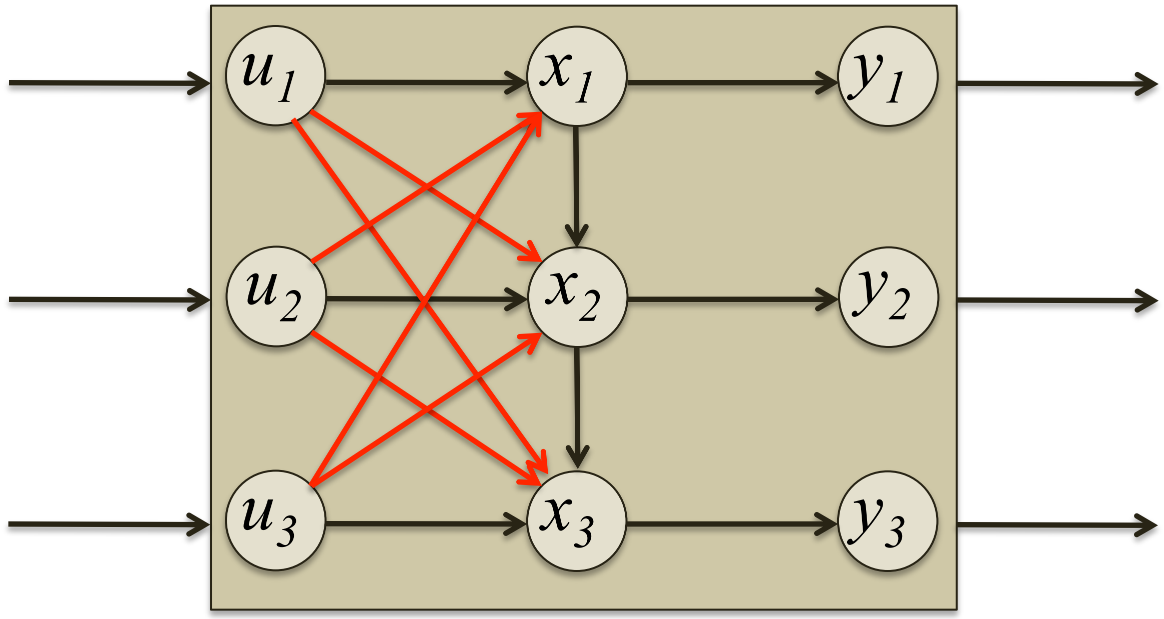

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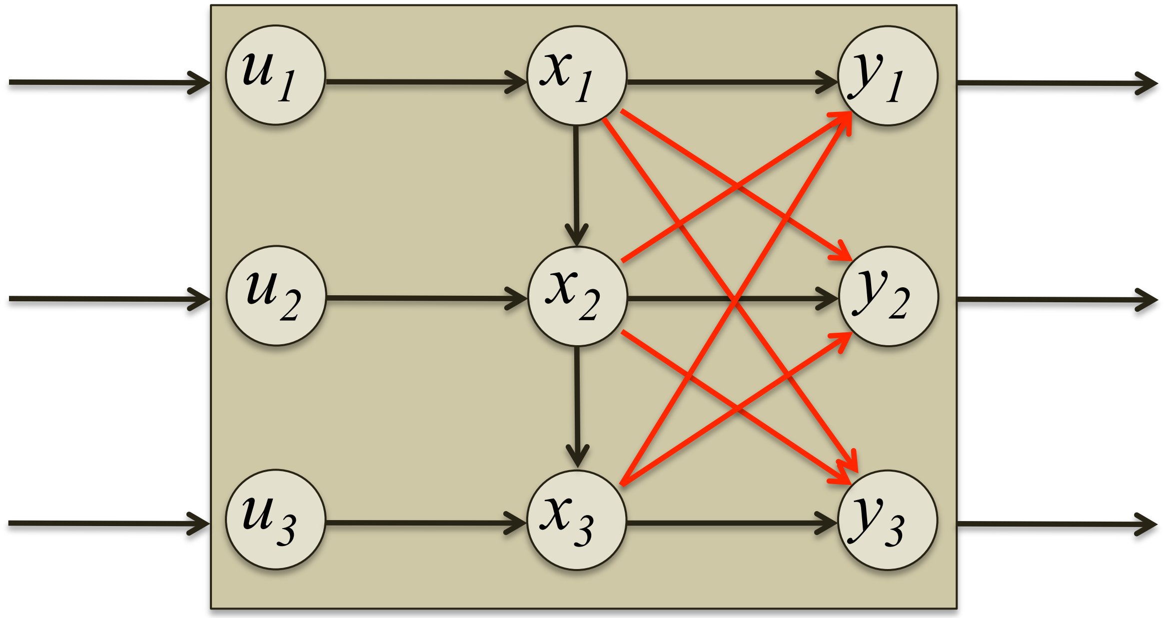

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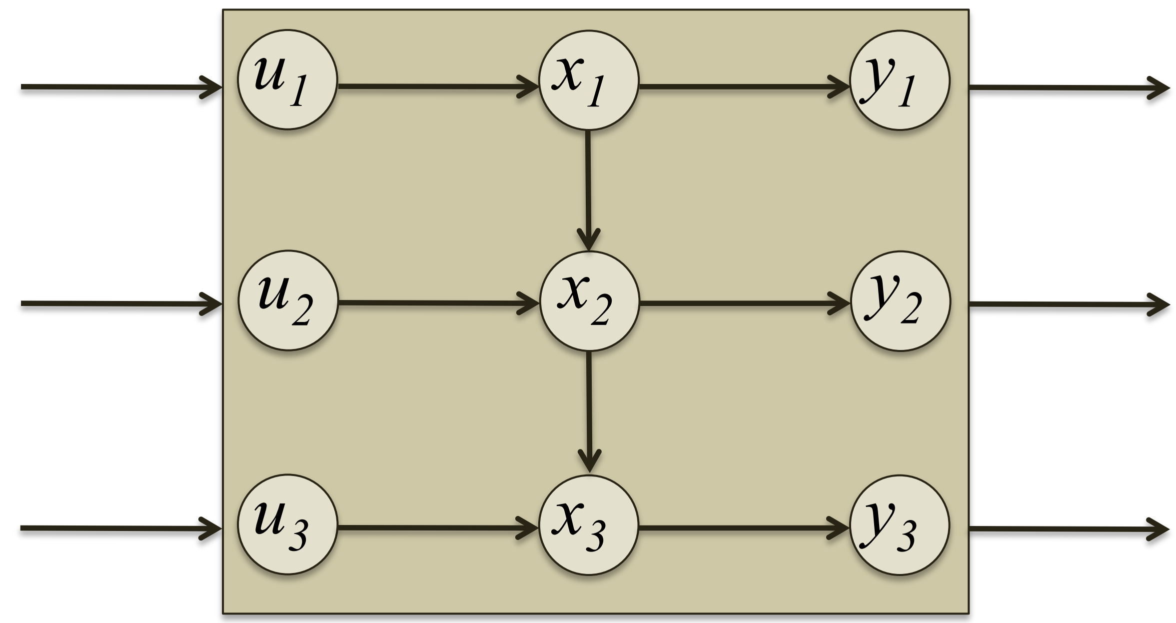

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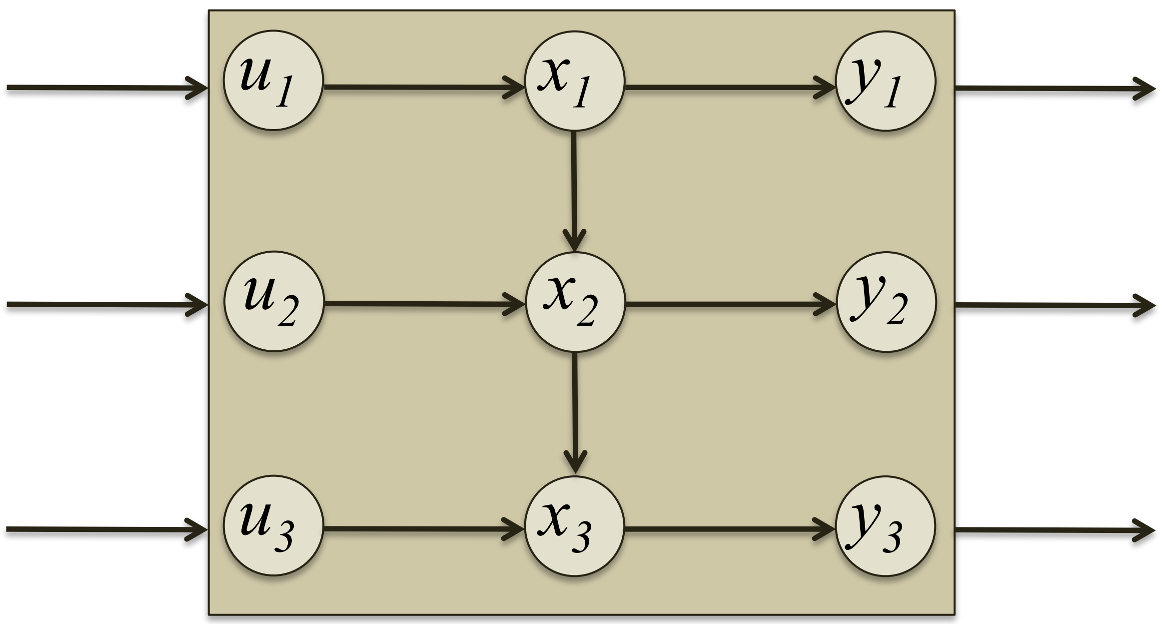
What is System Structure?

Sparsity Pattern of the Transfer Function



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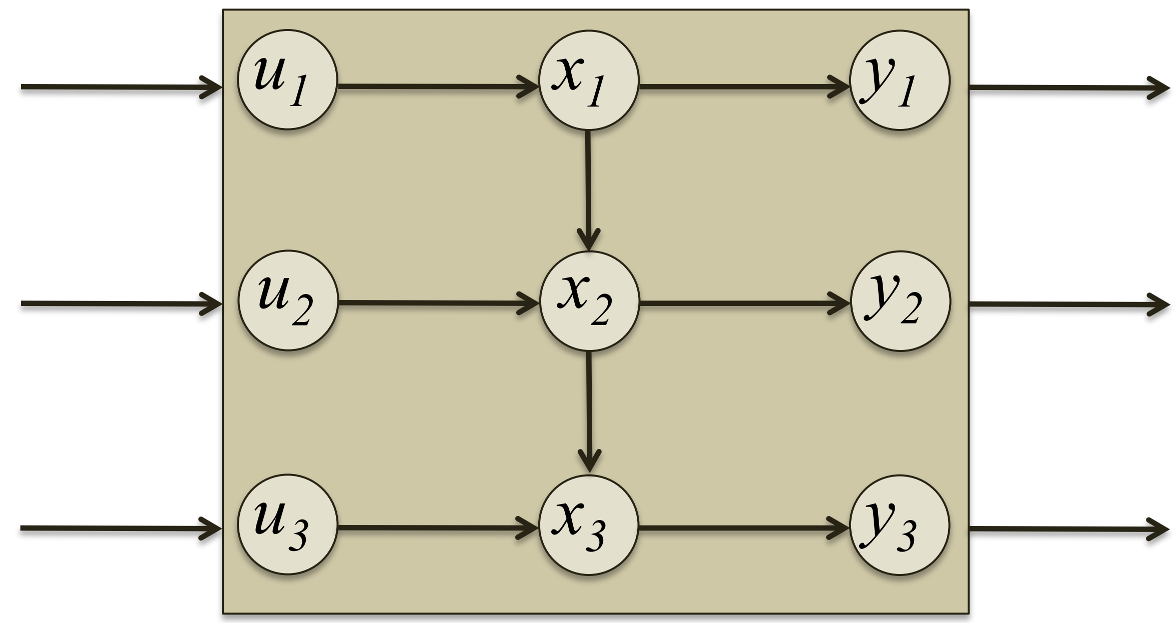
Complete Computational Structure



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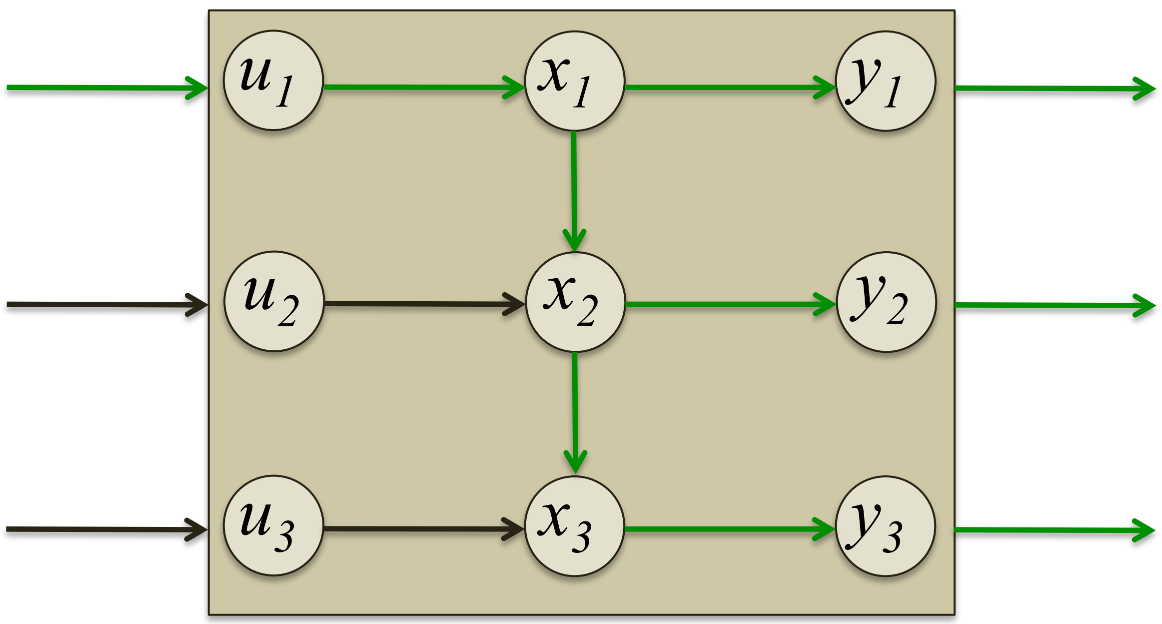

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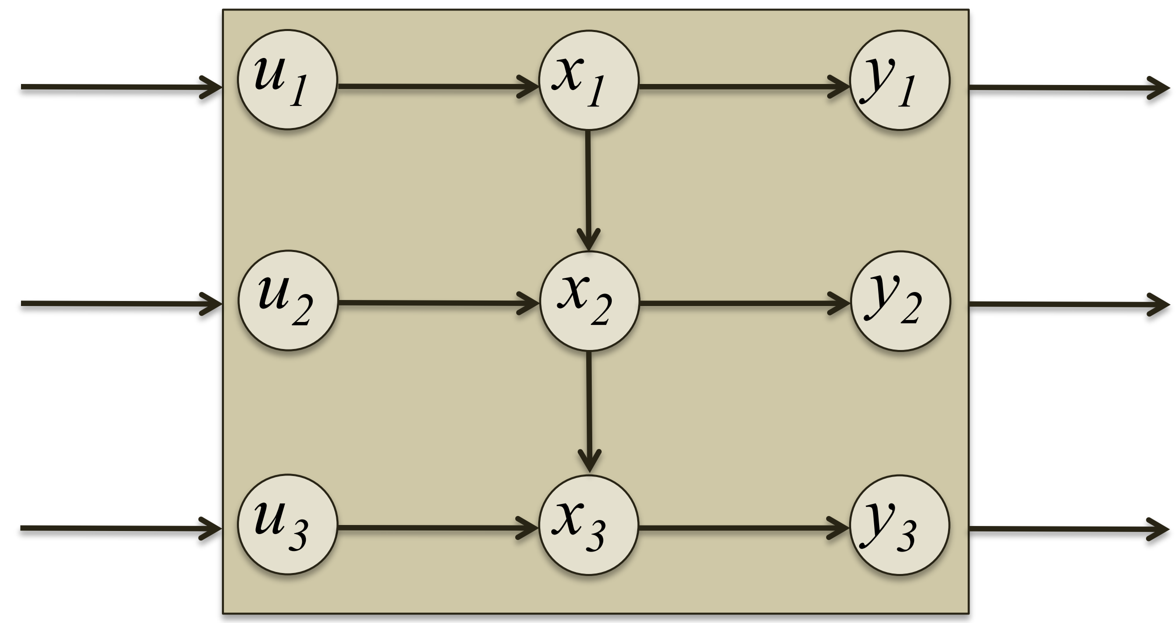

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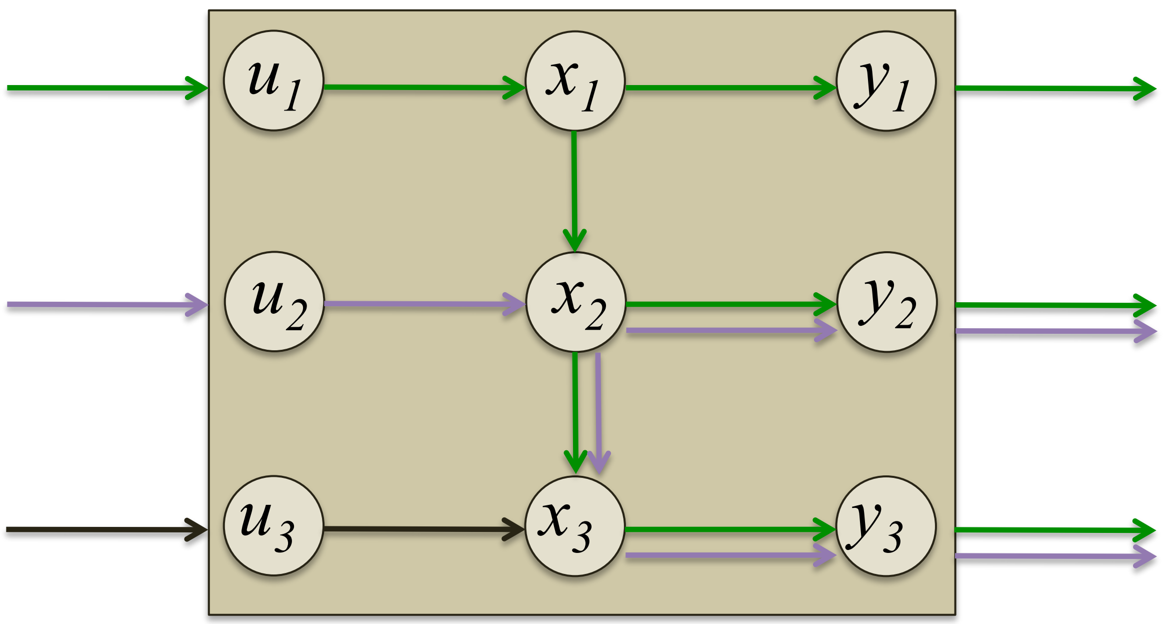

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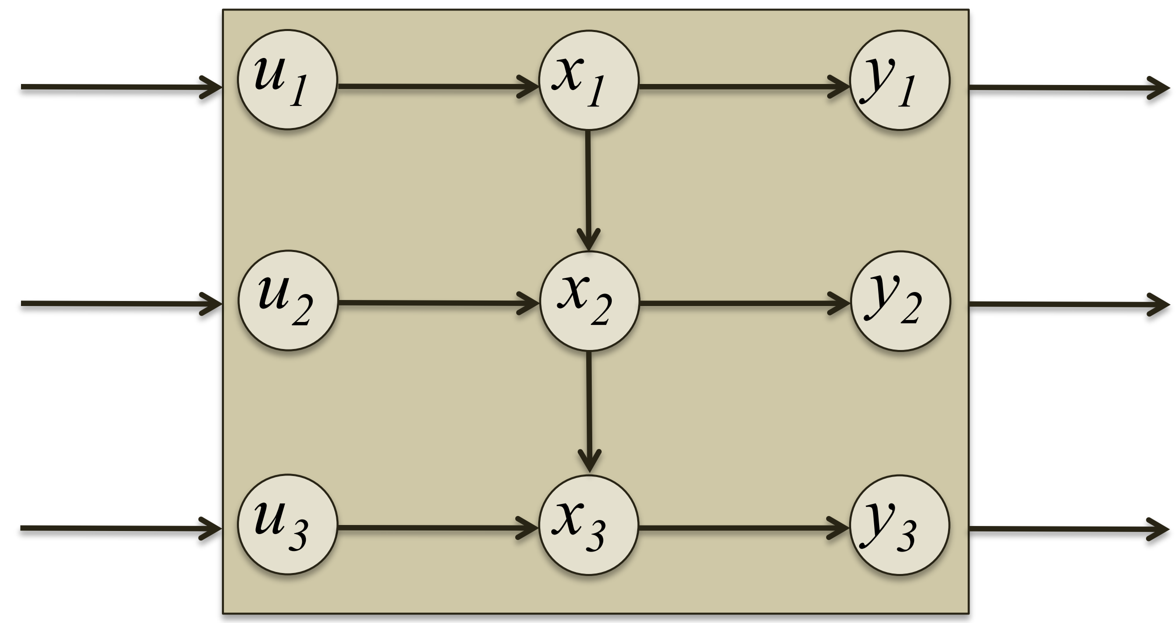

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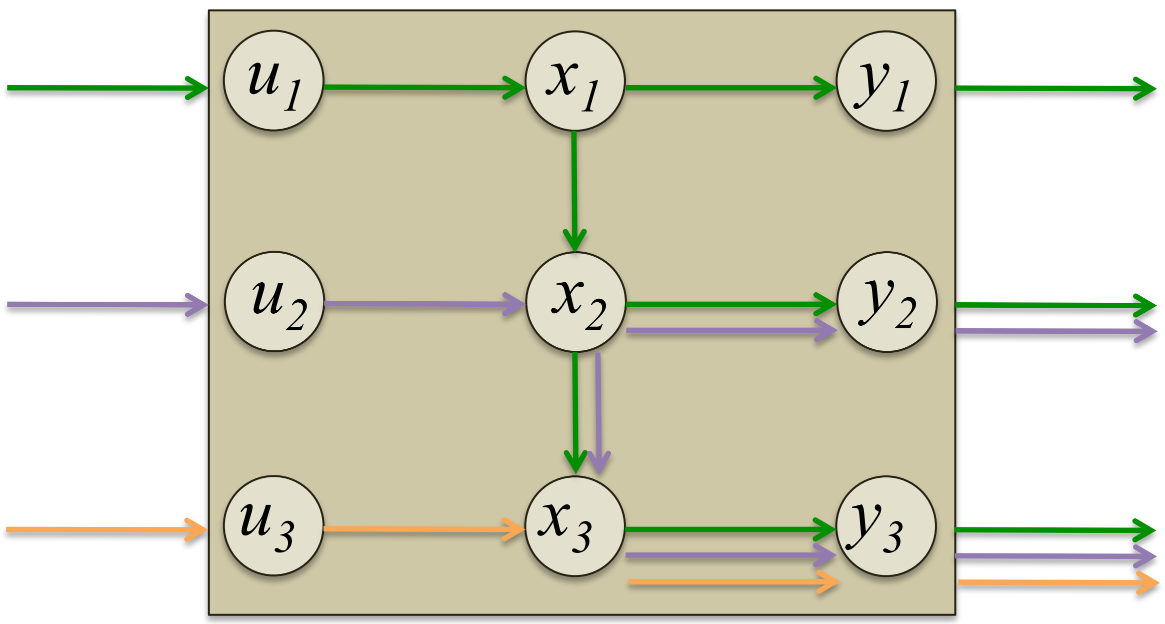

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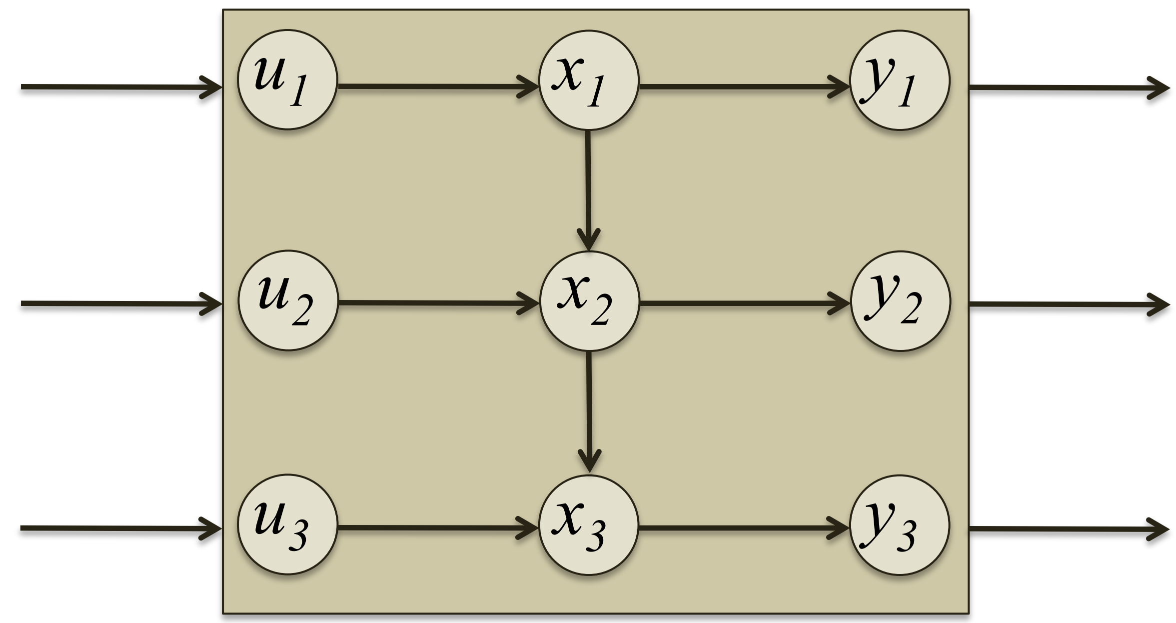

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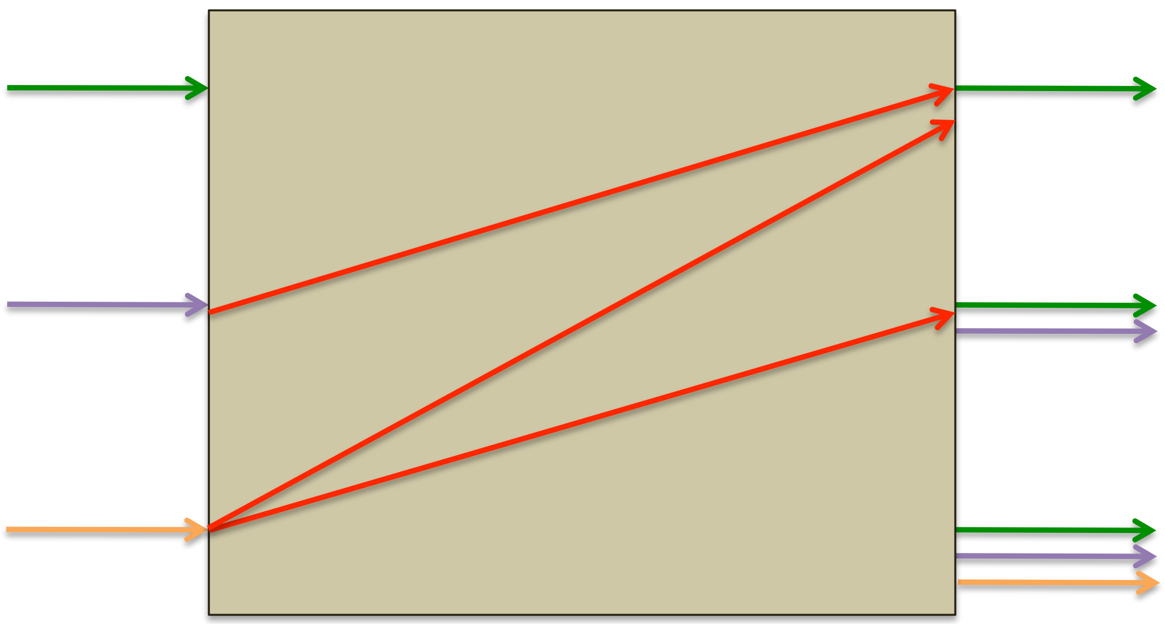
State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

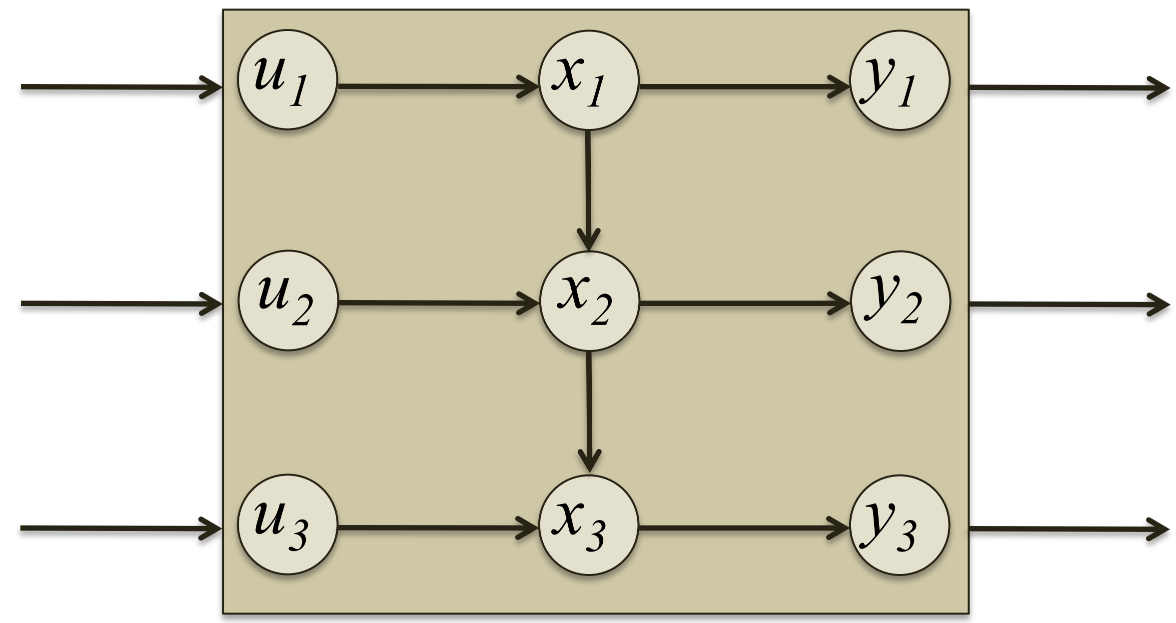
What is System Structure?

Sparsity Pattern of the Transfer Function



(*paths* from inputs to outputs)

Complete Computational Structure



(physical interconnection)

Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

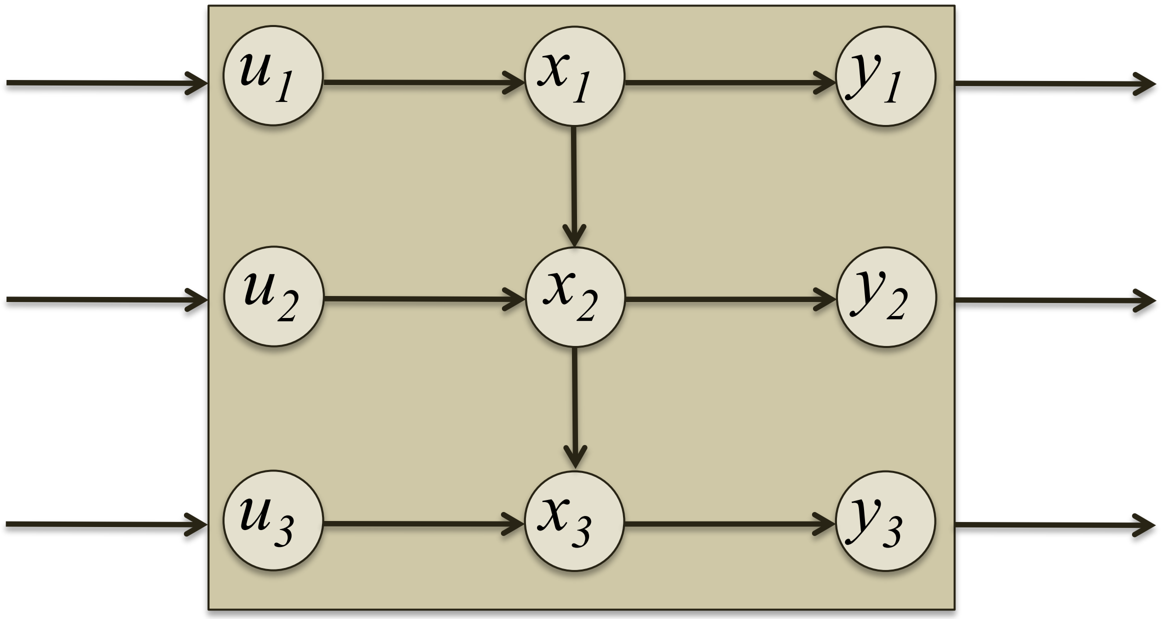
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

What is System Structure?

Sparsity Pattern of the Transfer Function

(*paths* from inputs to outputs)

Complete Computational Structure



(physical interconnection)

Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

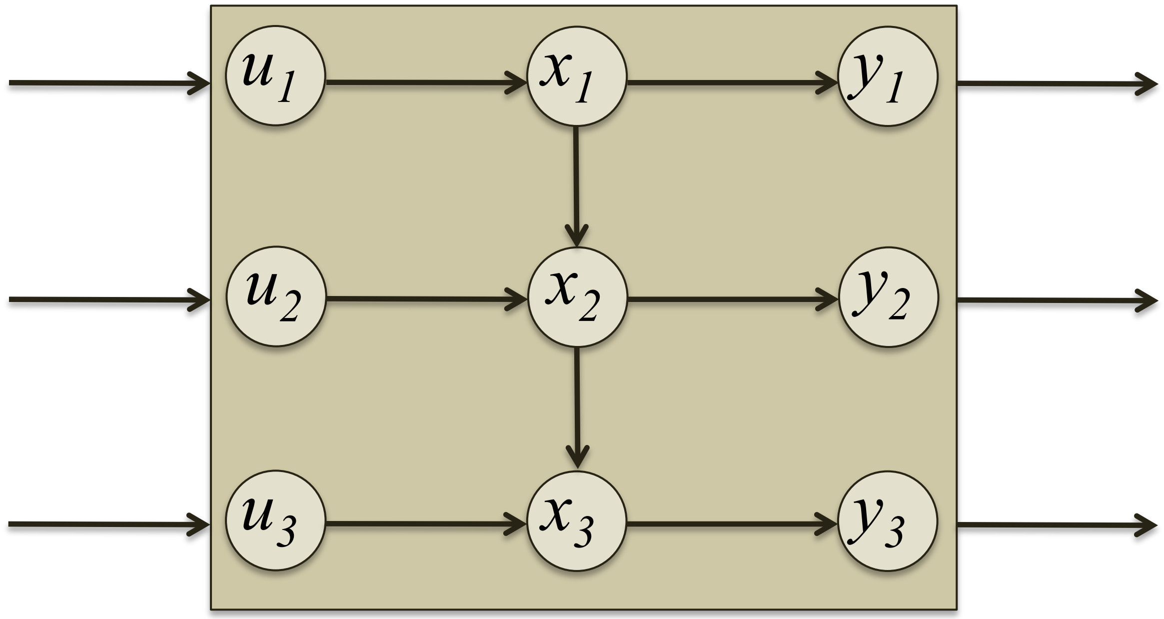
$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

What is System Structure?

Sparsity Pattern of the Transfer Function

Complete Computational Structure



(physical interconnection)

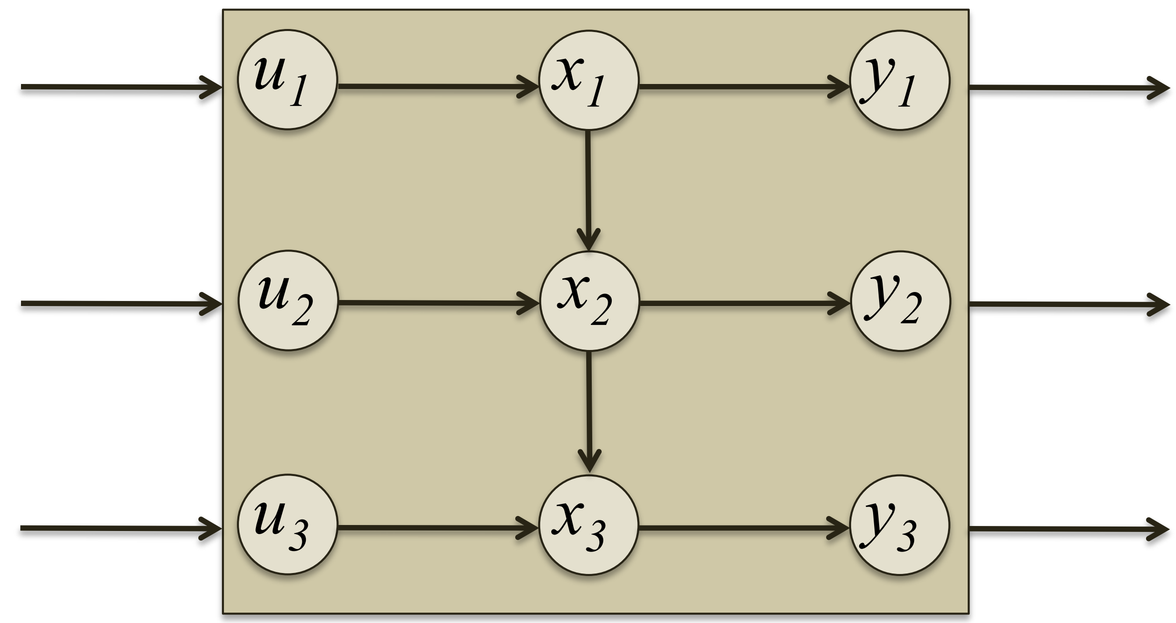
- These "structures" are weaker/stronger versions of each other
  - Weak: paths relating manifest variables (inputs/outputs)
  - Strong: direct interaction among physical (fundamental) components

What is System Structure?

Sparsity Pattern of the Transfer Function

(*paths* from inputs to outputs)

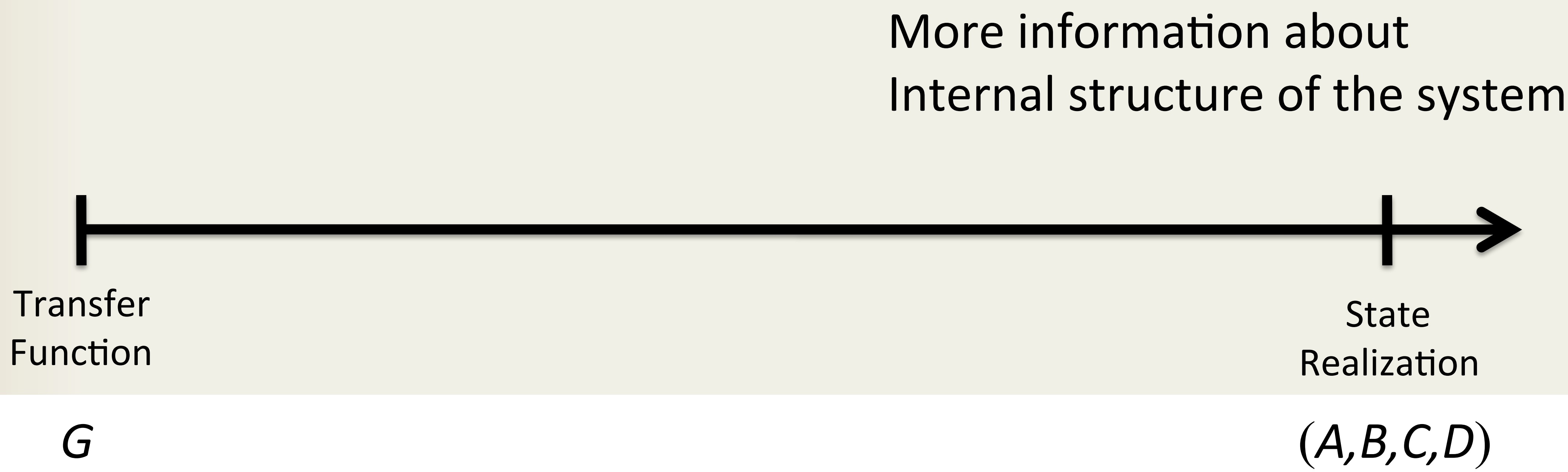
Complete Computational Structure



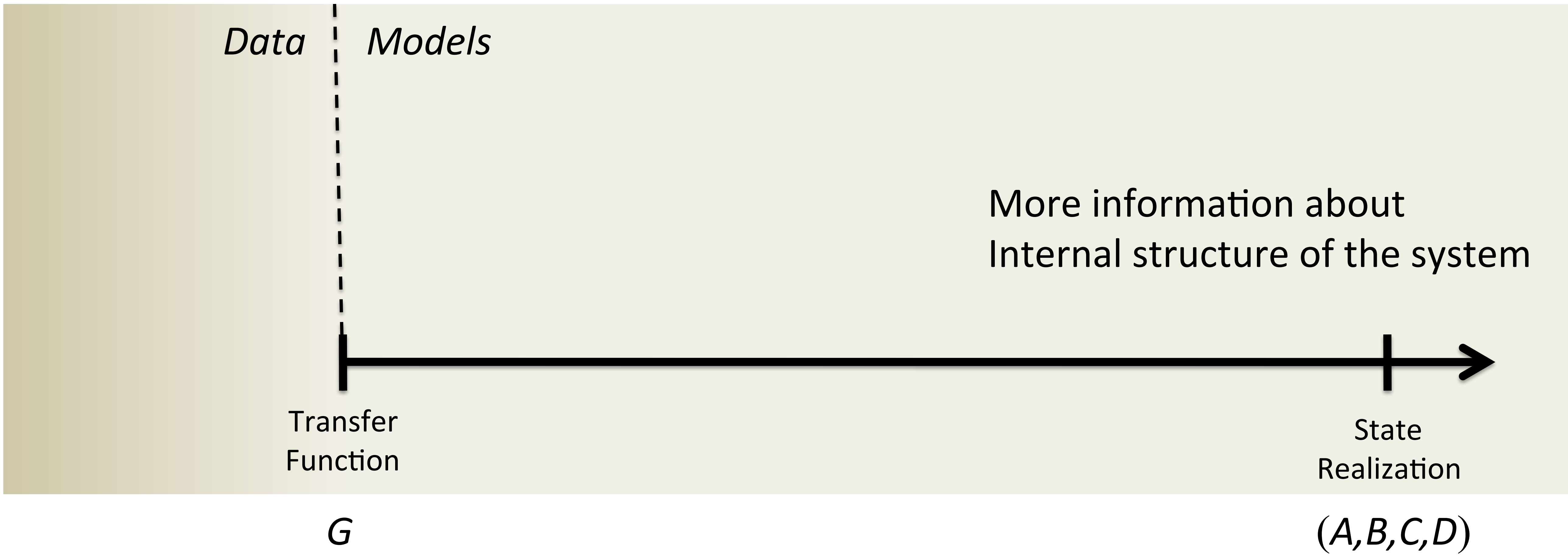
(physical interconnection)

- These “structures” are weaker/stronger versions of each other
  – Weak: paths relating manifest variables (inputs/outputs)
  – Strong: direct interaction among physical (fundamental) components
- Which kind of “structure” do network reconstruction algorithms try to find?

Network Reconstruction



Network Reconstruction

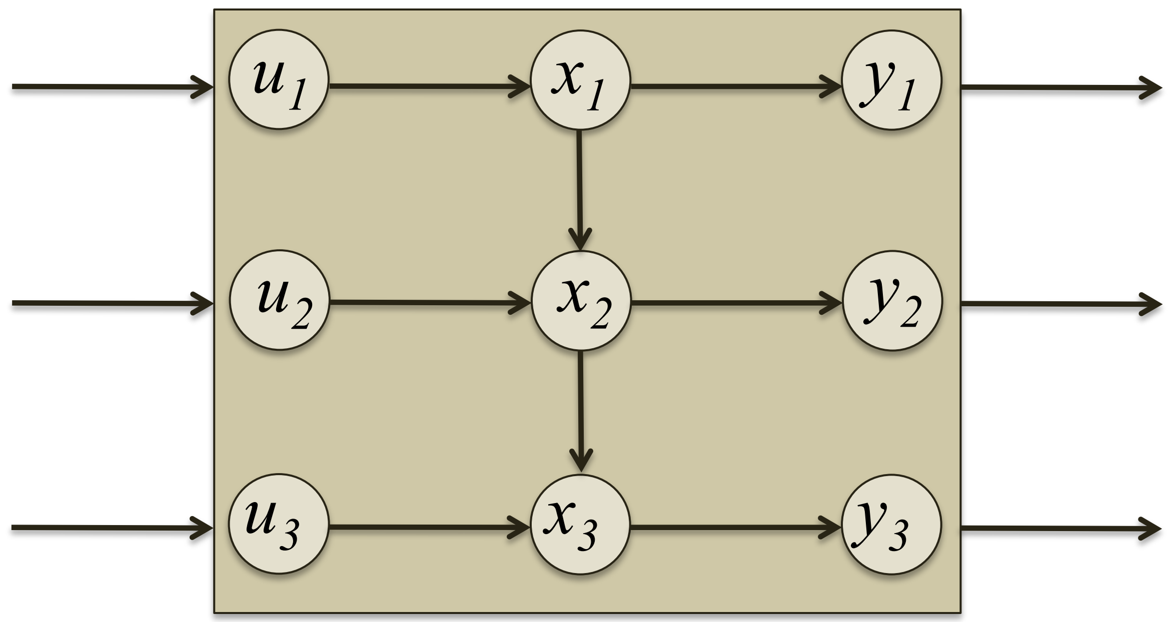


Network Reconstruction

G (A,B,C,D)

- System Identification characterizes the paths relating manifest variables
  - Lots of technical issues dealing with stochasticity, unmodeled dynamics, sufficiency of excitation, sample complexity, etc.
  - Weak characterization of the system's internal structure
  - Many network reconstruction techniques are implicitly or explicitly looking for this notion of structure e.g. correlation and mutual information methods

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

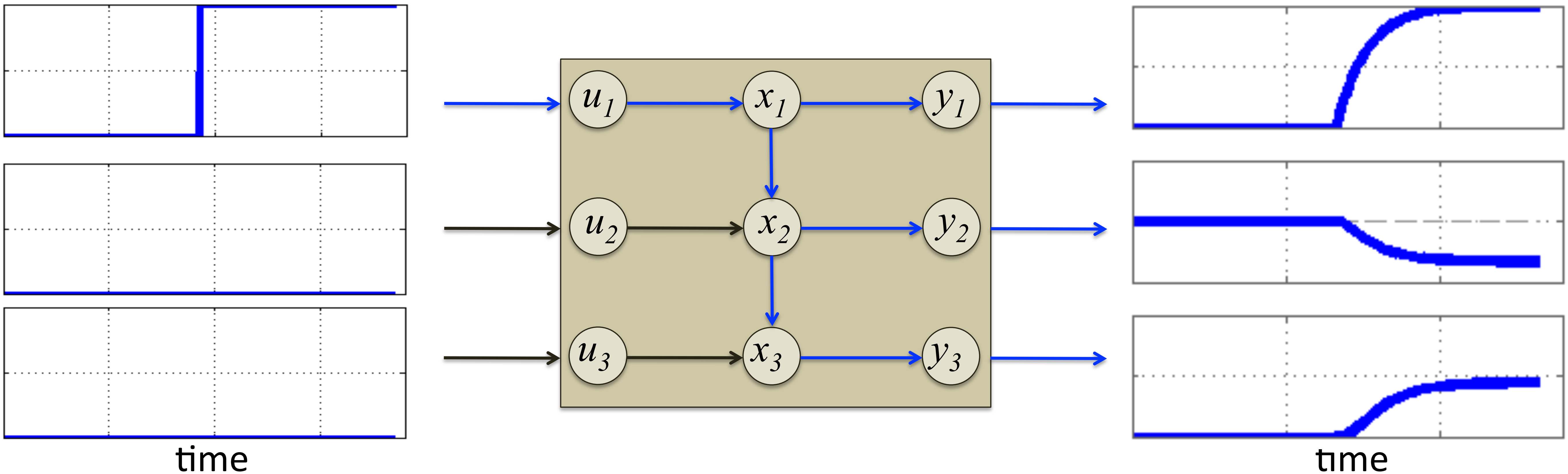
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realization

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

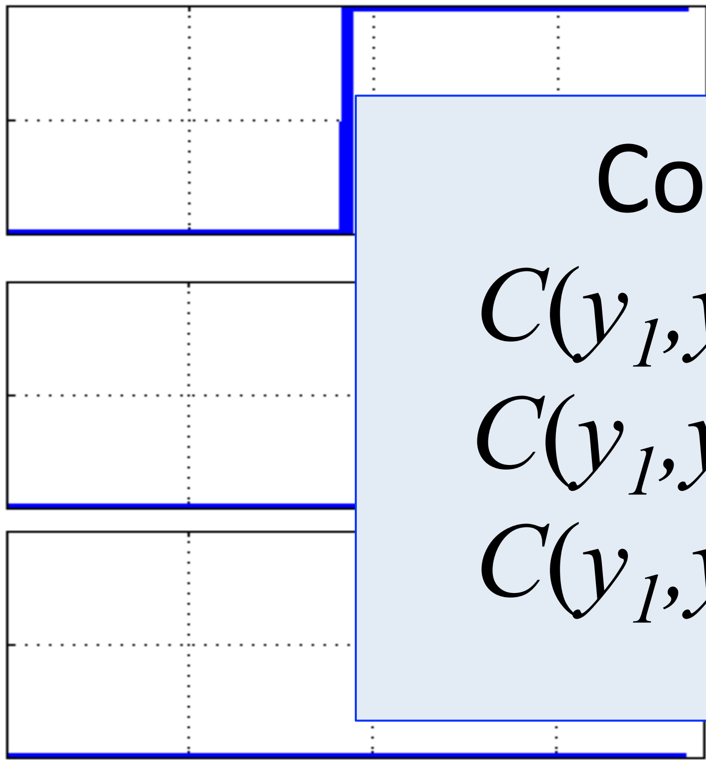
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

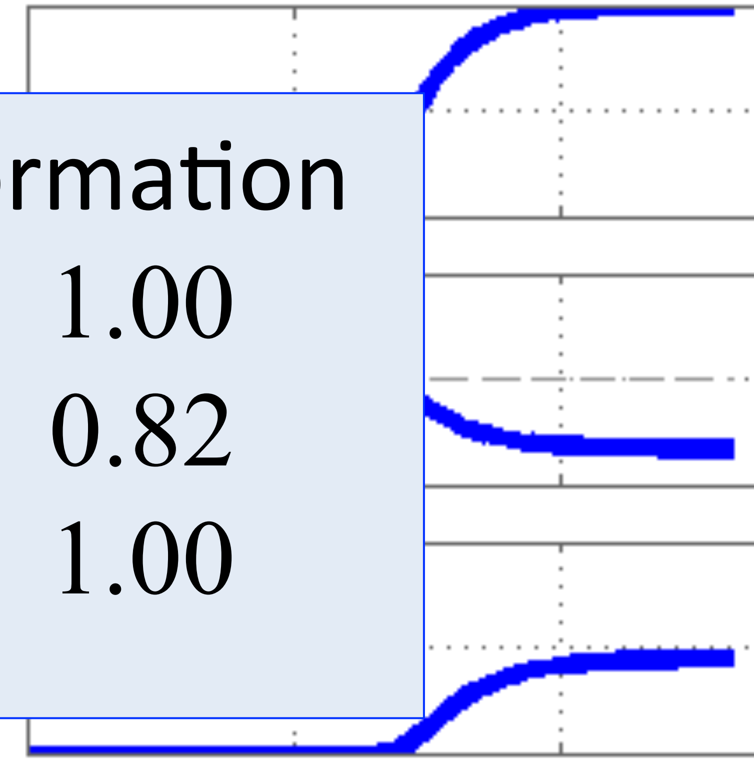
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



time

Correlations	Mutual Information
$C(y_1,y_1) = 1.0000$	$I(y_1,y_1) = 1.00$
$C(y_1,y_2) = -0.9898$	$I(y_1,y_2) = 0.82$
$C(y_1,y_3) = 0.9621$	$I(y_1,y_3) = 1.00$



time

Transfer Function

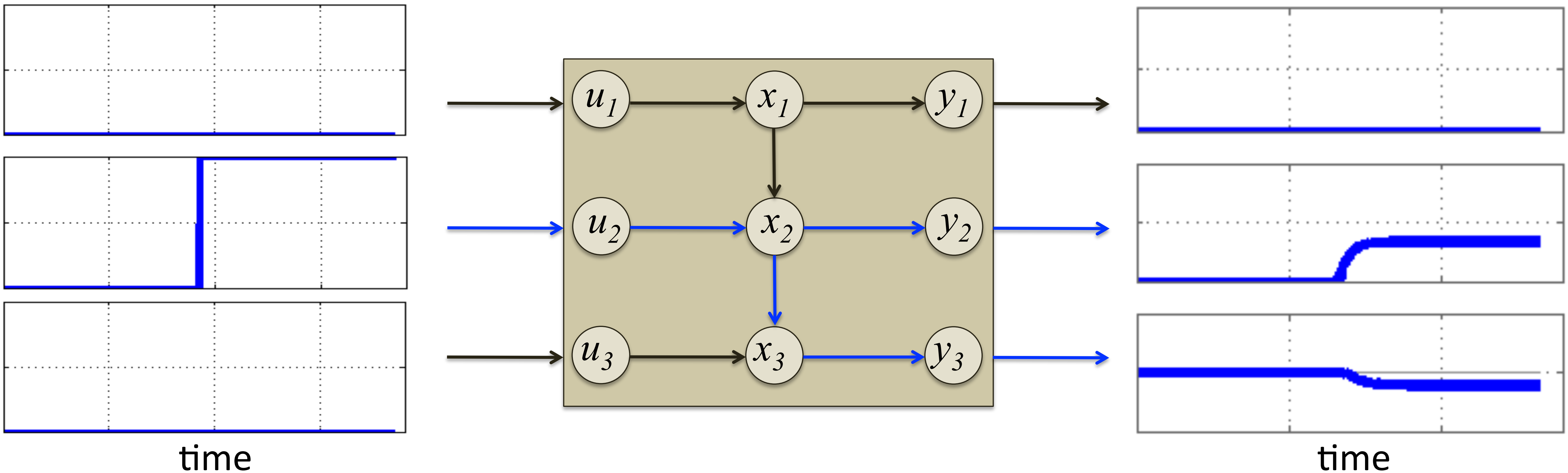
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

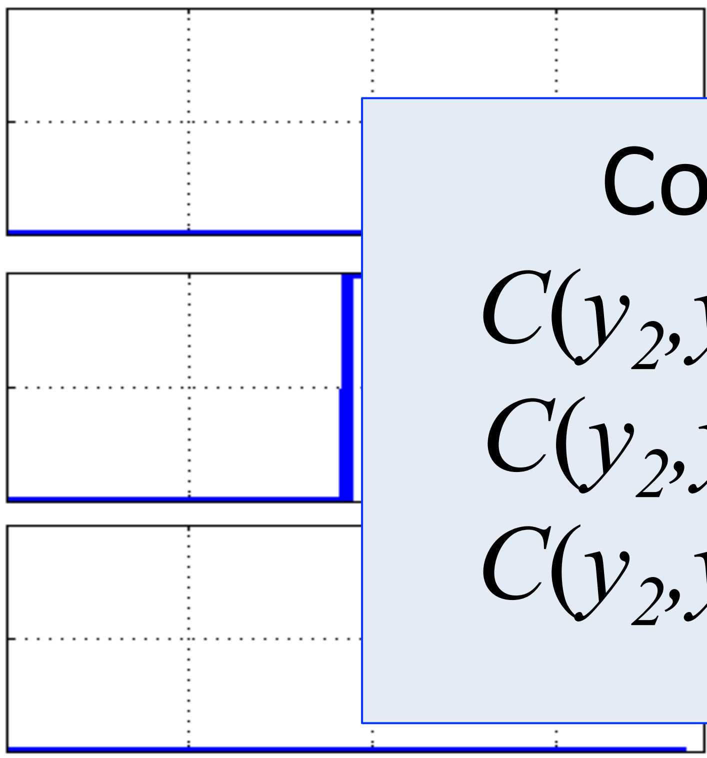
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

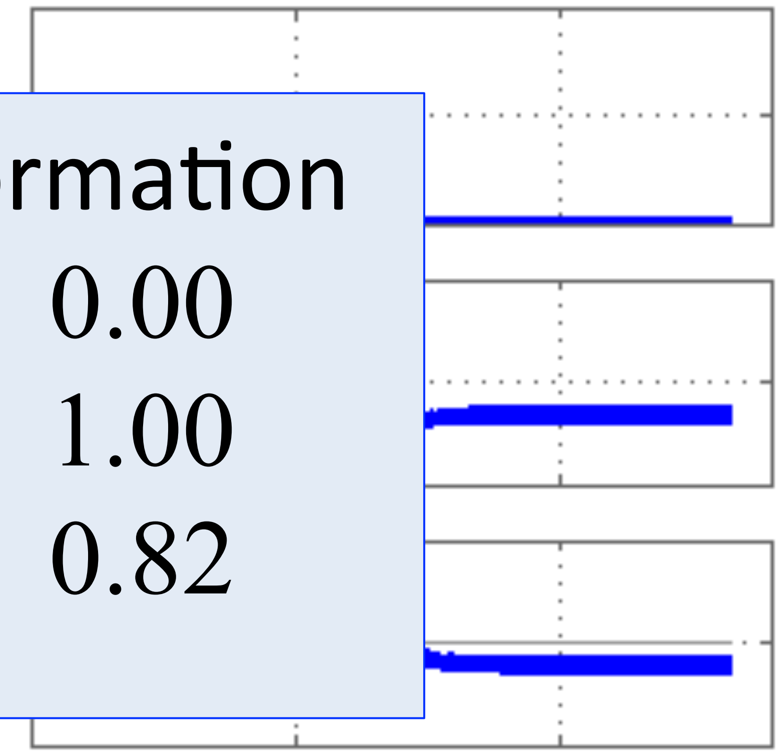
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



time

Correlations	Mutual Information
$C(y_2,y_1) = -0.0000$	$I(y_2,y_1) = 0.00$
$C(y_2,y_2) = 1.0000$	$I(y_2,y_2) = 1.00$
$C(y_2,y_3) = -0.9407$	$I(y_2,y_3) = 0.82$



time

Transfer Function

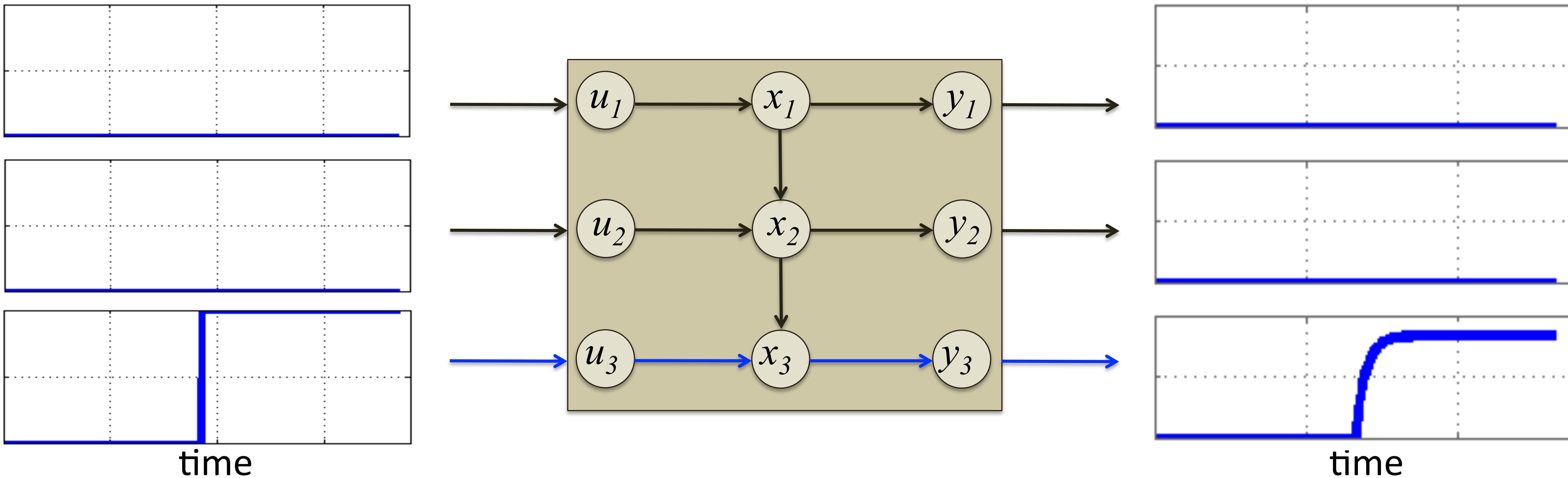
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

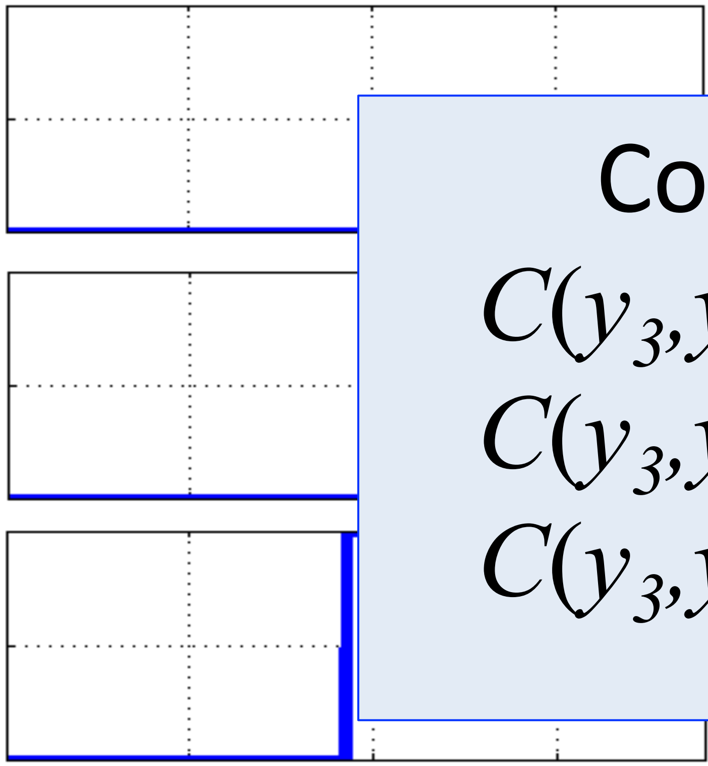
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

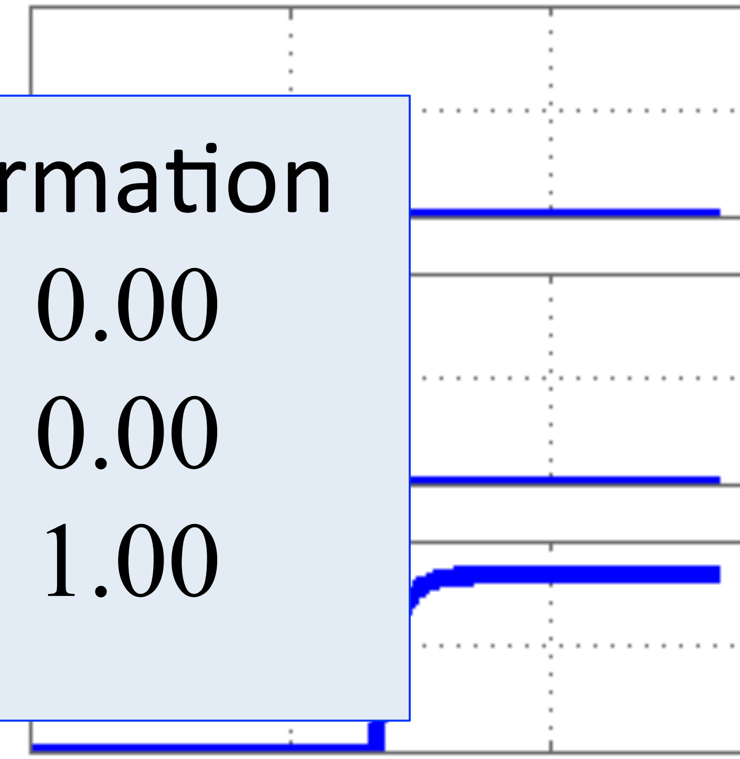
$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Correlations	Mutual Information
$C(y_3,y_1) = 0.0000$	$I(y_3,y_1) = 0.00$
$C(y_3,y_2) = 0.0000$	$I(y_3,y_2) = 0.00$
$C(y_3,y_3) = 1.0000$	$I(y_3,y_3) = 1.00$



time

time

Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods

Correlations

$$\begin{bmatrix} 1.000 & 0.0000 & 0.0000 \\ -0.9898 & 1.000 & 0.0000 \\ 0.9621 & -0.9407 & 1.000 \end{bmatrix}$$

Mutual Information

$$\begin{bmatrix} 1.00 & 0.00 & 0.00 \\ 0.82 & 1.00 & 0.00 \\ 1.00 & 1.82 & 1.00 \end{bmatrix}$$

Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods

Correlations

$$\begin{bmatrix} 1.000 & 0.0000 & 0.0000 \\ -0.9898 & 1.000 & 0.0000 \\ 0.9621 & -0.9407 & 1.000 \end{bmatrix}$$

Mutual Information

$$\begin{bmatrix} 1.00 & 0.00 & 0.00 \\ 0.82 & 1.00 & 0.00 \\ 1.00 & 1.82 & 1.00 \end{bmatrix}$$

Transfer Function

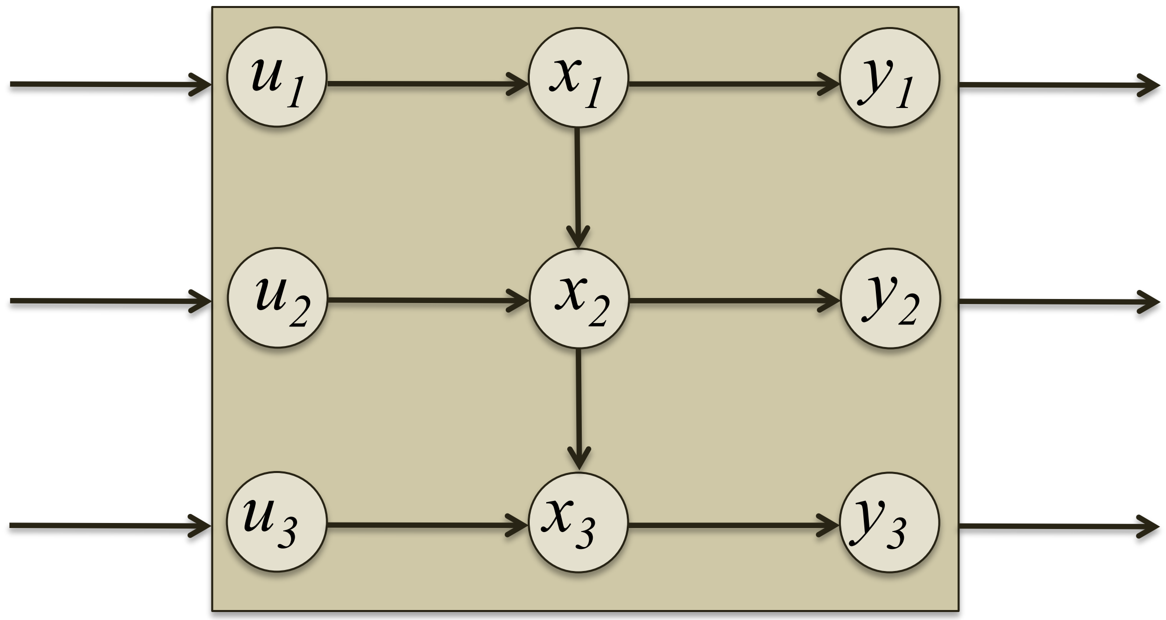
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

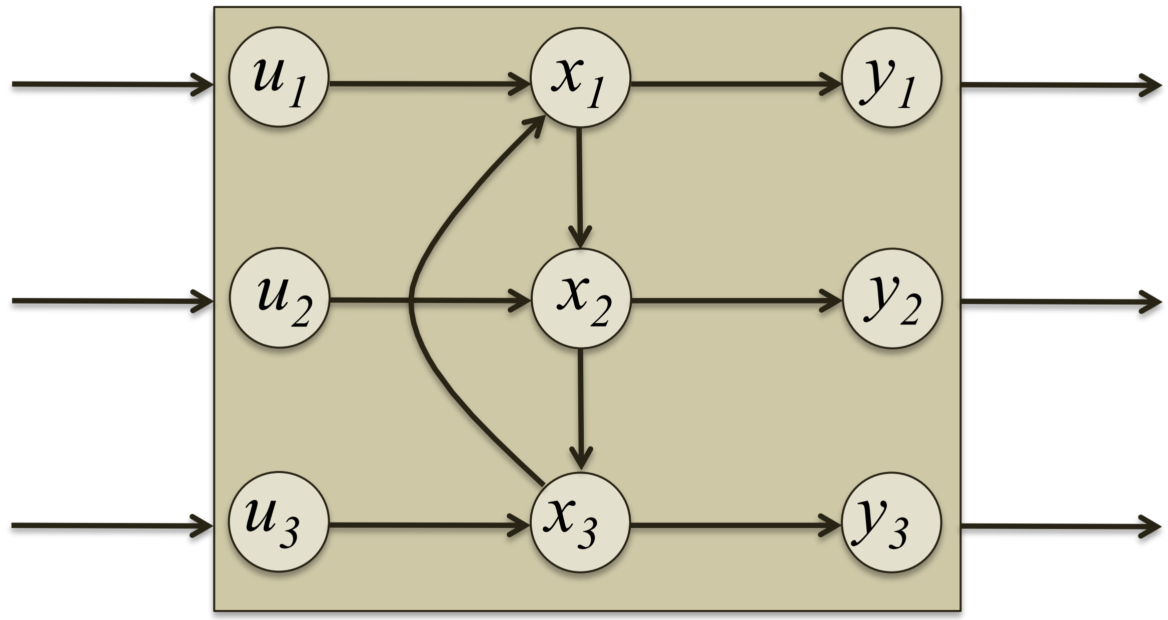
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{s+1} & 0 & 0 \\ \frac{-2}{(s+1)(s+3)} & \frac{1}{s+3} & 0 \\ \frac{4}{(s+1)(s+3)^2} & \frac{-2}{(s+3)^2} & \frac{1}{s+3} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

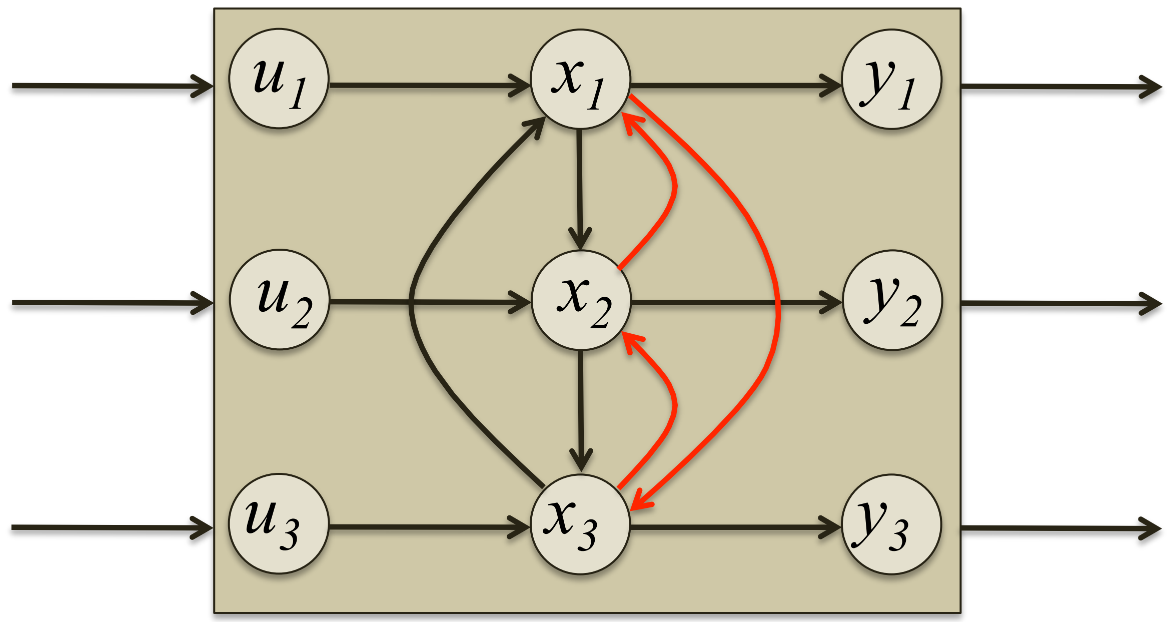
$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{(s+3)^2}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} & \frac{-(s+3)}{(s+1)^2(s+4)} \\ \frac{-2(s+3)}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} \\ \frac{4}{(s+1)^2(s+4)} & \frac{-2s}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -1 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Network Reconstruction Examples: Correlation and Information Methods



Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{(s+3)^2}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} & \frac{-(s+3)}{(s+1)^2(s+4)} \\ \frac{-2(s+3)}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} \\ \frac{4}{(s+1)^2(s+4)} & \frac{-2s}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

State Space Realisation

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -1 \\ -2 & -3 & 0 \\ 0 & -2 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

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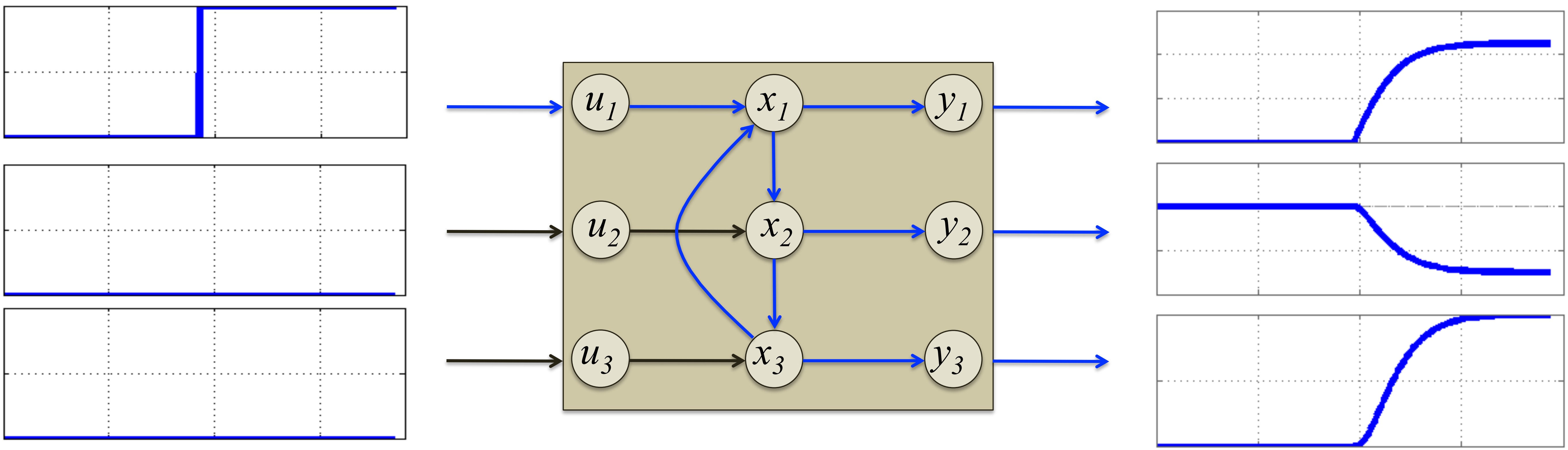
Network Reconstruction Examples: Correlation and Information Methods



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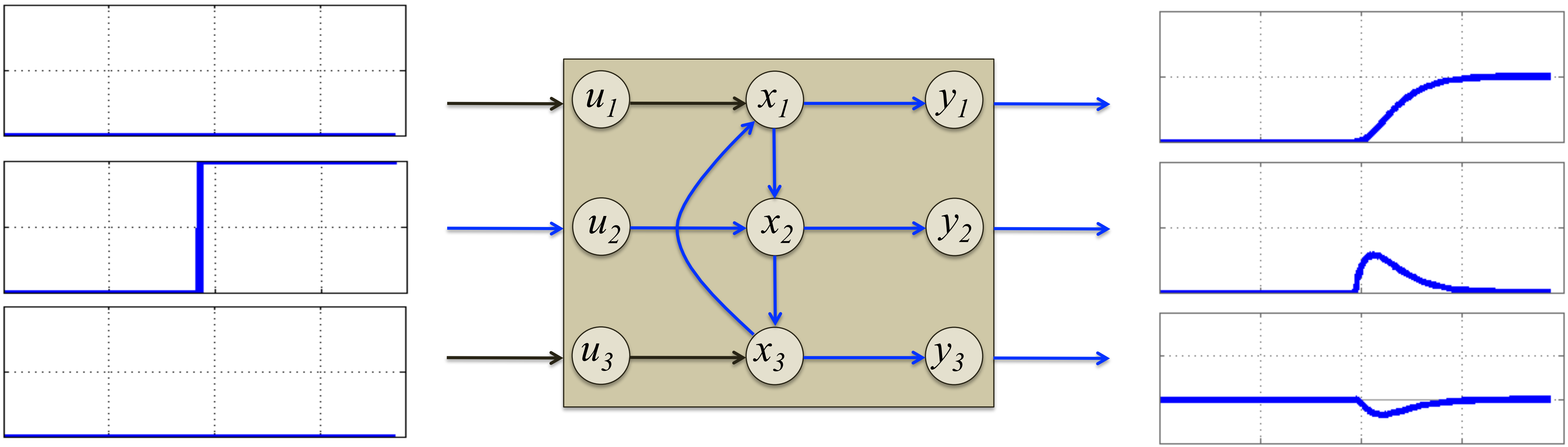

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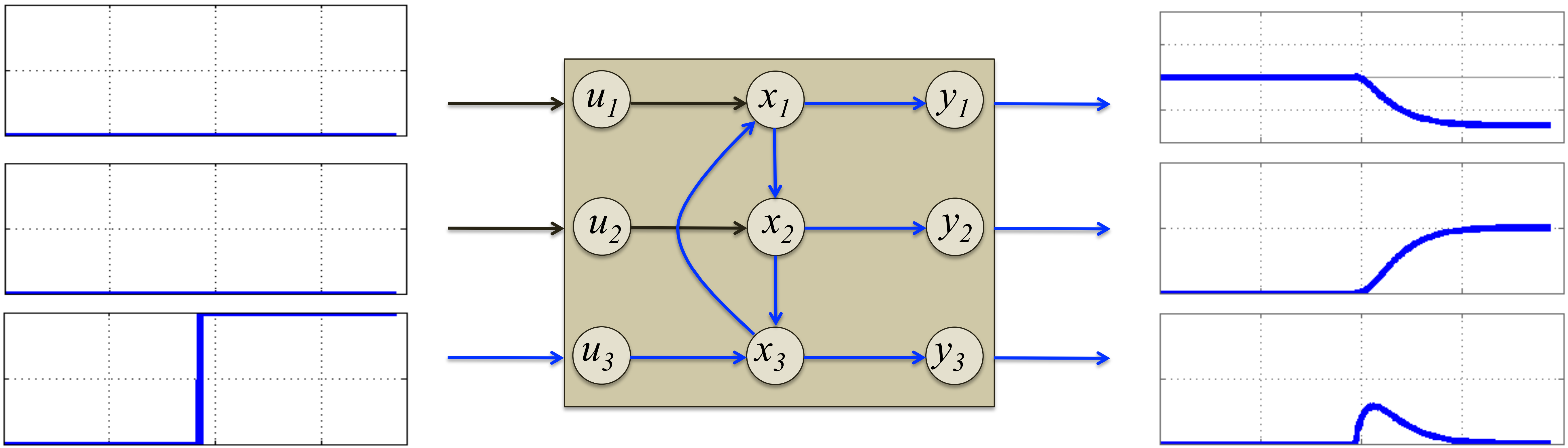

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Network Reconstruction Examples: Correlation and Information Methods

Correlations

$$\begin{bmatrix} 1.000 & -0.8391 & 0.7852 \\ -0.9953 & 1.000 & -0.8391 \\ 0.9815 & -0.9296 & 1.000 \end{bmatrix}$$

Mutual Information

$$\begin{bmatrix} 1.00 & 0.71 & 0.77 \\ 0.79 & 1.00 & 0.71 \\ 1.00 & 0.73 & 1.00 \end{bmatrix}$$

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Network Reconstruction Examples: Correlation and Information Methods

- Try to find sparsity pattern in the input-output map, or Transfer Function

Transfer Function

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Network Reconstruction Examples: Correlation and Information Methods

- Try to find sparsity pattern in the input-output map, or Transfer Function
- Do not find the internal sparsity pattern of the underlying State Space Realisation

Transfer Function

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} \frac{(s+3)^2}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} & \frac{-(s+3)}{(s+1)^2(s+4)} \\ \frac{-2(s+3)}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} & \frac{2}{(s+1)^2(s+4)} \\ \frac{4}{(s+1)^2(s+4)} & \frac{-2s}{(s+1)^2(s+4)} & \frac{s(s+3)}{(s+1)^2(s+4)} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

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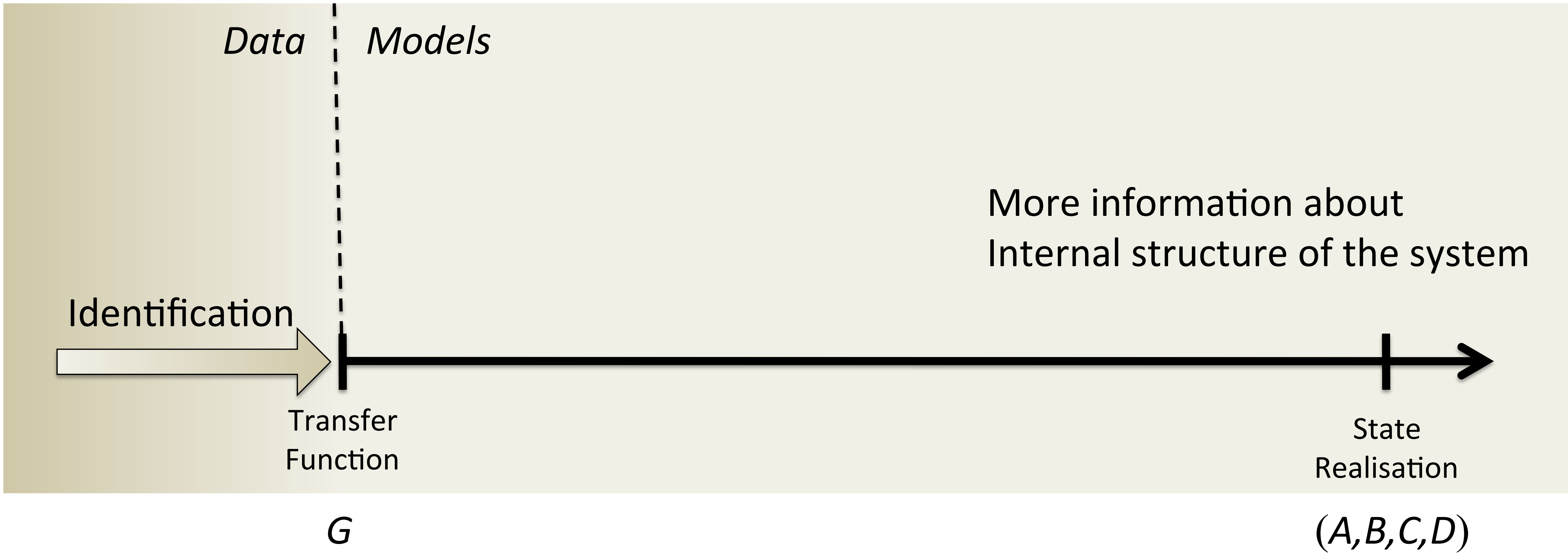
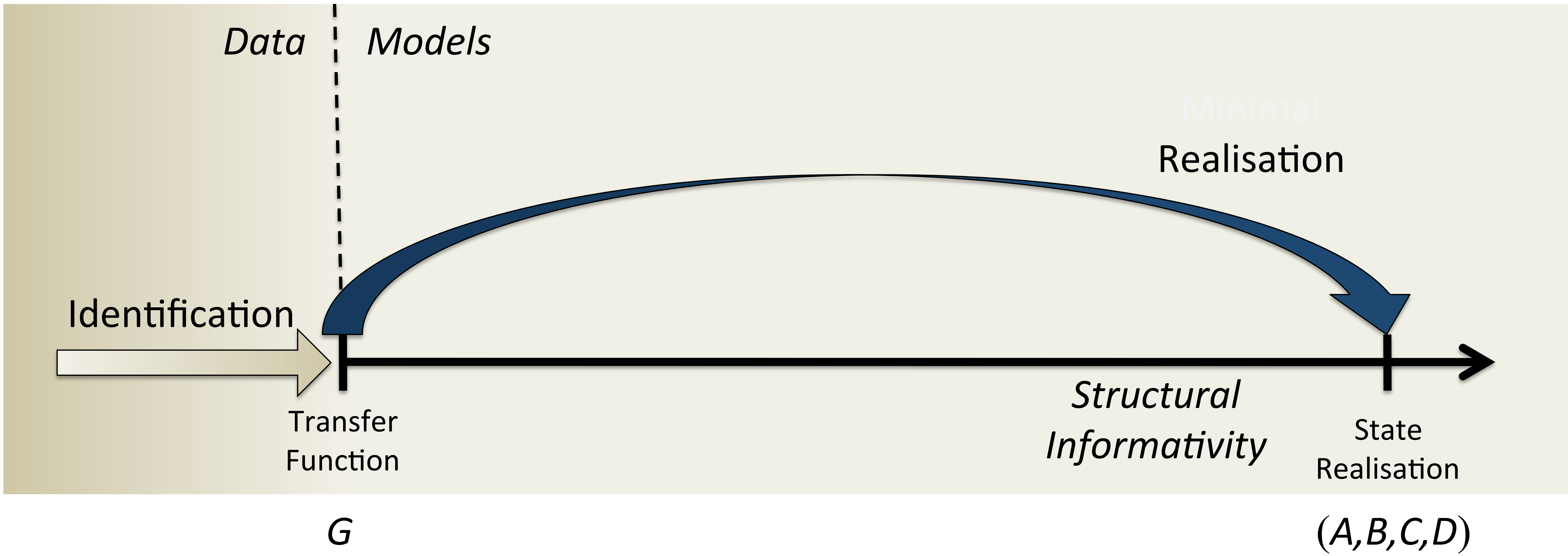
Network Reconstruction

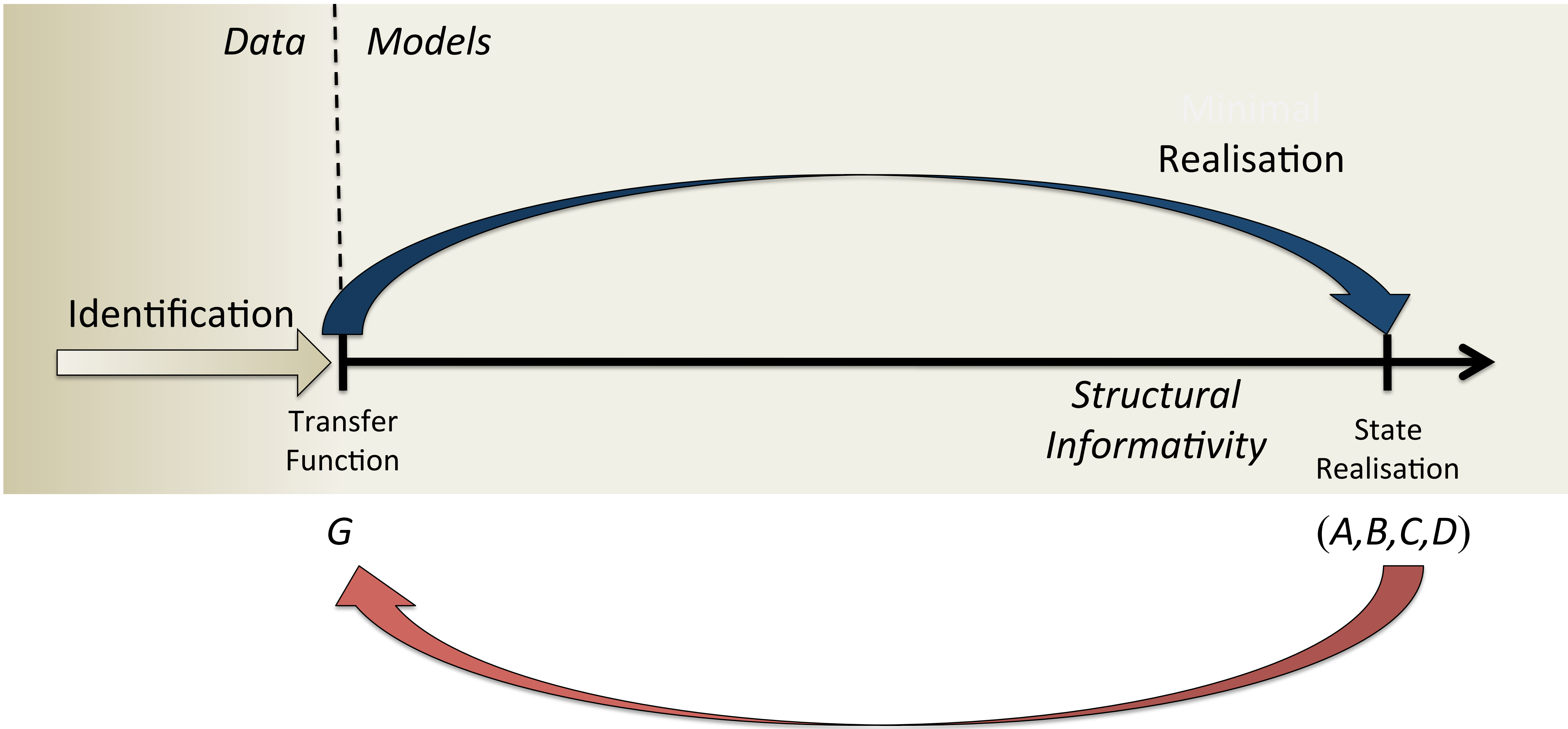


Bellman and Astrom, 1970. Lessard, Kristalny and Rantzer, submitted, 2012

Network Reconstruction



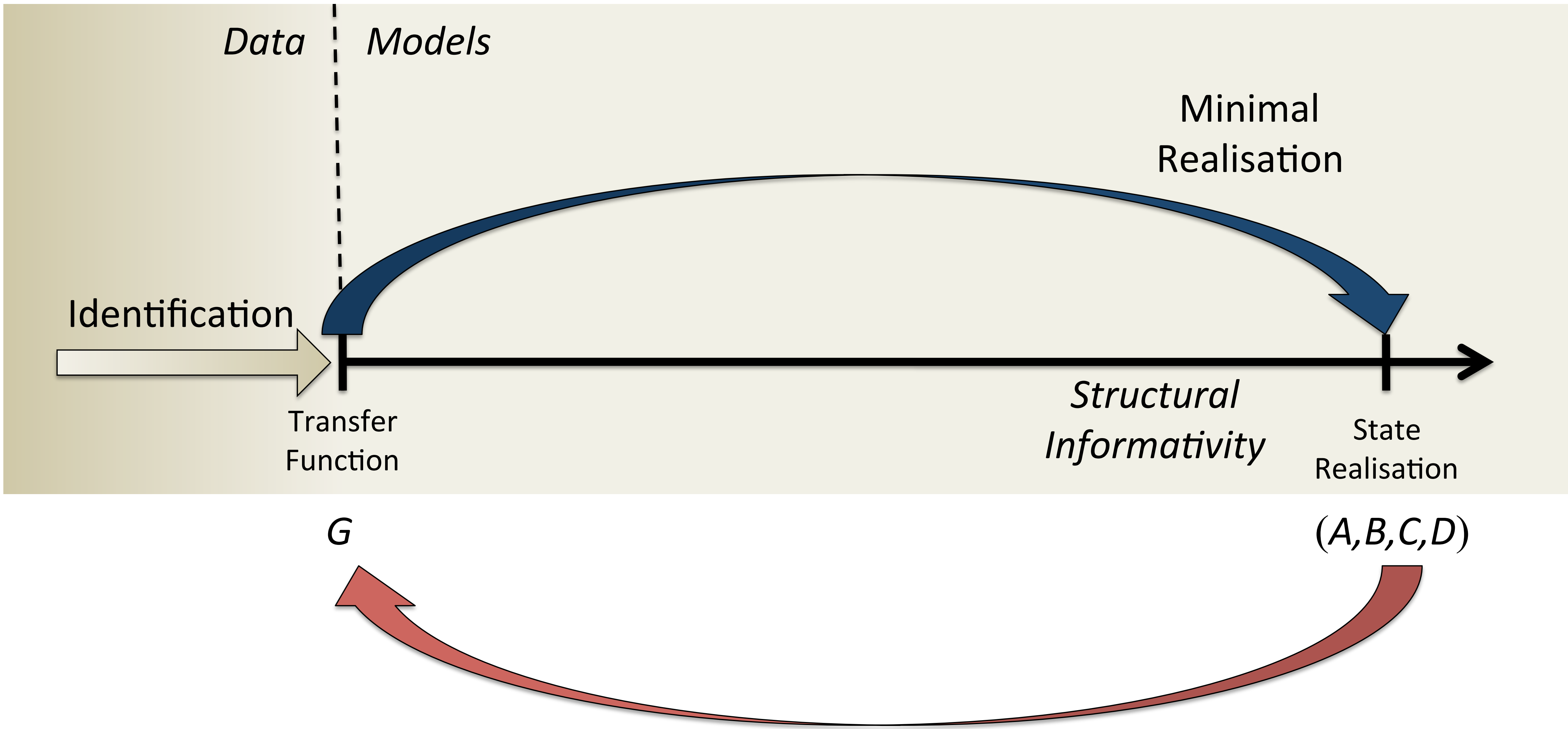
Network Reconstruction



Uniquely Specified:

$$G(s) = C(sI - A)^{-1}B + D$$

Network Reconstruction



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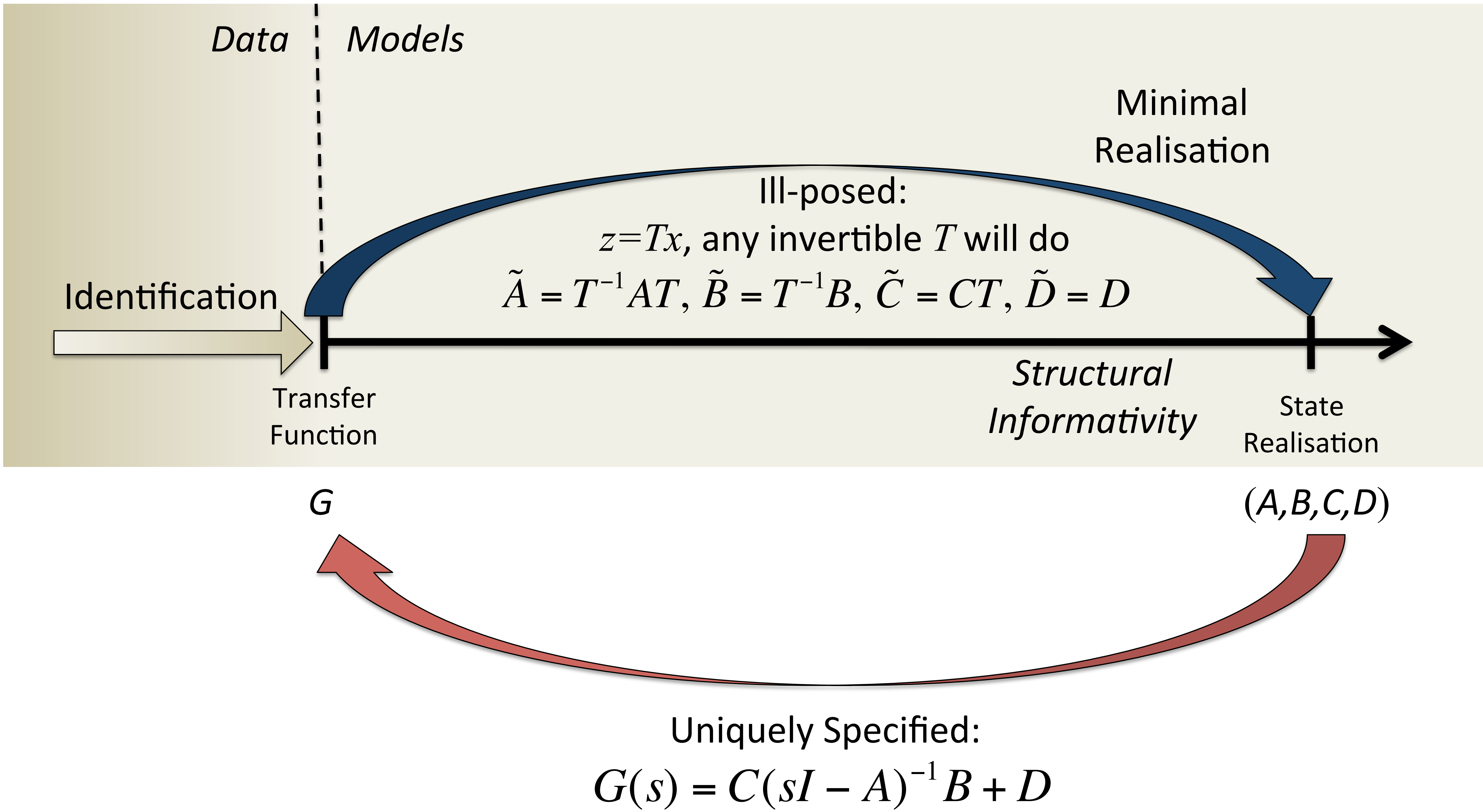
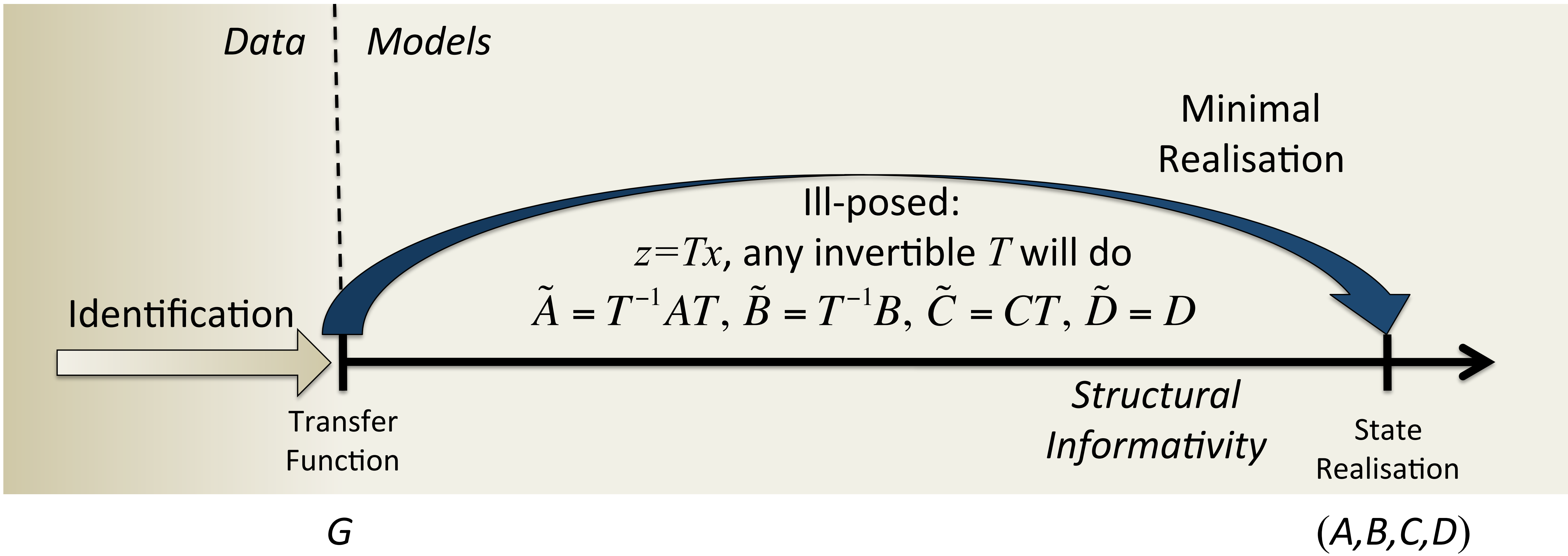
Network Reconstruction

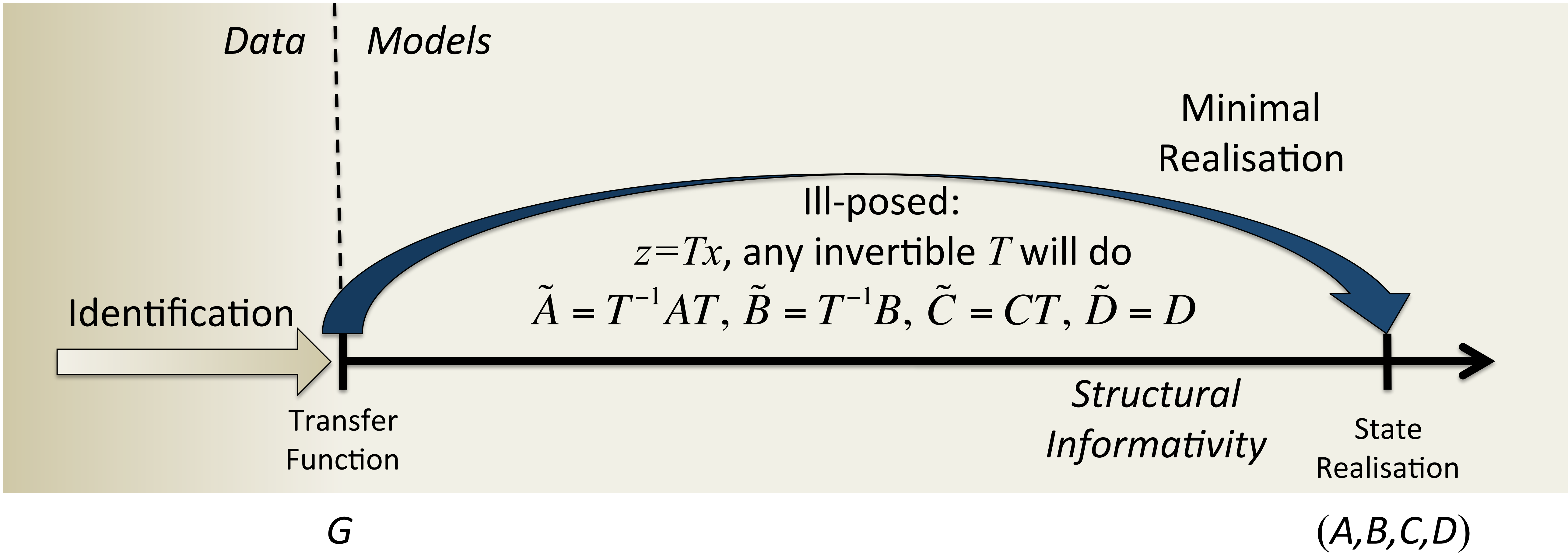


Network Reconstruction



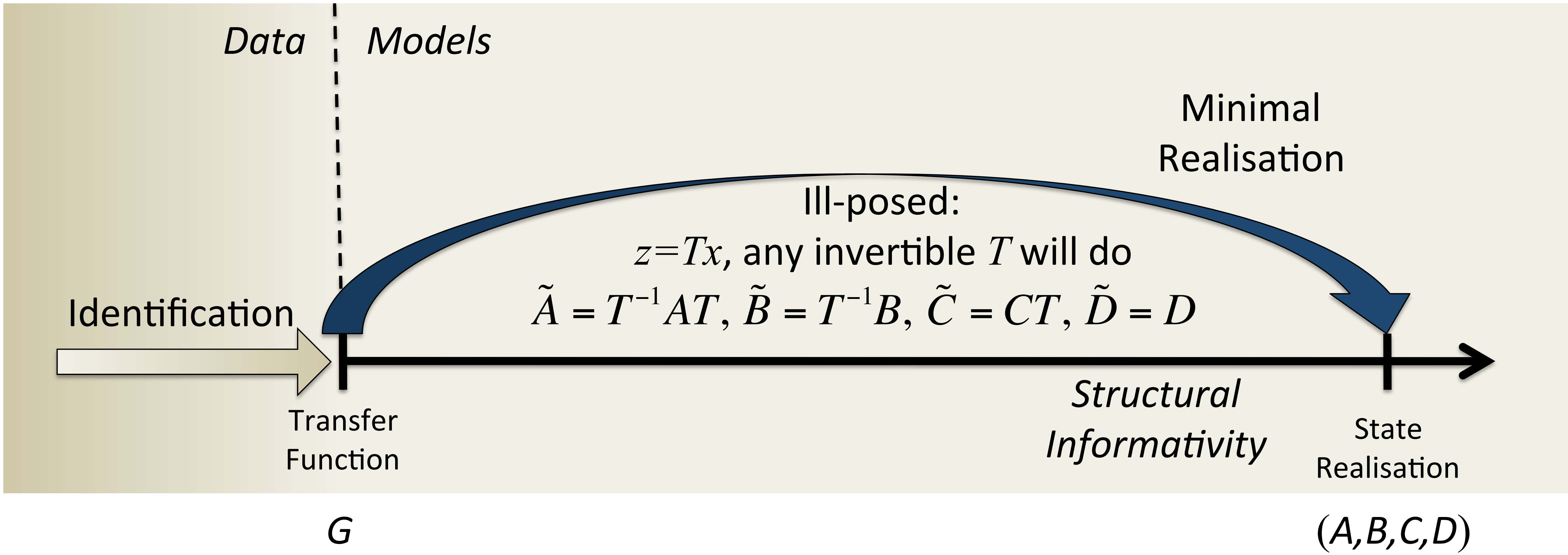
- How do network reconstruction methods find the true *(A, B, C, D)* from data when many *(A, B, C, D)* generate the same *G*?

Network Reconstruction



- How do network reconstruction methods find the true (A, B, C, D) from data when many (A, B, C, D) generate the same G?
- Assume full state measurements i.e. $C = I$, $D = 0$.

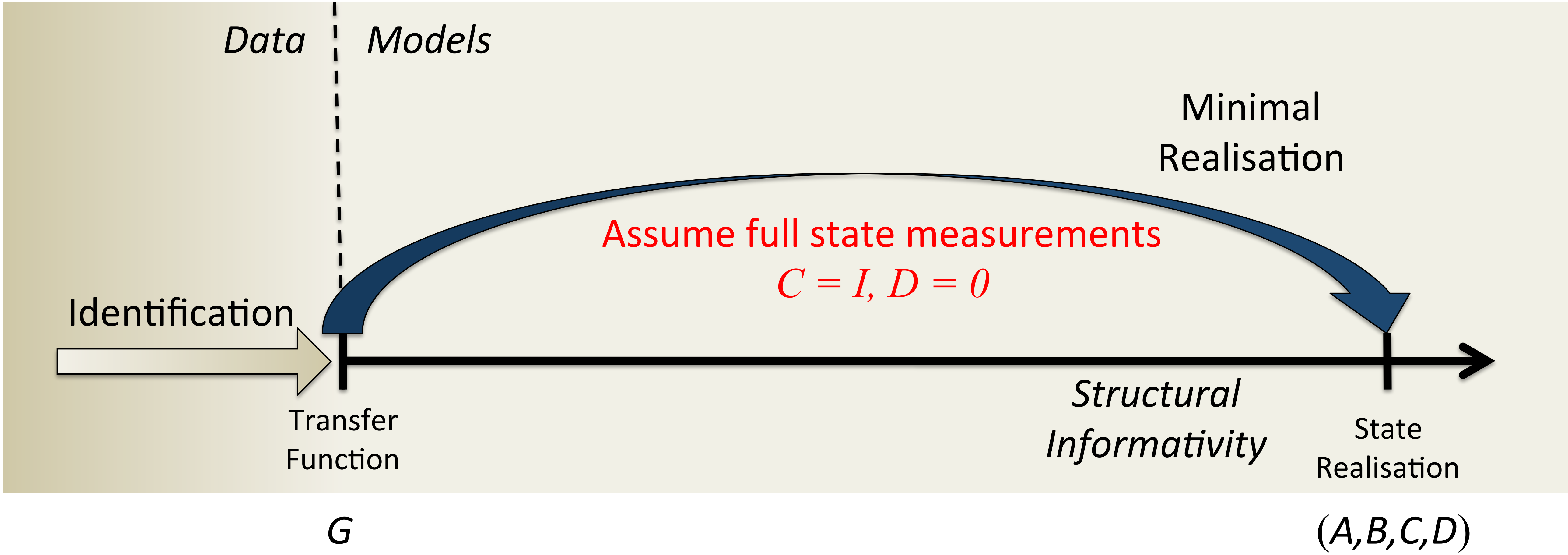
Network Reconstruction



- How do network reconstruction methods find the true *(A, B, C, D)* from data when many *(A, B, C, D)* generate the same *G*?
- Assume full state measurements i.e. $C = I$, $D = 0$.
- Fact: If $C = I$, $D = 0$ then there is a unique minimal state realisation for every transfer function G. **$A=sI-G^{-1}$ when B=I**

Julius, Zavlanos, Boyd, Pappas, 2011. Chang, Tomlin, 2012.

Network Reconstruction

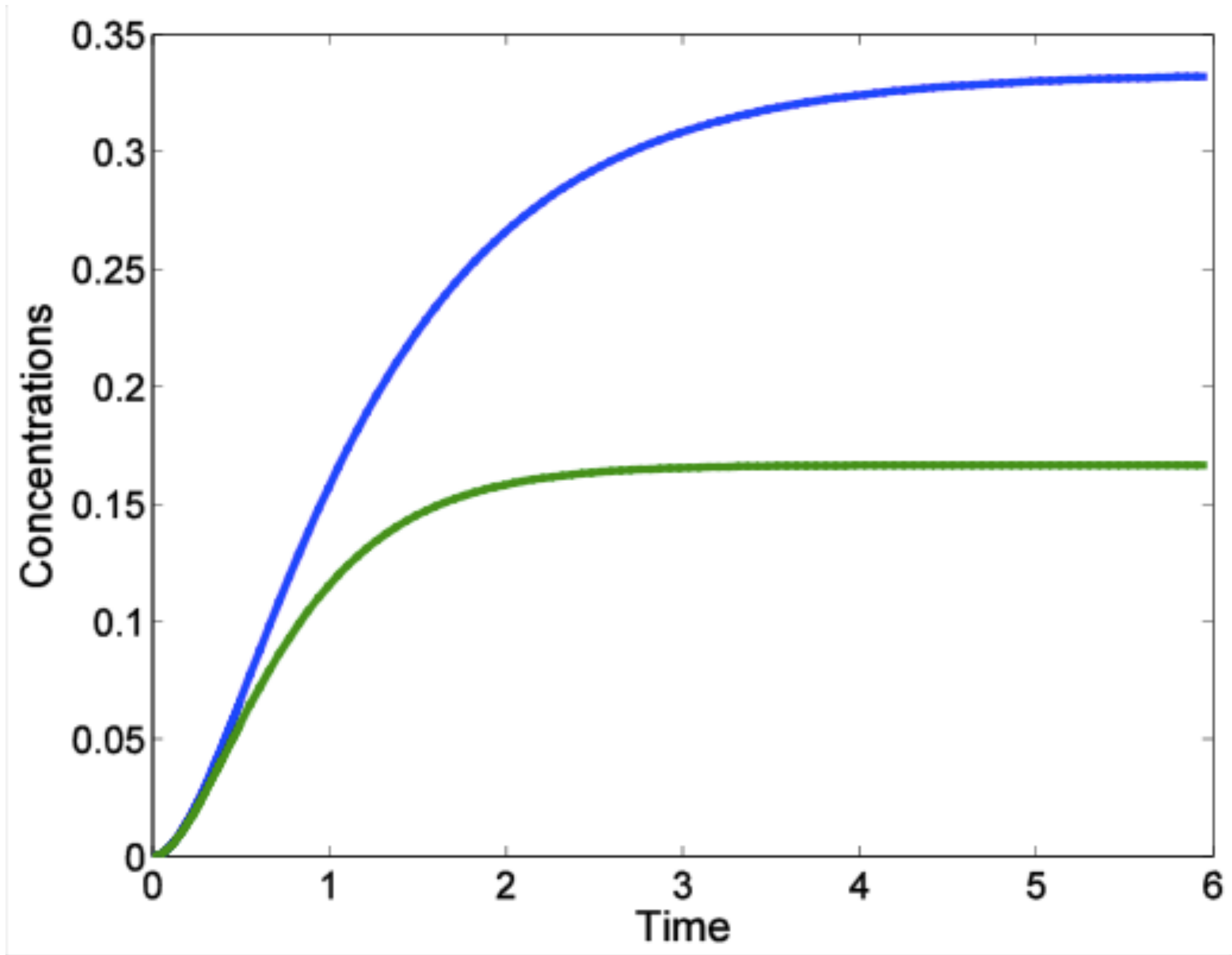


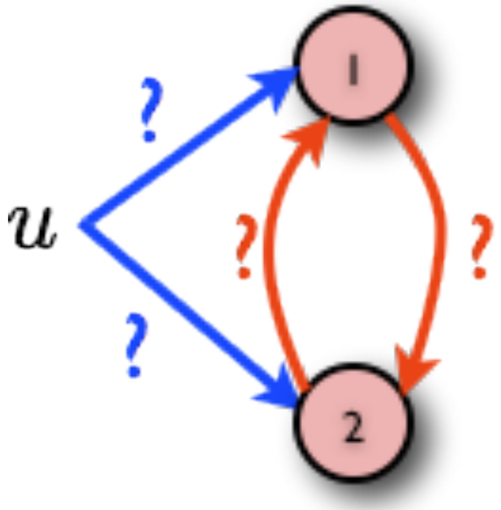
- What if we mistakenly assume full state measurements?
- If we only miss one “hidden” state, will our conclusions be “close”?

Network Reconstruction Example: Missing Just One Hidden State

Conclusions can be arbitrarily wrong!

$$G(s) = \frac{1}{s+3}\begin{bmatrix} \frac{1}{s+1} \\ \frac{1}{s+2} \end{bmatrix}$$



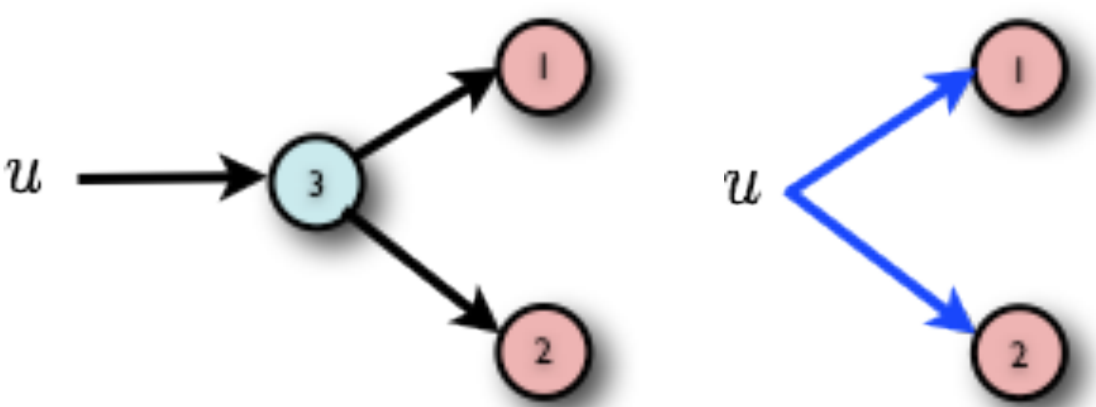


Network Reconstruction Example: Missing Just One Hidden State

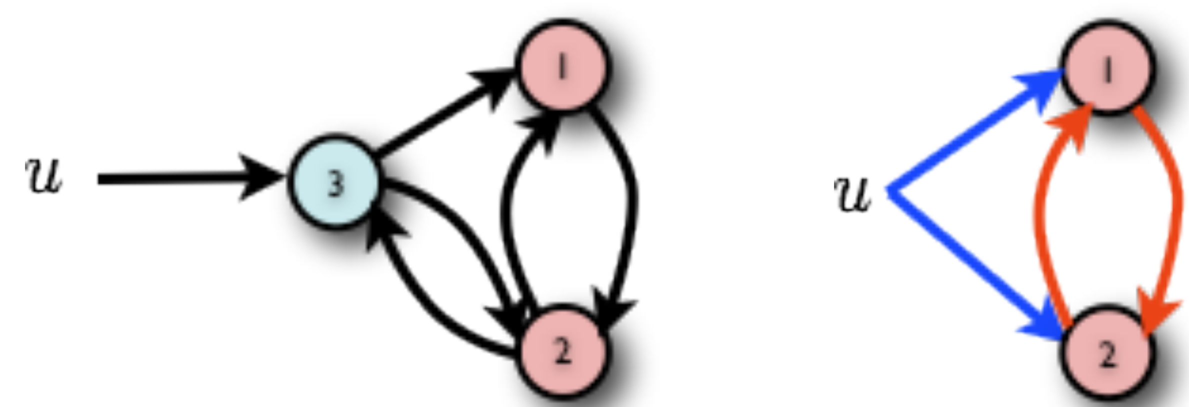
Conclusions can be arbitrarily wrong!

$$B = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^T \text{ and } C = \begin{bmatrix} I & 0 \end{bmatrix}$$

$$A = \begin{bmatrix} -1 & 0 & 1 \\ 0 & -2 & 1 \\ 0 & 0 & -3 \end{bmatrix}$$



$$A = \begin{bmatrix} -2 & -1 & 1 \\ -1 & -3 & 1 \\ 0 & -1 & -1 \end{bmatrix}$$



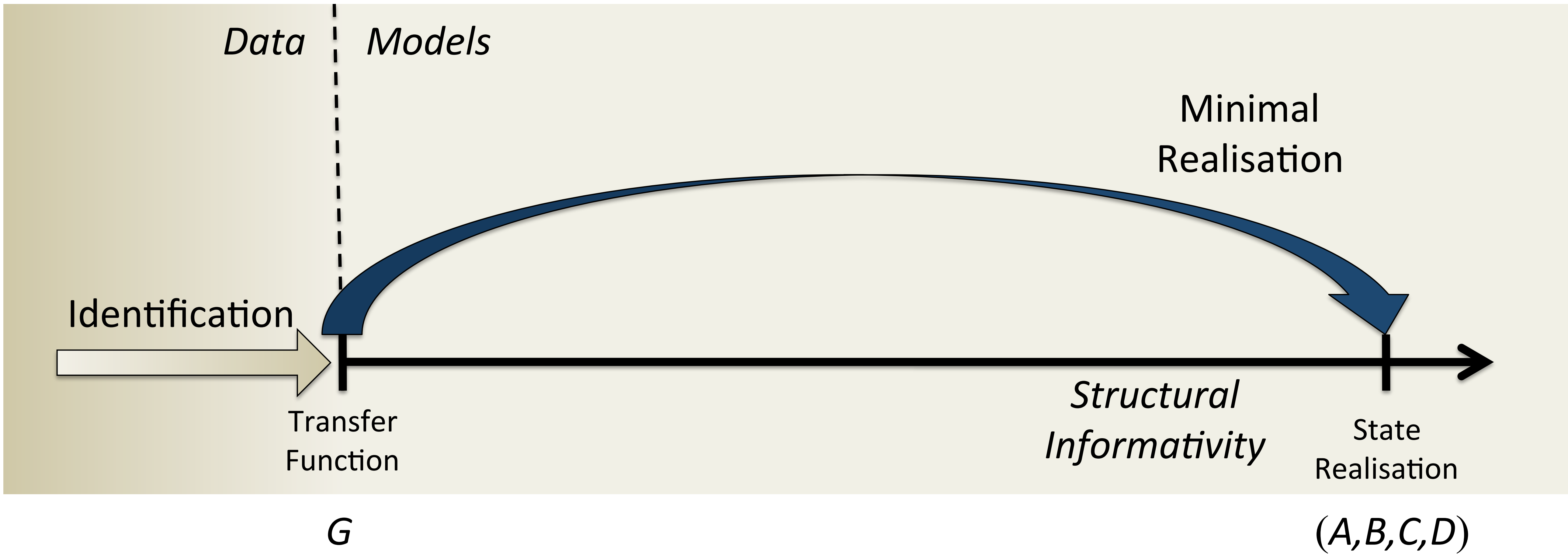
Both realisations are minimal

Outline

- Motivation
- Introduction of dynamical structure function
- How it can be used to solve this network reconstruction problem?


盲人摸象

Network Reconstruction



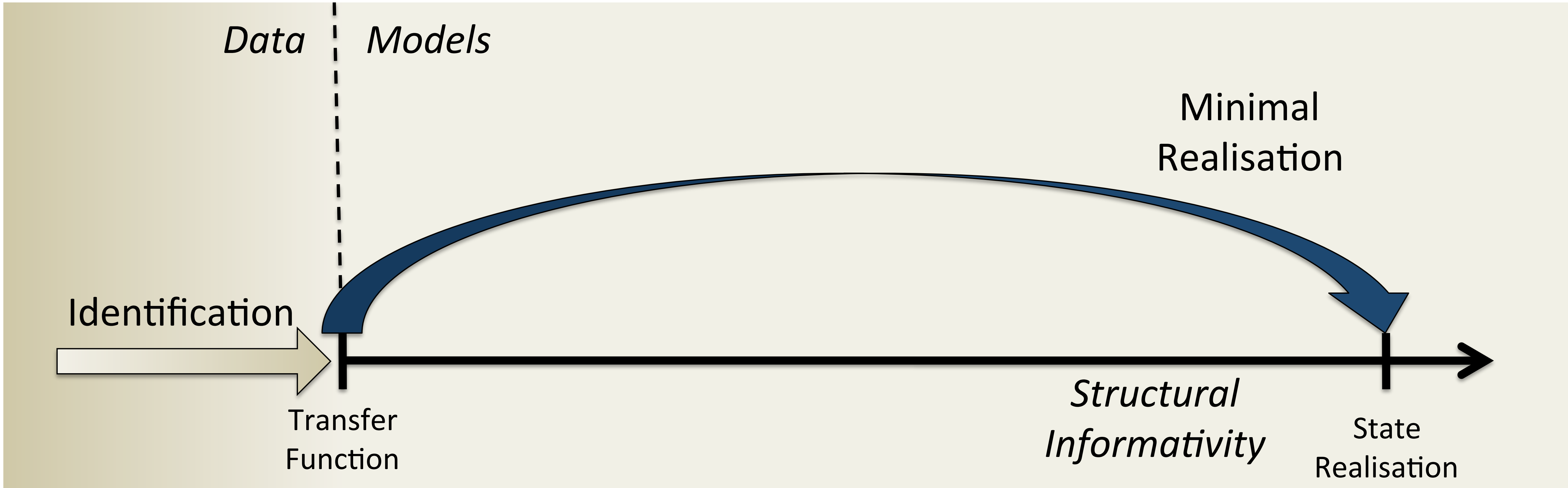
I/O Methods

Weak characterization of internal structure

State Space Methods

Demand unreasonable assumptions--like full state measurement

Network Reconstruction



G

(A,B,C,D)

I/O Methods

Weak characterization of internal structure

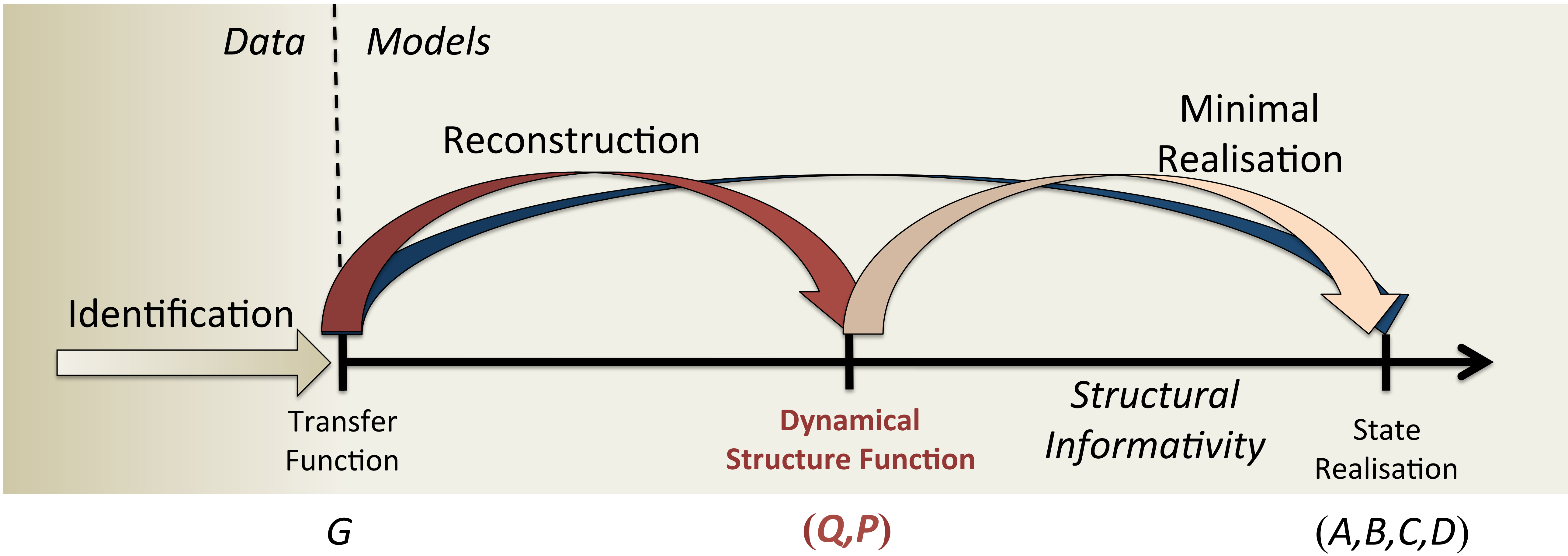
Need an intermediate system representation:

- more structure than TF
- Fewer assumptions than State Space

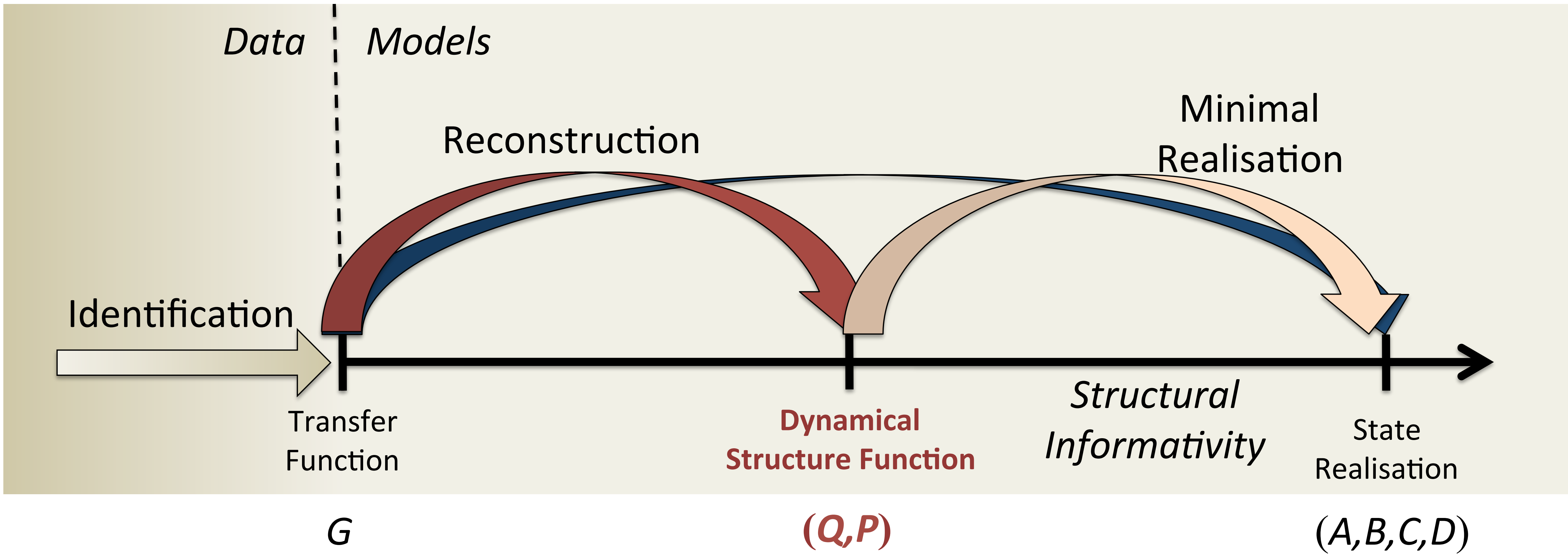
State Space Methods

Demand unreasonable assumptions--like full state measurement

Dynamical Structure Functions



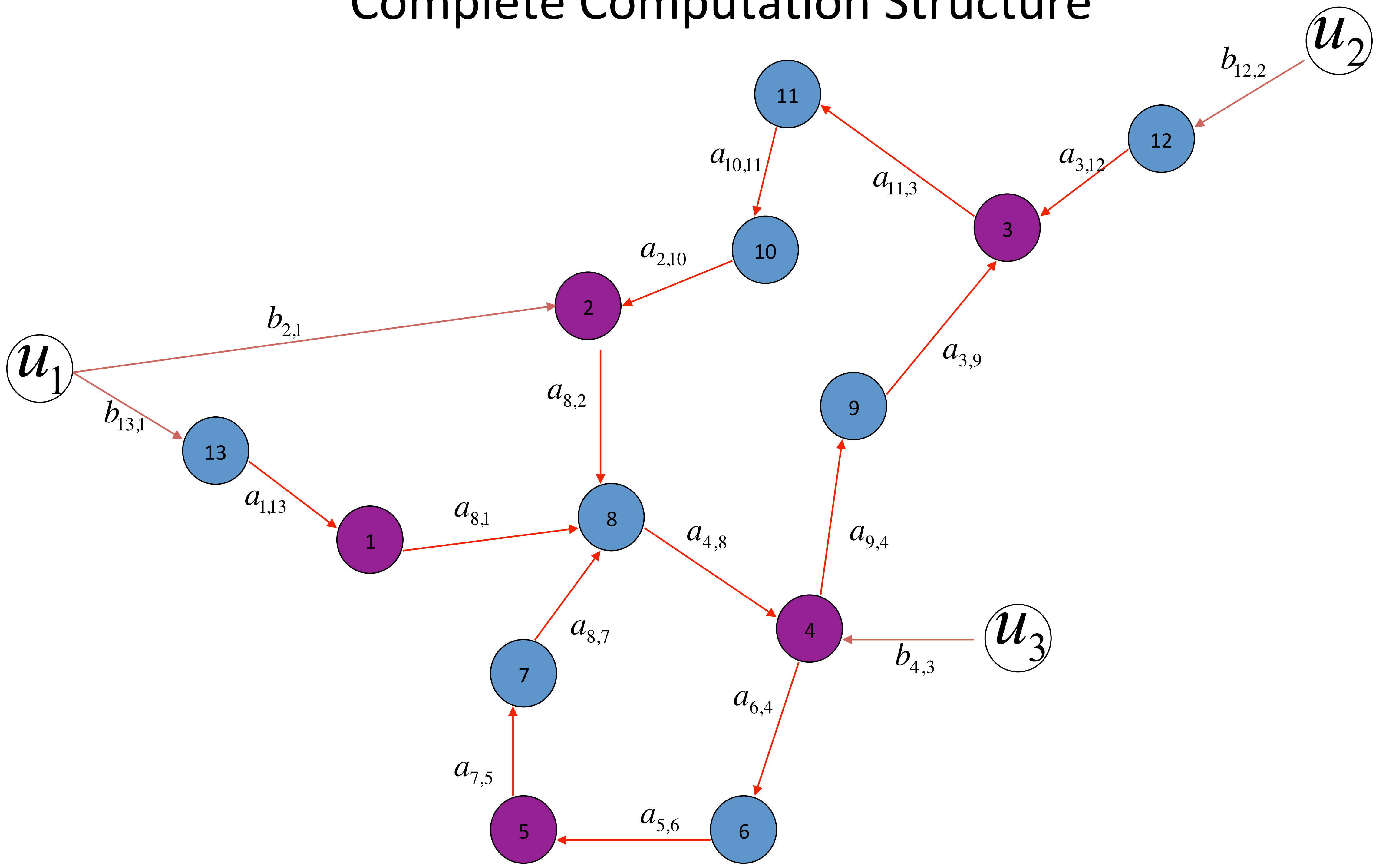
Dynamical Structure Functions



- Dynamical Structure Functions (DSF)
  - New representation for systems
  - More structurally informative than the input-output map
  - Less restrictive to reconstruct from data than the full state realisation

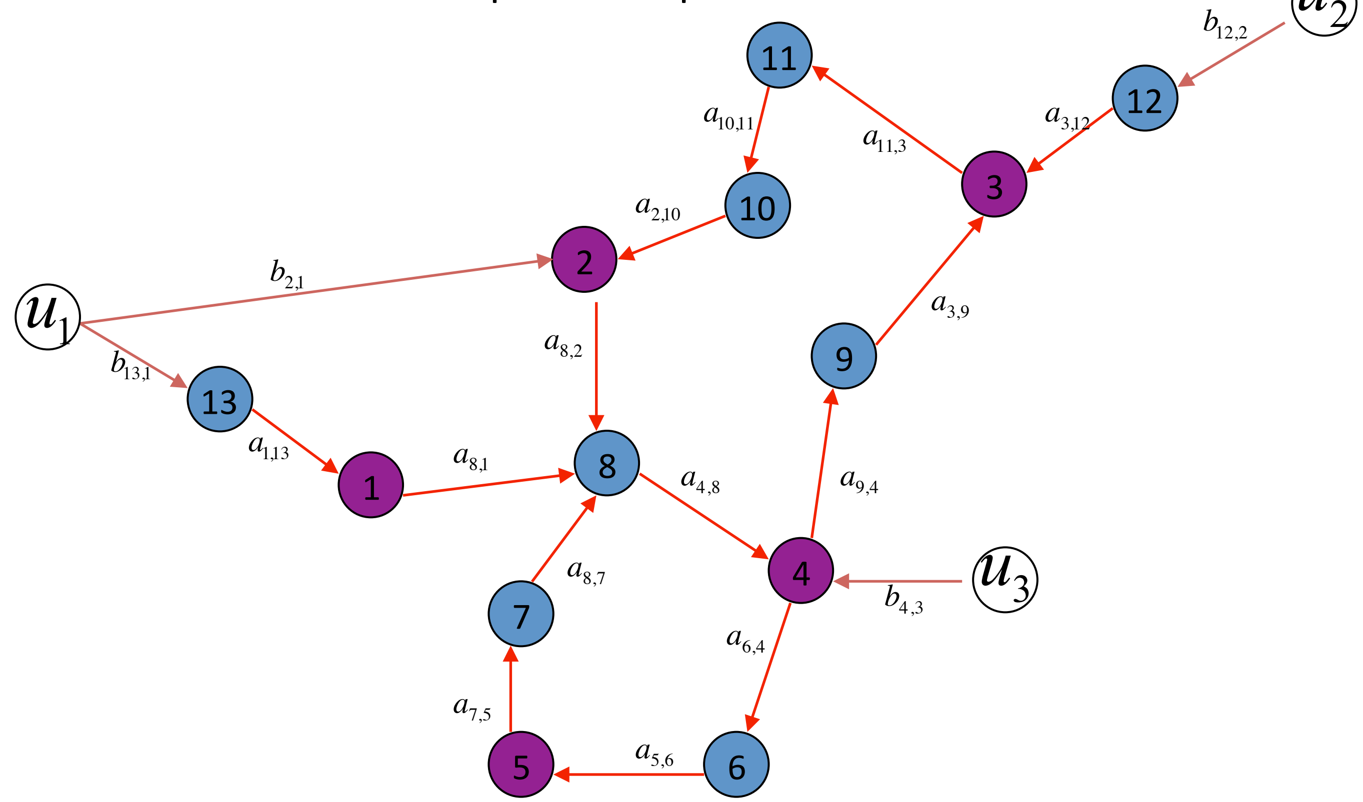
Dynamical Structure Function Example

Complete Computation Structure



Dynamical Structure Function Example

Complete Computation Structure



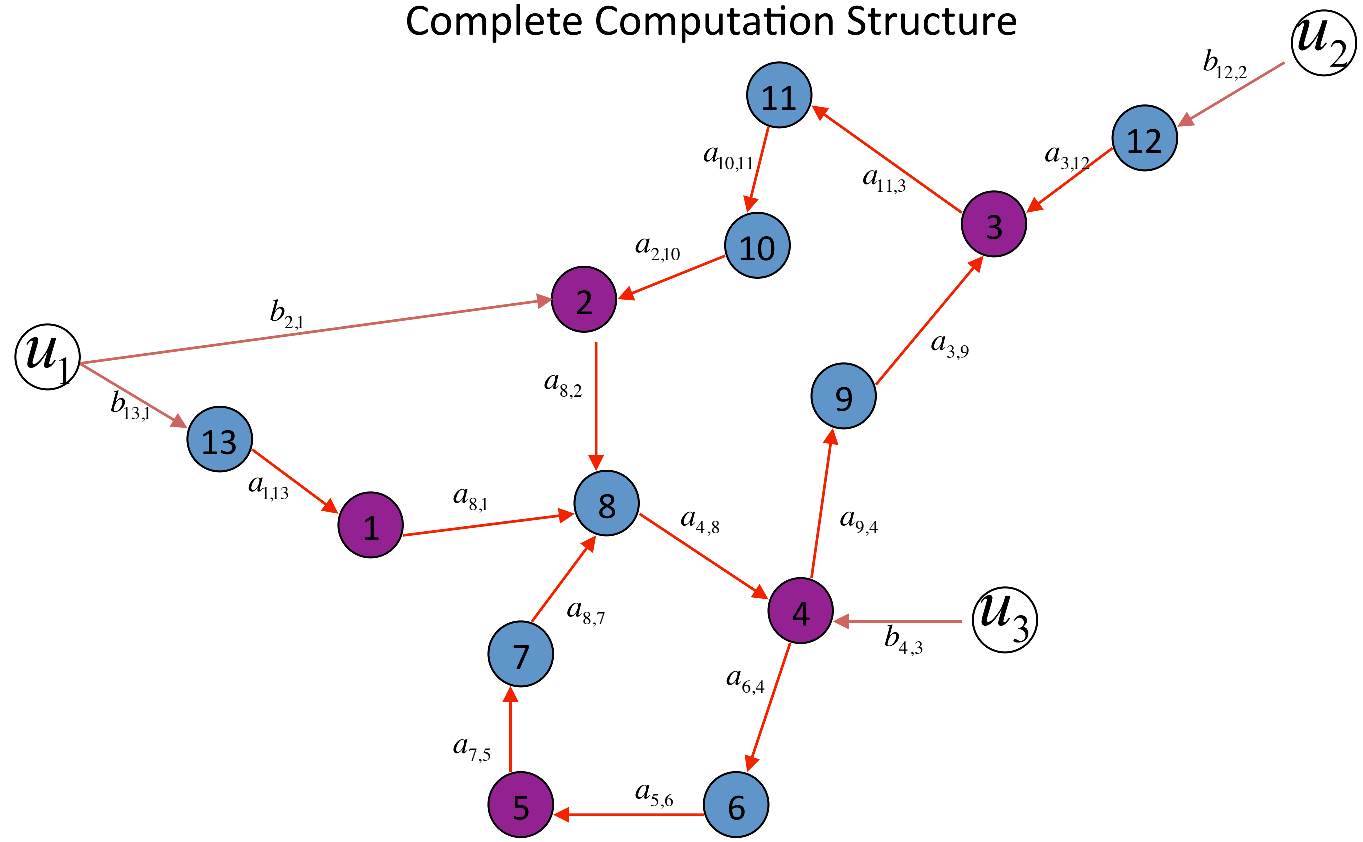
$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \\ \dot{x}_6 \\ \dot{x}_7 \\ \dot{x}_8 \\ \dot{x}_9 \\ \dot{x}_{10} \\ \dot{x}_{11} \\ \dot{x}_{12} \\ \dot{x}_{13} \end{bmatrix}
=
\begin{bmatrix}
a_{1,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{1,13} \\
0 & a_{2,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{2,10} & 0 & 0 & 0 \\
0 & 0 & a_{3,3} & 0 & 0 & 0 & 0 & 0 & a_{3,9} & 0 & 0 & a_{3,12} & 0 \\
0 & 0 & 0 & a_{4,4} & 0 & 0 & 0 & a_{4,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{5,5} & a_{5,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{6,4} & 0 & a_{6,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{7,5} & 0 & a_{7,7} & 0 & 0 & 0 & 0 & 0 & 0 \\
a_{8,1} & a_{8,2} & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{9,4} & 0 & 0 & 0 & 0 & a_{9,9} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,10} & a_{10,11} & 0 & 0 \\
0 & 0 & a_{11,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{11,11} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{12,12} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{13,13}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 \\
b_{2,1} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & b_{4,3} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & b_{12,2} & 0 \\
b_{13,1} & 0 & 0
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}
$$

State Space Realisation

Dynamical Structure Function Example

- Signal Structure
  - Makes no assumptions about hidden states
  - Describes the causal dependencies among manifest variables

Complete Computation Structure



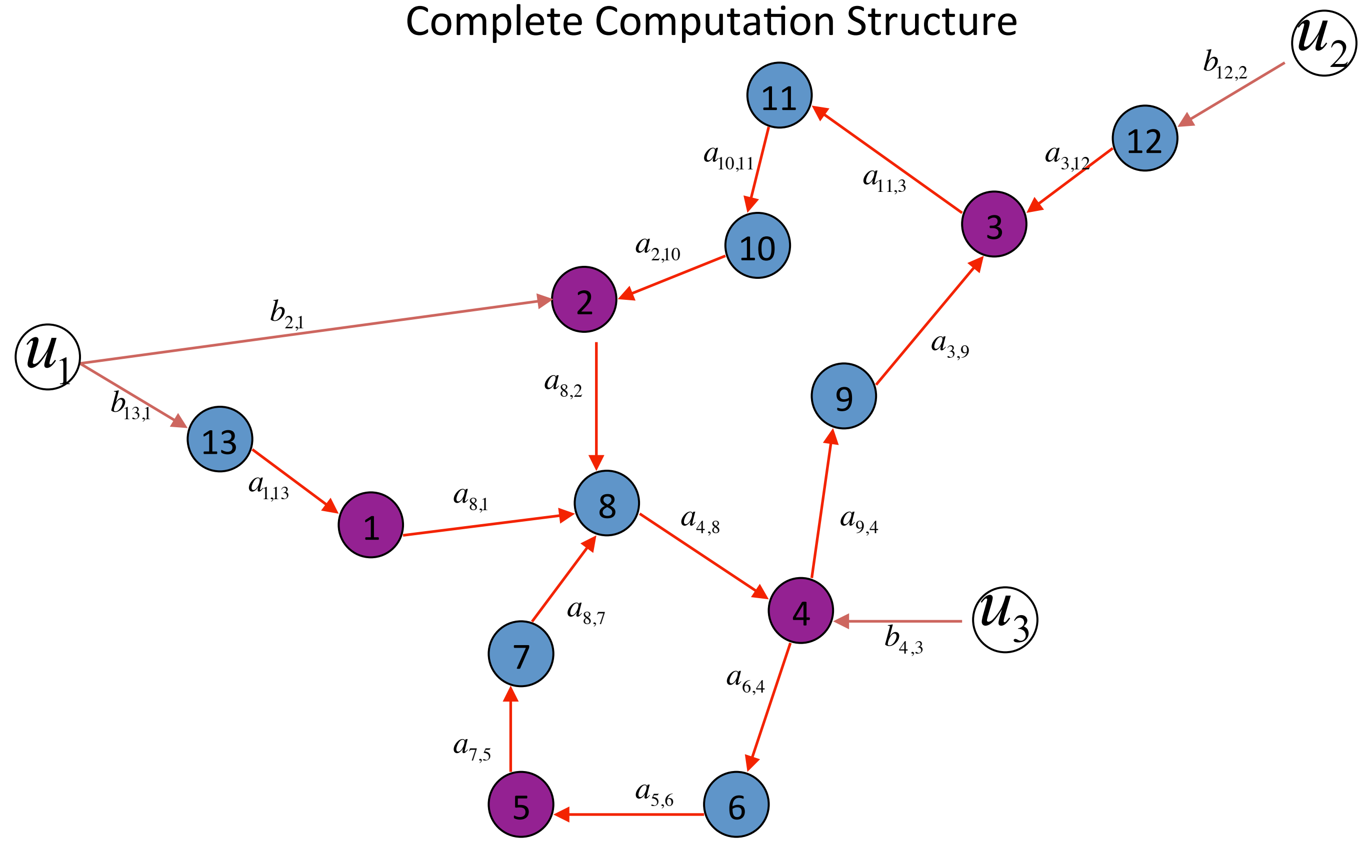
$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \\ \dot{x}_6 \\ \dot{x}_7 \\ \dot{x}_8 \\ \dot{x}_9 \\ \dot{x}_{10} \\ \dot{x}_{11} \\ \dot{x}_{12} \\ \dot{x}_{13} \end{bmatrix}
=
\begin{bmatrix}
a_{1,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{1,13} \\
0 & a_{2,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{2,10} & 0 & 0 & 0 \\
0 & 0 & a_{3,3} & 0 & 0 & 0 & 0 & 0 & a_{3,9} & 0 & 0 & a_{3,12} & 0 \\
0 & 0 & 0 & a_{4,4} & 0 & 0 & 0 & a_{4,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{5,5} & a_{5,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{6,4} & 0 & a_{6,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{7,5} & 0 & a_{7,7} & 0 & 0 & 0 & 0 & 0 & 0 \\
a_{8,1} & a_{8,2} & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{9,4} & 0 & 0 & 0 & 0 & a_{9,9} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,10} & a_{10,11} & 0 & 0 \\
0 & 0 & a_{11,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{11,11} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{12,12} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{13,13}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 \\
b_{2,1} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & b_{4,3} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & b_{12,2} & 0 \\
b_{13,1} & 0 & 0
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}
$$

State Space Realisation

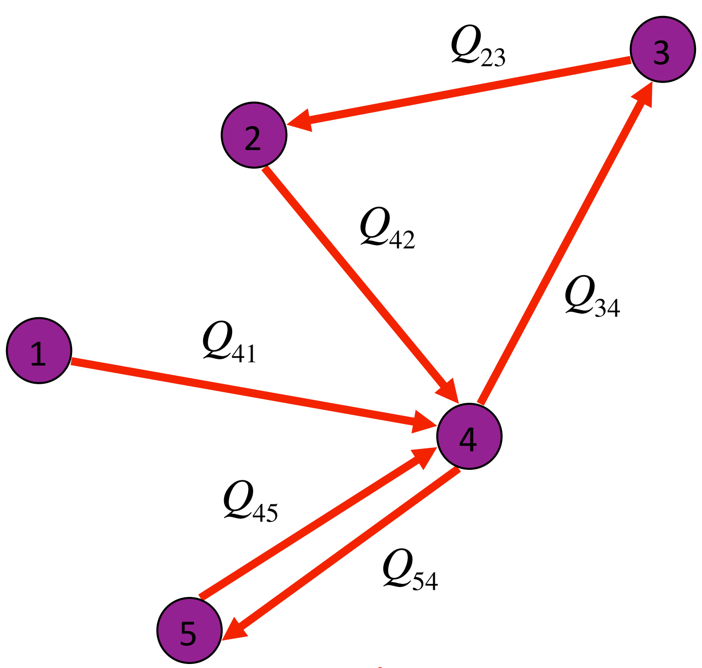
Dynamical Structure Function Example

- Signal Structure
  - Makes no assumptions about hidden states
  - Describes the causal dependencies among manifest variables

Complete Computation Structure



Signal Structure



Internal Structure

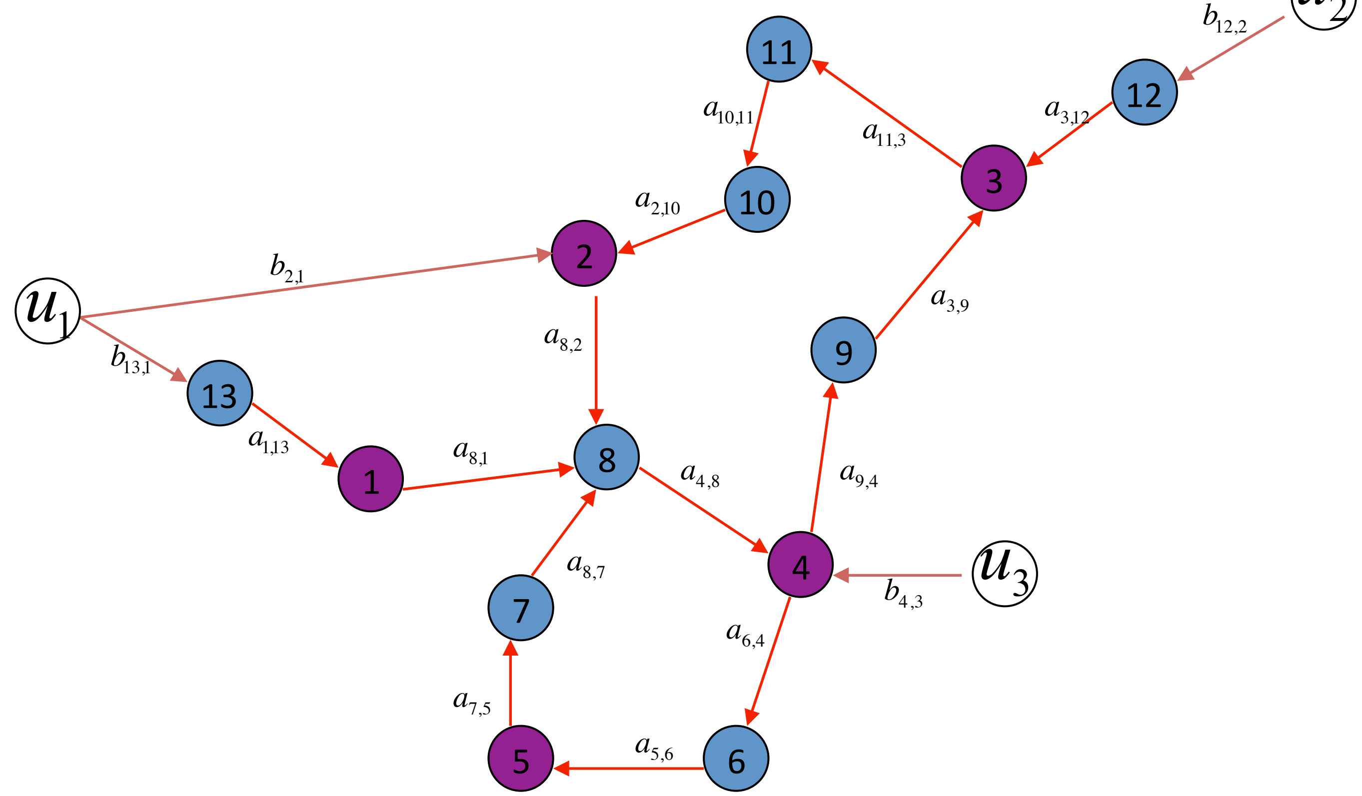
$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \\ \dot{x}_6 \\ \dot{x}_7 \\ \dot{x}_8 \\ \dot{x}_9 \\ \dot{x}_{10} \\ \dot{x}_{11} \\ \dot{x}_{12} \\ \dot{x}_{13} \end{bmatrix}
=
\begin{bmatrix}
a_{1,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{1,13} \\
0 & a_{2,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{2,10} & 0 & 0 & 0 \\
0 & 0 & a_{3,3} & 0 & 0 & 0 & 0 & 0 & a_{3,9} & 0 & 0 & a_{3,12} & 0 \\
0 & 0 & 0 & a_{4,4} & 0 & 0 & 0 & a_{4,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{5,5} & a_{5,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{6,4} & 0 & a_{6,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{7,5} & 0 & a_{7,7} & 0 & 0 & 0 & 0 & 0 & 0 \\
a_{8,1} & a_{8,2} & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{9,4} & 0 & 0 & 0 & 0 & a_{9,9} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,10} & a_{10,11} & 0 & 0 \\
0 & 0 & a_{11,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{11,11} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{12,12} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{13,13}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 \\
b_{2,1} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & b_{4,3} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & b_{12,2} & 0 \\
b_{13,1} & 0 & 0
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}
$$

State Space Realisation

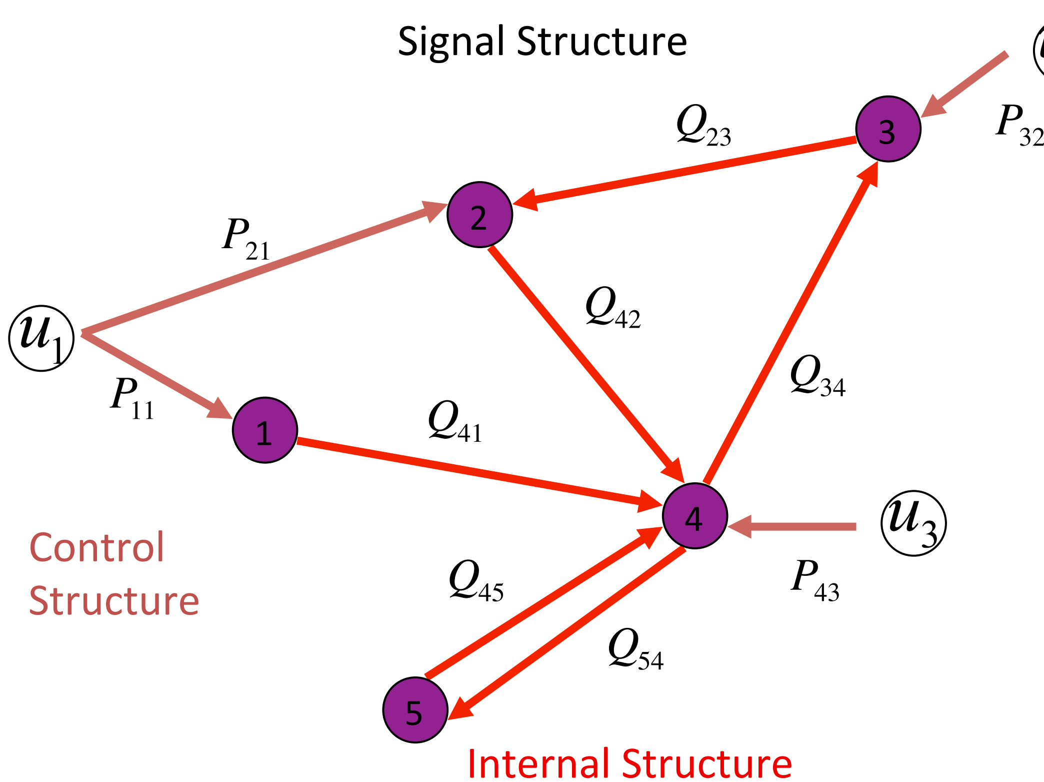
Dynamical Structure Function Example

- Signal Structure
  - Makes no assumptions about hidden states
  - Describes the causal dependencies among manifest variables

Complete Computation Structure



Signal Structure



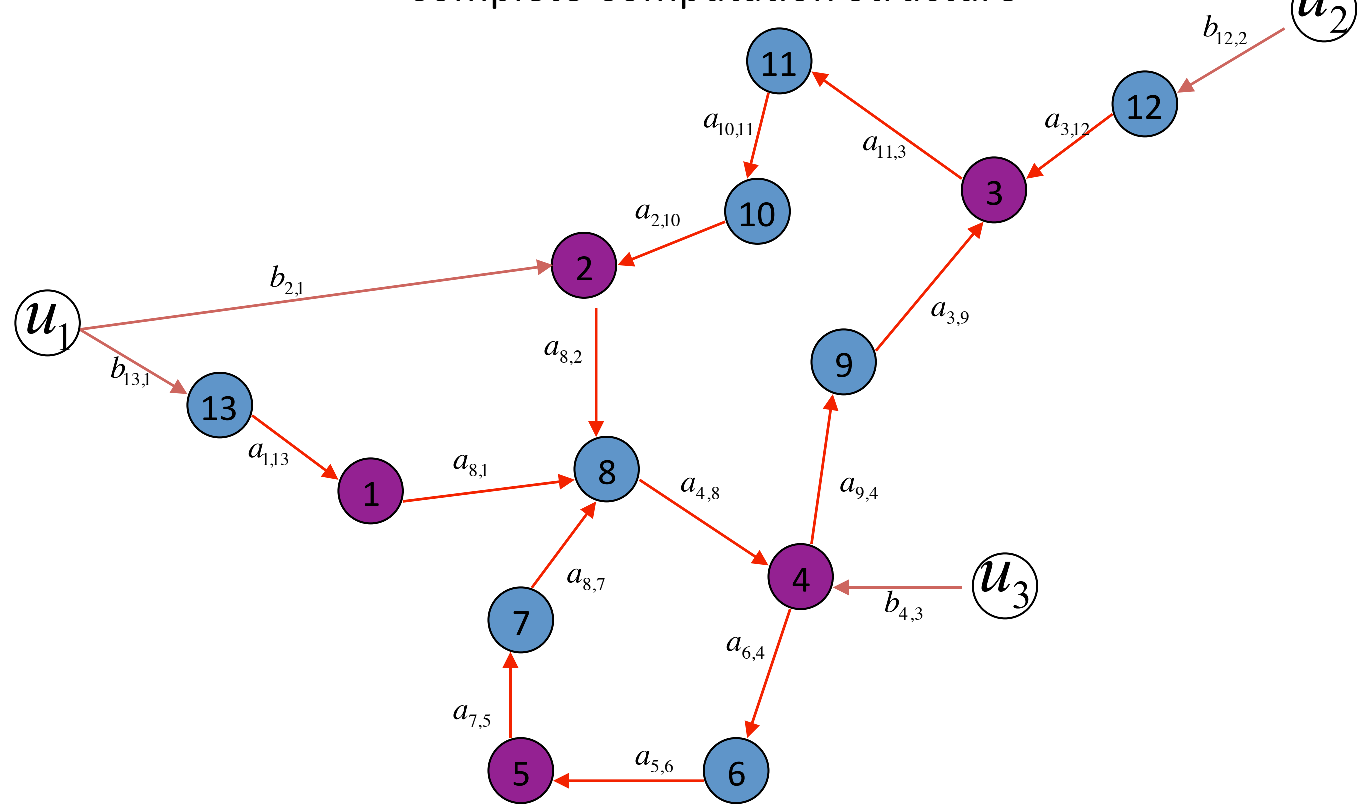
$$
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \\ \dot{x}_5 \\ \dot{x}_6 \\ \dot{x}_7 \\ \dot{x}_8 \\ \dot{x}_9 \\ \dot{x}_{10} \\ \dot{x}_{11} \\ \dot{x}_{12} \\ \dot{x}_{13} \end{bmatrix}
=
\begin{bmatrix}
a_{1,1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{1,13} \\
0 & a_{2,2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{2,10} & 0 & 0 & 0 \\
0 & 0 & a_{3,3} & 0 & 0 & 0 & 0 & 0 & a_{3,9} & 0 & 0 & a_{3,12} & 0 \\
0 & 0 & 0 & a_{4,4} & 0 & 0 & 0 & a_{4,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{5,5} & a_{5,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{6,4} & 0 & a_{6,6} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & a_{7,5} & 0 & a_{7,7} & 0 & 0 & 0 & 0 & 0 & 0 \\
a_{8,1} & a_{8,2} & 0 & 0 & 0 & 0 & a_{8,7} & a_{8,8} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_{9,4} & 0 & 0 & 0 & 0 & a_{9,9} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{10,10} & a_{10,11} & 0 & 0 \\
0 & 0 & a_{11,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{11,11} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{12,12} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a_{13,13}
\end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \end{bmatrix}
+
\begin{bmatrix}
0 & 0 & 0 \\
b_{2,1} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & b_{4,3} \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & b_{12,2} & 0 \\
b_{13,1} & 0 & 0
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}
$$

State Space Realisation

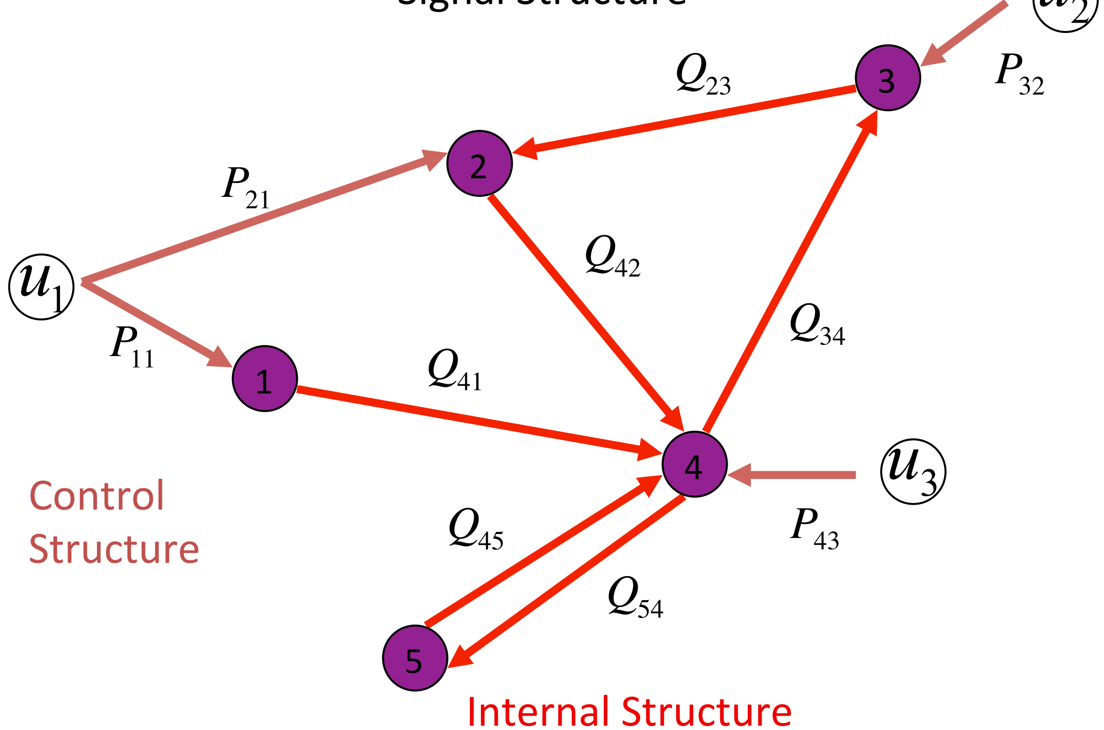
Dynamical Structure Function Example

- Signal Structure
  - Makes no assumptions about hidden states
  - Describes the causal dependencies among manifest variables

Complete Computation Structure



Signal Structure



$$Y = QY + PU$$

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & Q_{23} & 0 & 0 \\ 0 & 0 & 0 & Q_{34} & 0 \\ Q_{41} & Q_{42} & 0 & 0 & Q_{45} \\ 0 & 0 & 0 & Q_{54} & 0 \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \\ Y_5 \end{bmatrix} + \begin{bmatrix} P_{11} & 0 & 0 \\ P_{21} & 0 & 0 \\ 0 & P_{32} & 0 \\ 0 & 0 & P_{43} \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

Internal Structure

Control Structure

Dynamical Structure Functions

- Consider the system:

$$\begin{bmatrix} \dot{y} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} u \quad \text{with}$$

$$y = \begin{bmatrix} I & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix}$$

$u(t) \in R^m$ inputs

$y(t) \in R^p$ measured states

$z(t) \in R^{n-p}$ hidden states

- Taking Laplace transforms:

$$\begin{bmatrix} sY \\ sZ \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} Y \\ Z \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} U$$

- Solving for hidden states in terms of measured states and inputs:

$$\Rightarrow Z = (sI - A_{22})^{-1} A_{21} Y + (sI - A_{22})^{-1} B_2 U$$

- Substitute for Z in first line:

$$sY = A_{11}Y + A_{12}\left[(sI - A_{22})^{-1} A_{21} Y + (sI - A_{22})^{-1} B_2 U\right] + B_1 U$$

$$sY = \underbrace{\left[A_{11} + A_{12}(sI - A_{22})^{-1} A_{21}\right]}_{W} Y + \underbrace{\left[A_{12}(sI - A_{22})^{-1} B_2 + B_1\right]}_{V} U$$

$$sY = WY + VU$$

- To solve for Y, let D be a matrix of the diagonal entries of W:

$$D = \text{diag}\left(W_{11}, W_{22}, \ldots, W_{pp}\right)$$

$$\Rightarrow (sI - D)Y = (W - D)Y + VU$$

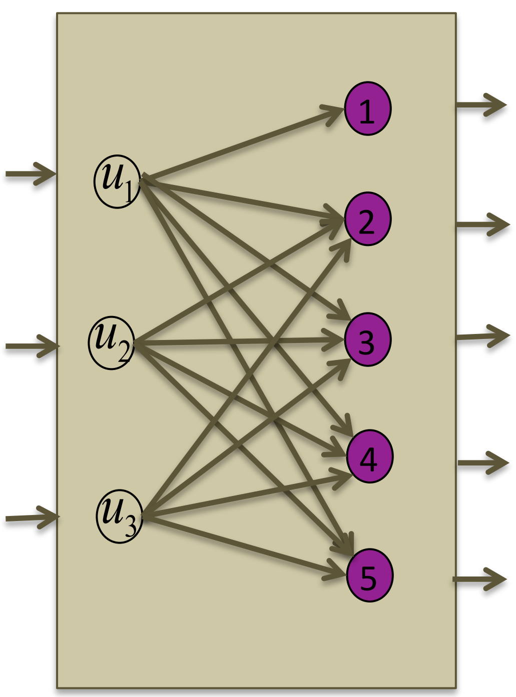
$$\Rightarrow Y = \underbrace{\left[(SI - D)^{-1}(W - D)\right]}_{Q} Y + \underbrace{\left[(SI - D)^{-1} V\right]}_{P} U$$

$$\boxed{Y = QY + PU}$$

Note Q is zero on the diagonal. It is a matrix of strictly proper transfer functions relating outputs to other outputs. P is a matrix of strictly proper transfer functions relating inputs to outputs *excluding dependence on any other output.*

Structures of System Representations

Sparsity Pattern of the Transfer Function

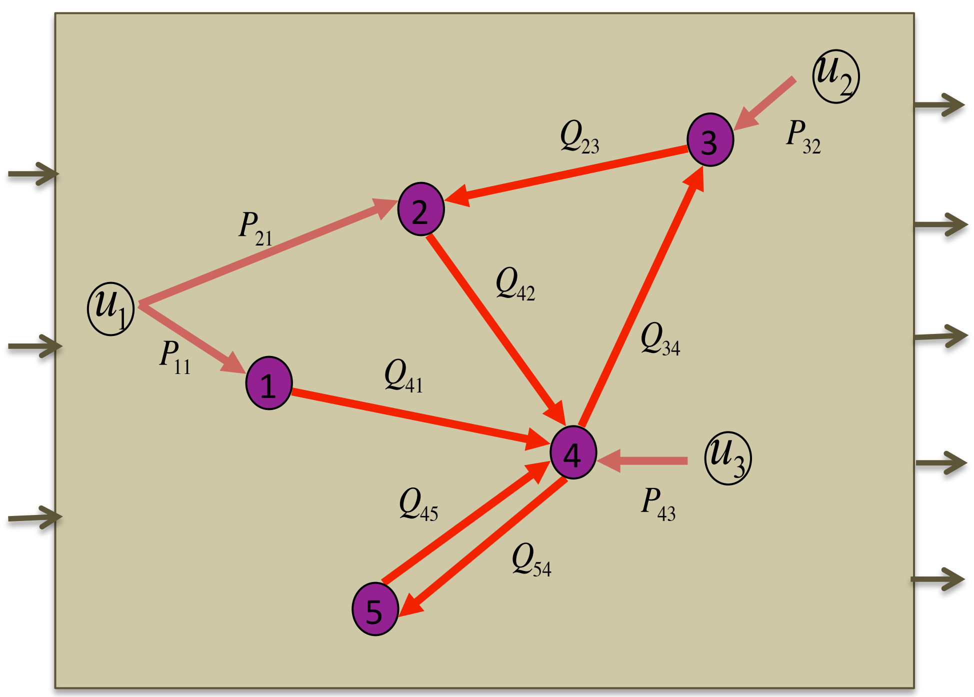


(closed-loop *paths* from inputs to outputs)

$$G$$

Transfer Function

Signal Structure

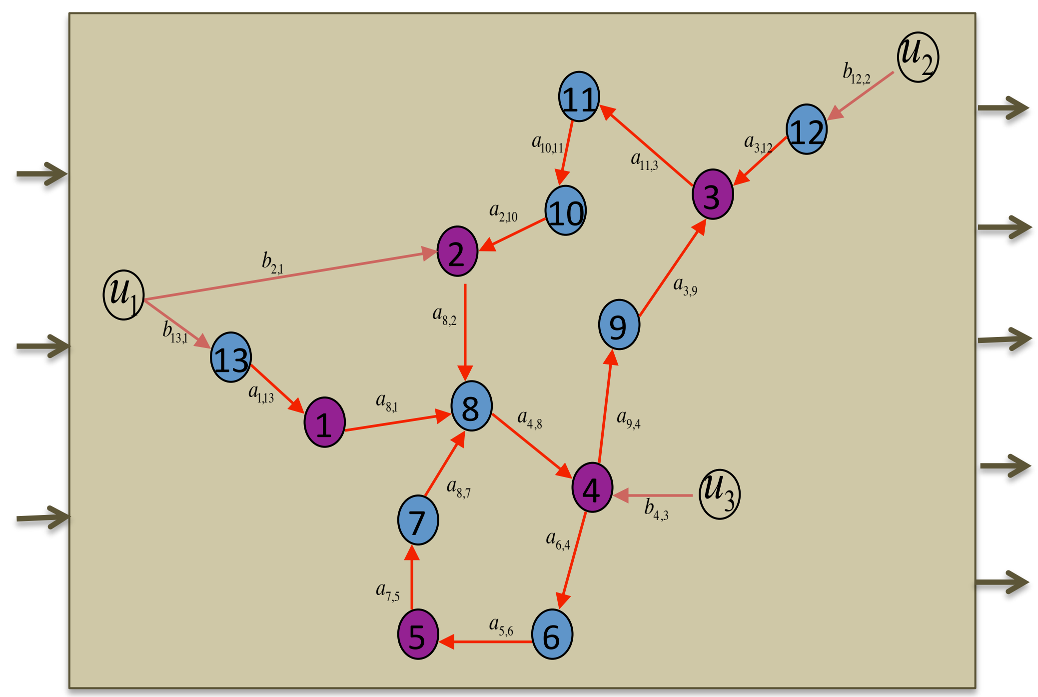


(*causal dependencies* among manifest variables)

$$(Q, P)$$

Dynamical Structure Function

Complete Computational Structure



(physical interconnection)

$$(A, B, C, D)$$

State Space Realisation

Outline

- Motivation
- Introduction of dynamical structure function
- How it can be used to solve this network reconstruction problem?

Dynamical network structure

Question: given input-output measurements from a system, can we reconstruct its dynamical or boolean structure?

$$Y = QY + PU$$

$$Y = GU$$

$$(I - Q)Y = PU \quad \Leftrightarrow (I - Q)GU = PU$$

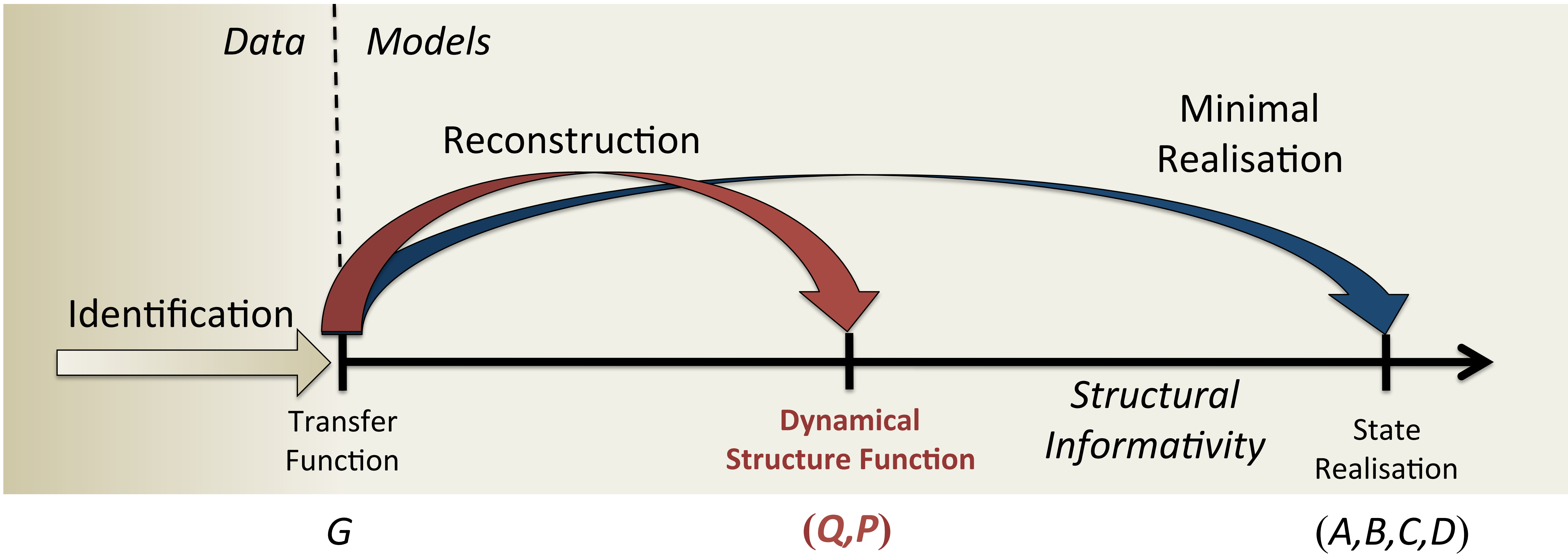
$$(I - Q)G = P$$

Every transfer function admits any internal structure

Given G and Q there is a P such that (Q,P) is consistent with G.

In particular, any transfer function has a realisation with an internal structure that is completely *de-coupled* (i.e. $Q = 0$) or *fully connected*.

Dynamical Structure Functions



- Reconstruction, like Realisation, is ill posed
  - Many (Q,P)s consistent with same G
  - Impossible without a priori structural information
    - For realisation, need knowledge of full state measurements
    - For reconstruction, target specificity is sufficient

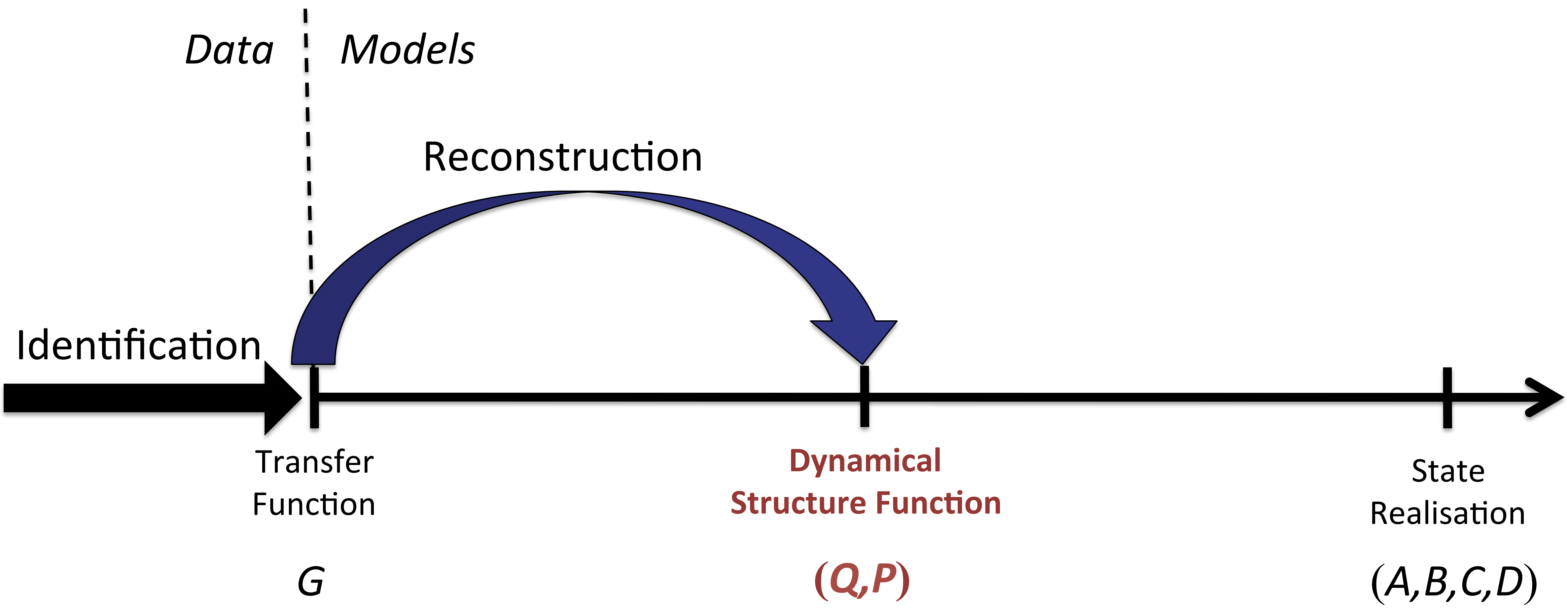
Network reconstruction

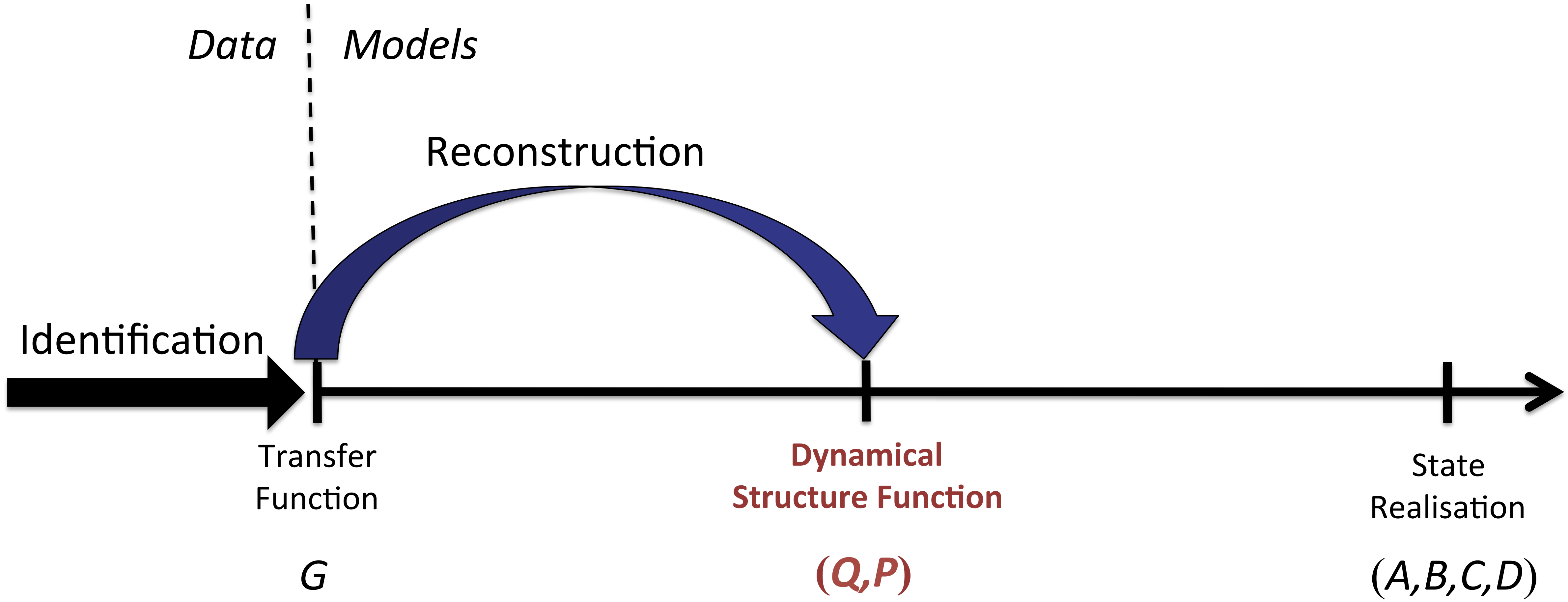
$$(I - Q)G = P$$

p – total number of measurements
m – total number of inputs

– There are pm equations
– There are $p^2 - p + pm$ unknowns

$\Rightarrow$ There are $p^2 - p$ degrees of freedom



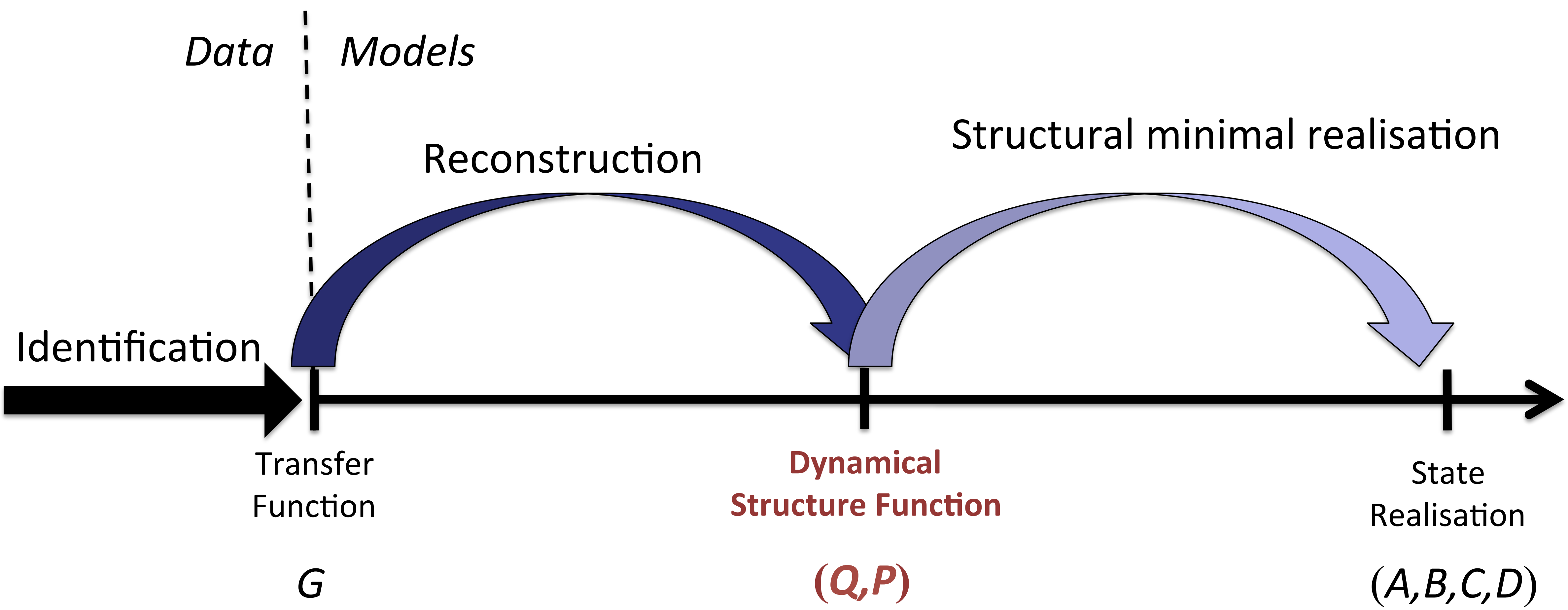


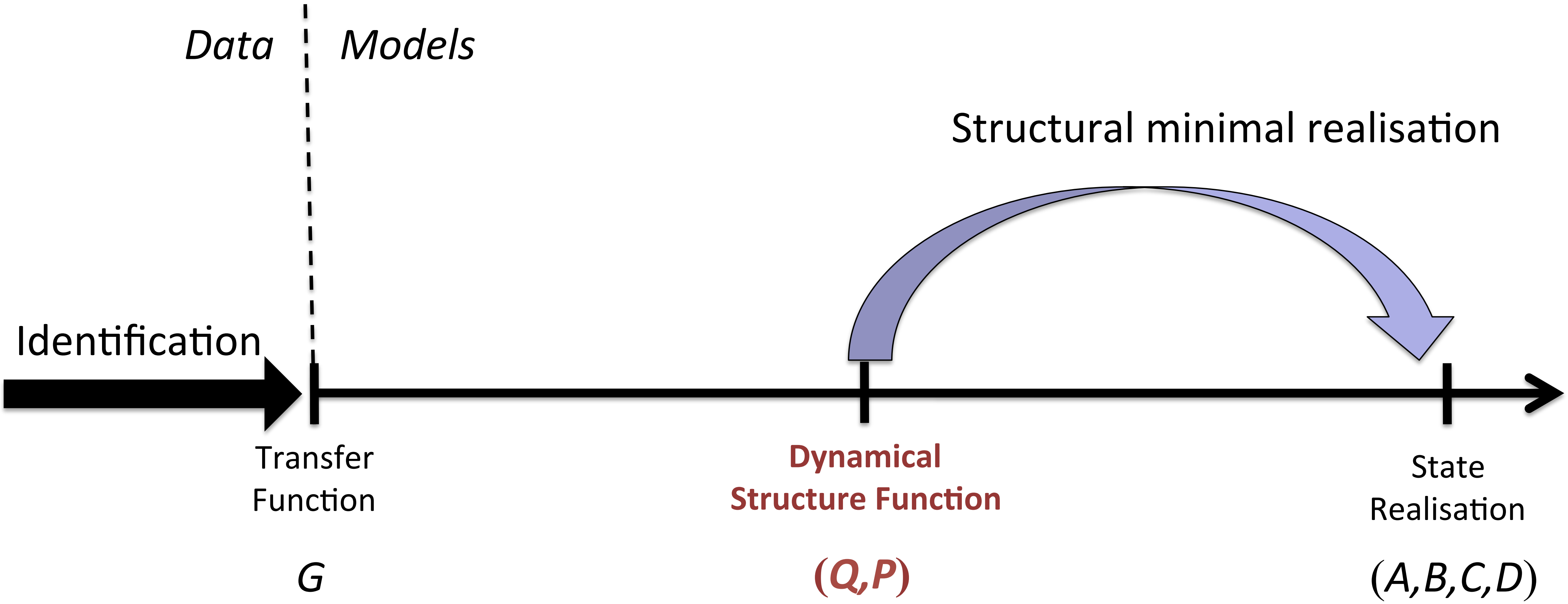
Experiment guideline for biological network reconstruction: (P is diagonal)

If nothing is known about the network of some measured species, then the experiments must be performed as follows:

1. For a network composed of p measured species, the same number of experiments p must be performed.
2. Each experiment must independently control a measured species. In other words, control input i must first affect measured species i.

- Motivation
- Introduction of dynamical structure function
- How it can be used to solve this network reconstruction problem?
- **What else?**





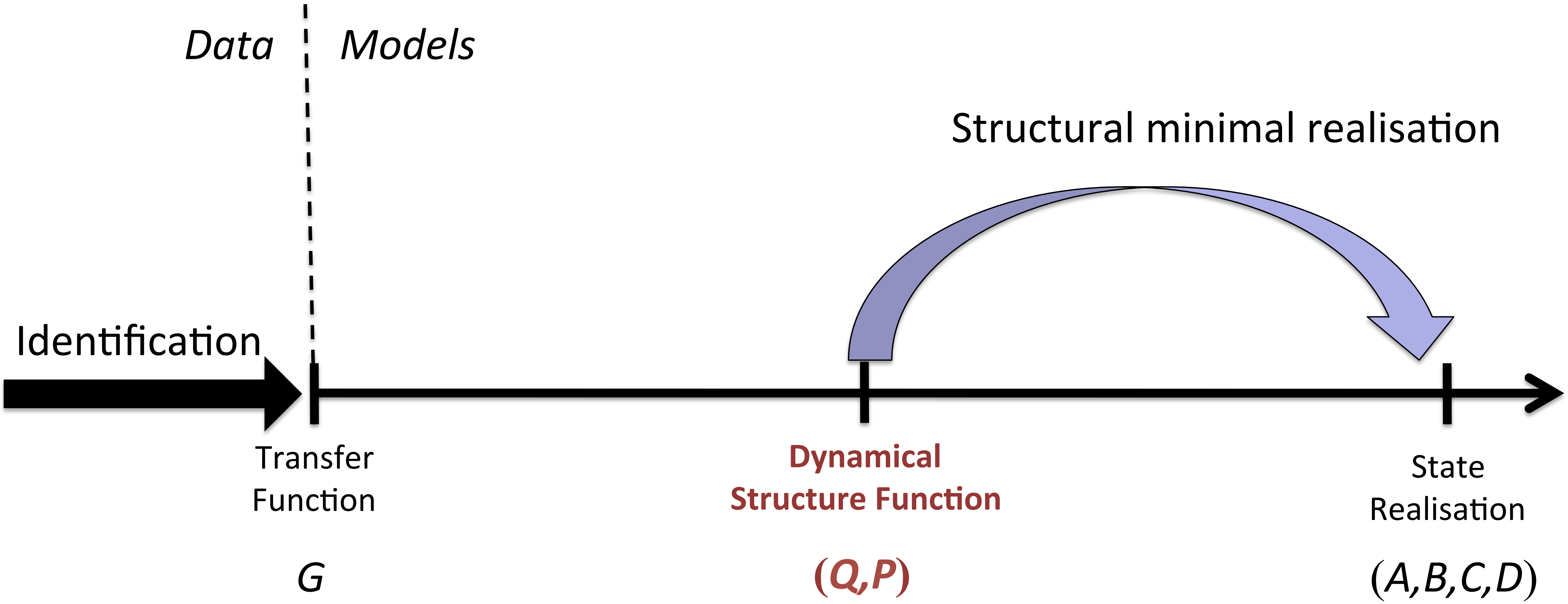
$$\lim_{s\to\infty} sQ(s) = A_{11} - \operatorname{diag} A_{11}$$

$$\lim_{s\to\infty} P(s) = B_1$$

$$\begin{bmatrix}\dot{y}\\ \dot{z}\end{bmatrix} = \begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix}\begin{bmatrix}y\\ z\end{bmatrix} + \begin{bmatrix}B_1\\ B_2\end{bmatrix}u$$

$$y = \begin{bmatrix} I & 0 \end{bmatrix}\begin{bmatrix}y\\ z\end{bmatrix}$$

<u>Theorem</u>: Let (A, B) be the matrices from the state-space representation of an LTI system, and (Q, P) its dynamical structure function. If $Q[i,j]$ is nonzero, then either $A_{11}[i,j]$ is nonzero or there exists a sequence $k_1, k_2, \ldots$ of indices corresponding to hidden states such that $A(i,k_1)$, $A(k_1,k_2) \ldots A(k_{m-1},k_m)$, $A(k_m,j)$ are nonzero.



Ill-posed:

$z=Tx$, any invertible T will do $\quad \tilde{A}=T^{-1}AT,\ \tilde{B}=T^{-1}B,\ \tilde{C}=CT,\ \tilde{D}=D$

$$T=\begin{bmatrix} I & 0 \\ 0 & \bar{T} \end{bmatrix} \quad \tilde{A}=\begin{bmatrix} A_{11} & \bar{T}^{-1}A_{12} \\ A_{21}\bar{T} & \bar{T}^{-1}A_{22}\bar{T} \end{bmatrix}$$

Consider the system:

$$\begin{bmatrix} \dot{y} \\ \dot{z} \end{bmatrix}=\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}\begin{bmatrix} y \\ z \end{bmatrix}+\begin{bmatrix} B_1 \\ B_2 \end{bmatrix}u$$

$$y=\begin{bmatrix} I & 0 \end{bmatrix}\begin{bmatrix} y \\ z \end{bmatrix}$$

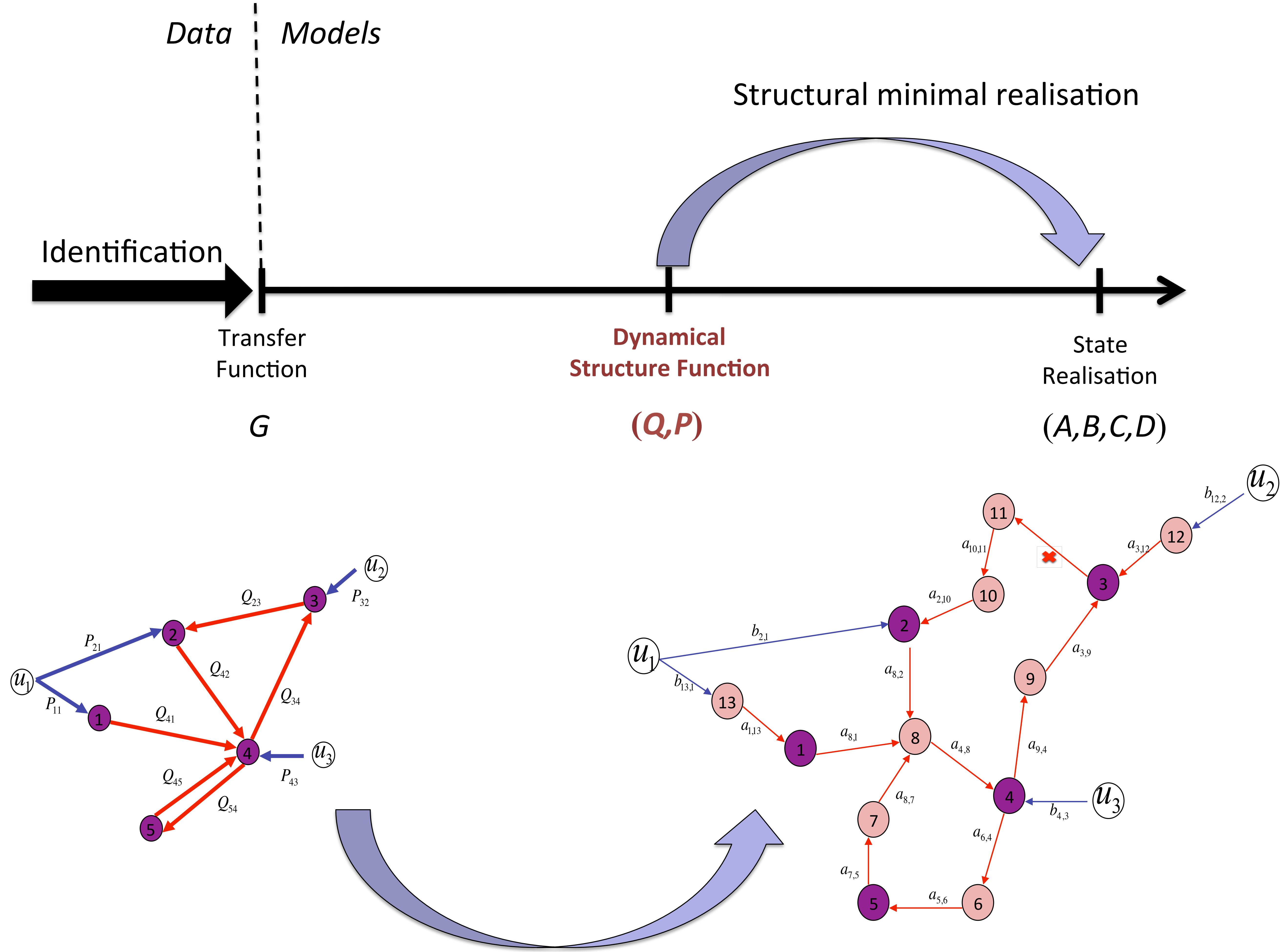
with

$u(t)\in R^m$ inputs

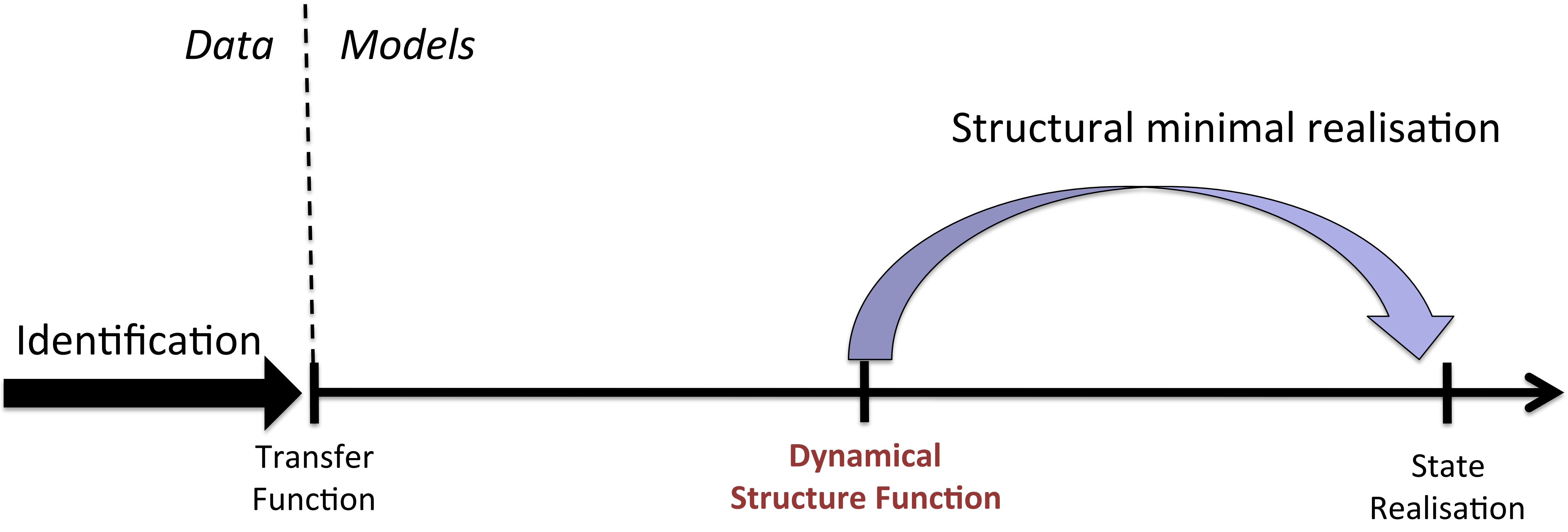
$y(t)\in R^p$ measured states

$z(t)\in R^{n-p}$ hidden states

Yuan et. al. arxiv 2011.



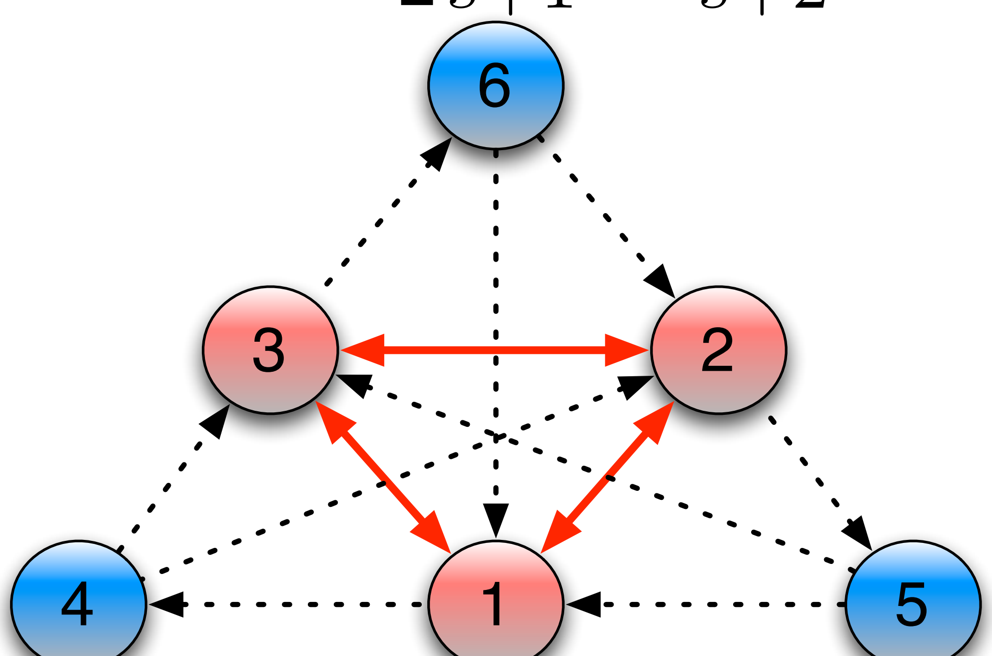
Yuan et. al. arxiv 2011.



Example: G (Q,P) (A,B,C,D)

$$[Q \mid P] = \left[\begin{array}{ccc|c} 0 & \frac{1}{s+2} & \frac{1}{s+3} & \frac{1}{s+4} \\ \frac{1}{s+1} & 0 & \frac{1}{s+3} & \frac{1}{s+4} \\ \frac{1}{s+1} & \frac{1}{s+2} & 0 & \frac{1}{s+4} \end{array}\right] .$$

$$G = \left[\begin{array}{c} \frac{(s+1)(s+3)}{s^3+6s^2+8s-2} \\ \frac{(s+2)^2}{s^3+6s^2+8s-2} \\ \frac{(s+2)(s+3)^2}{(s+4)(s^3+6s^2+8s-2)} \end{array}\right]$$

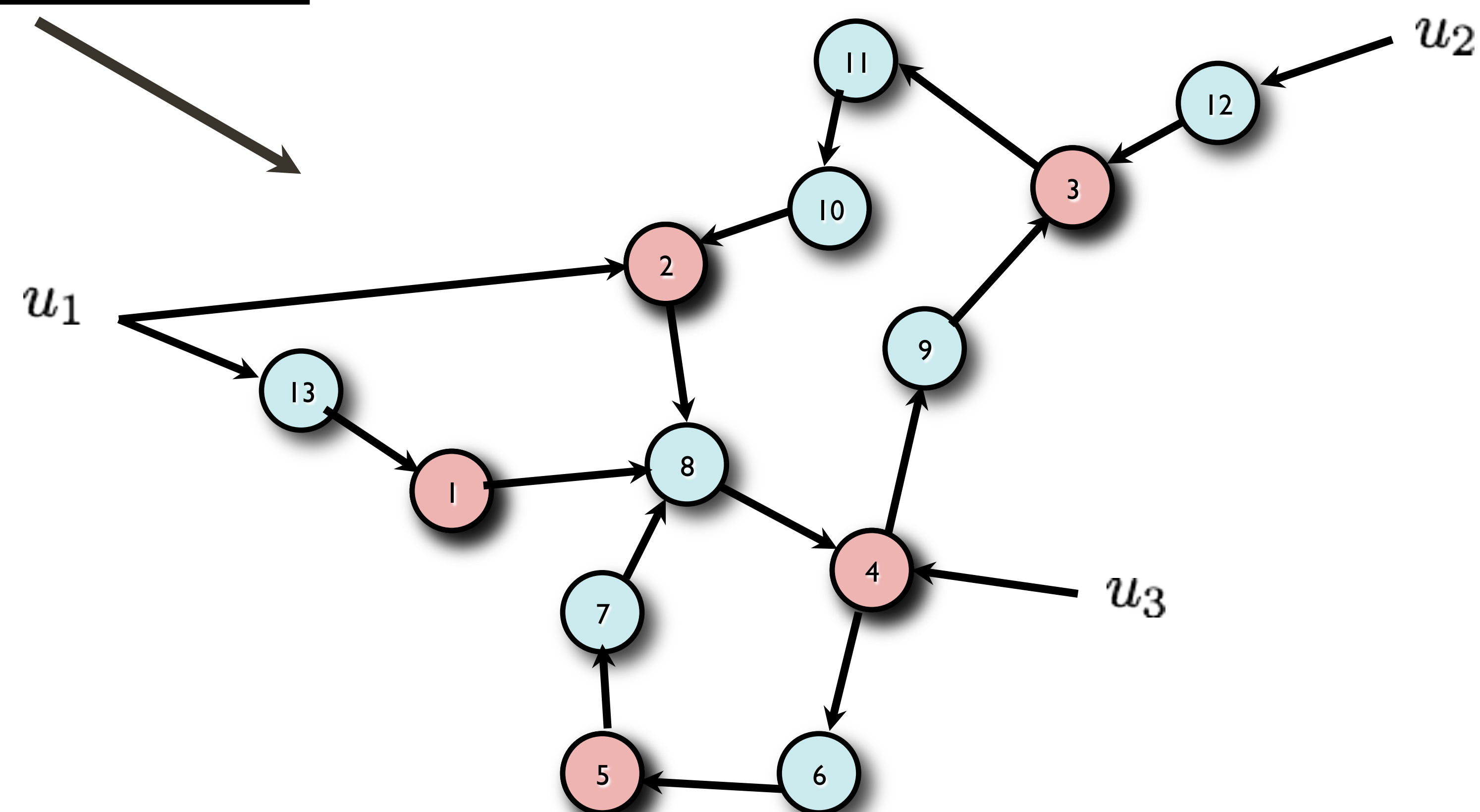


Yuan et. al. arxiv 2011.

Small perturbation at steady state! keep it linear!

I-O DATA [U, Y]

ALGORITHM (?)

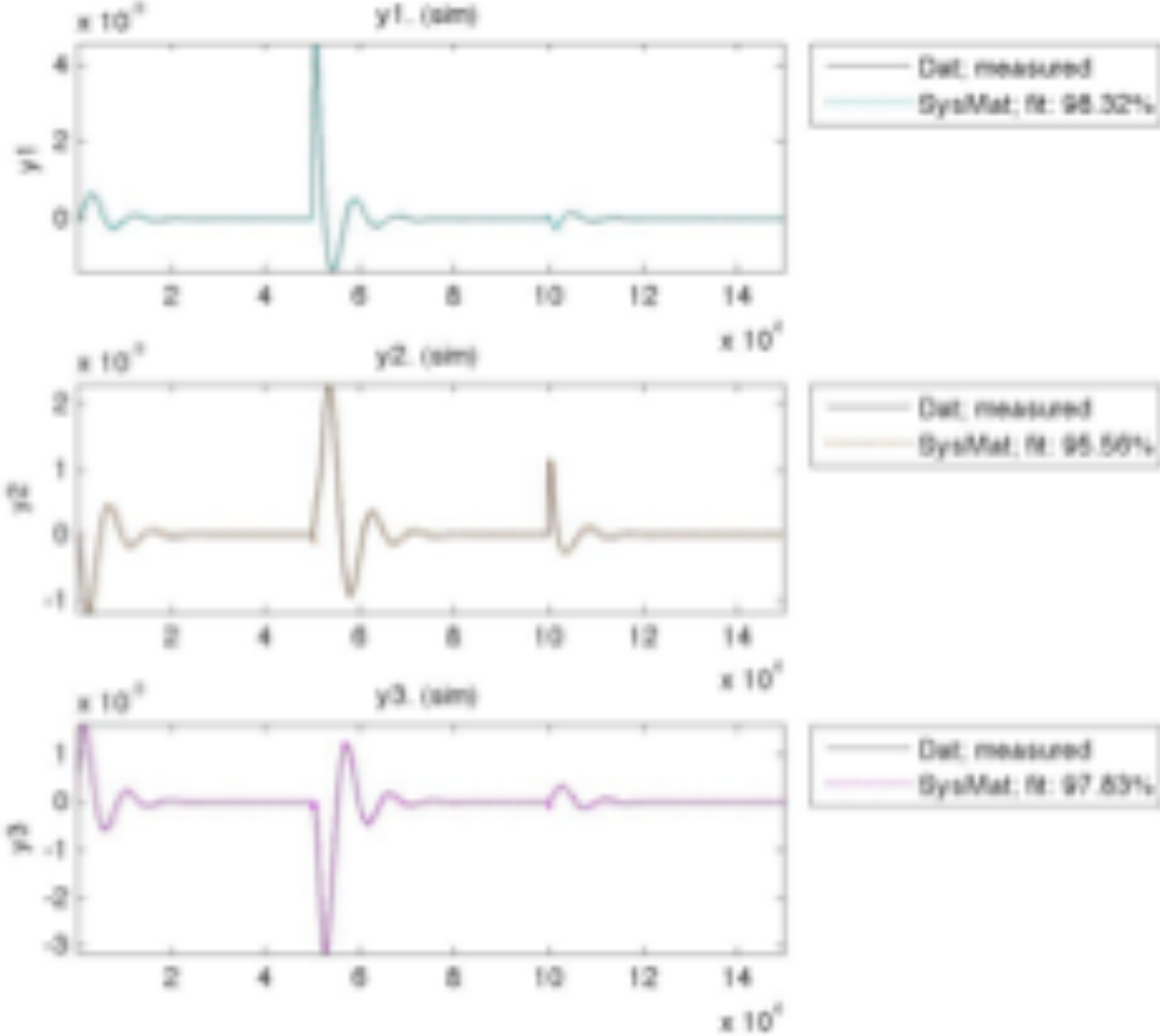


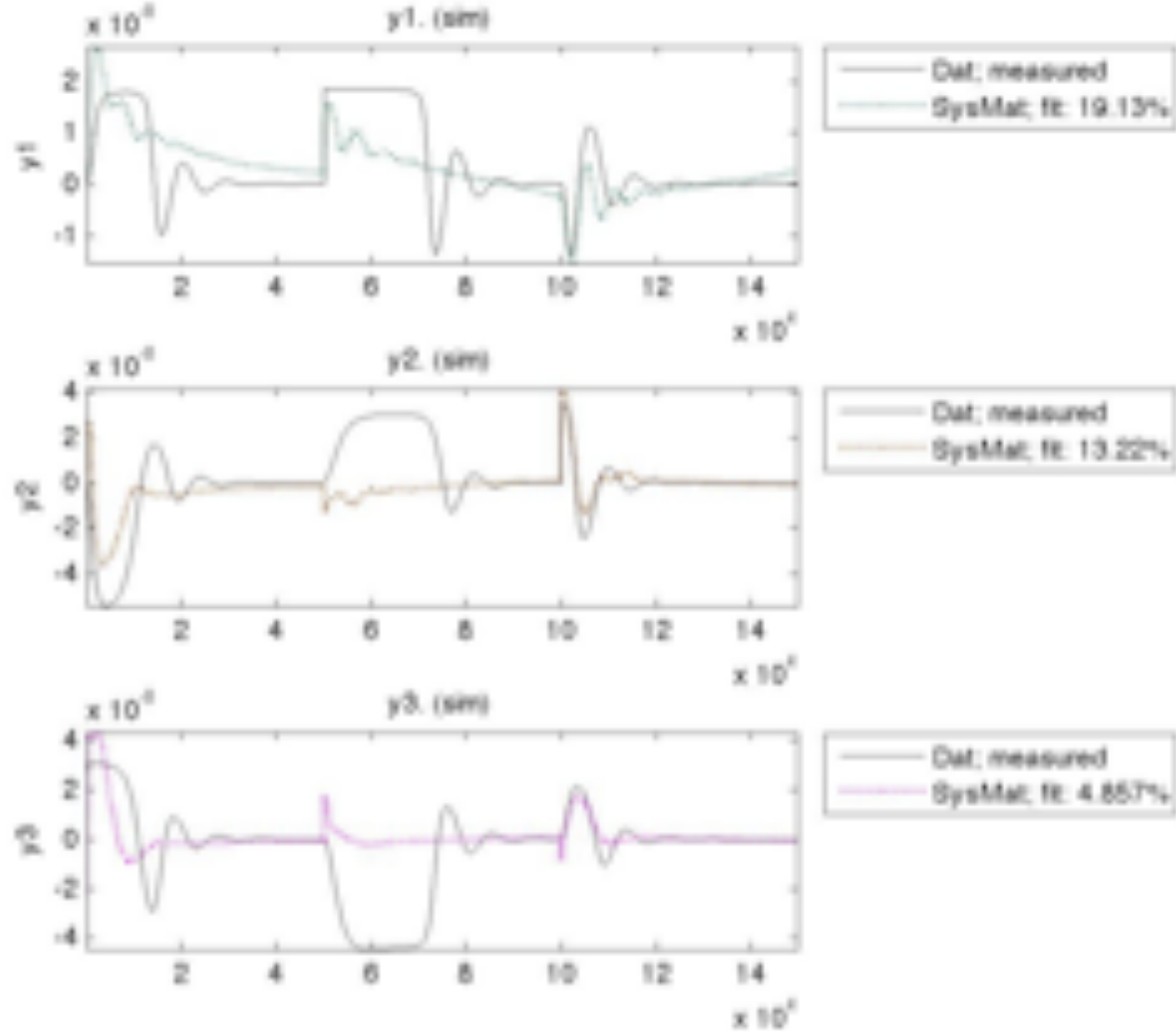
ISSUES:

- INFORMATION
- HIDDEN/LATENT NODES
- NONLINEARITY
- ROBUSTNESS

Pan, Yuan, Goncalves, Stan, CDC 2012

In Silico: Small Perturbation vs. Knockout





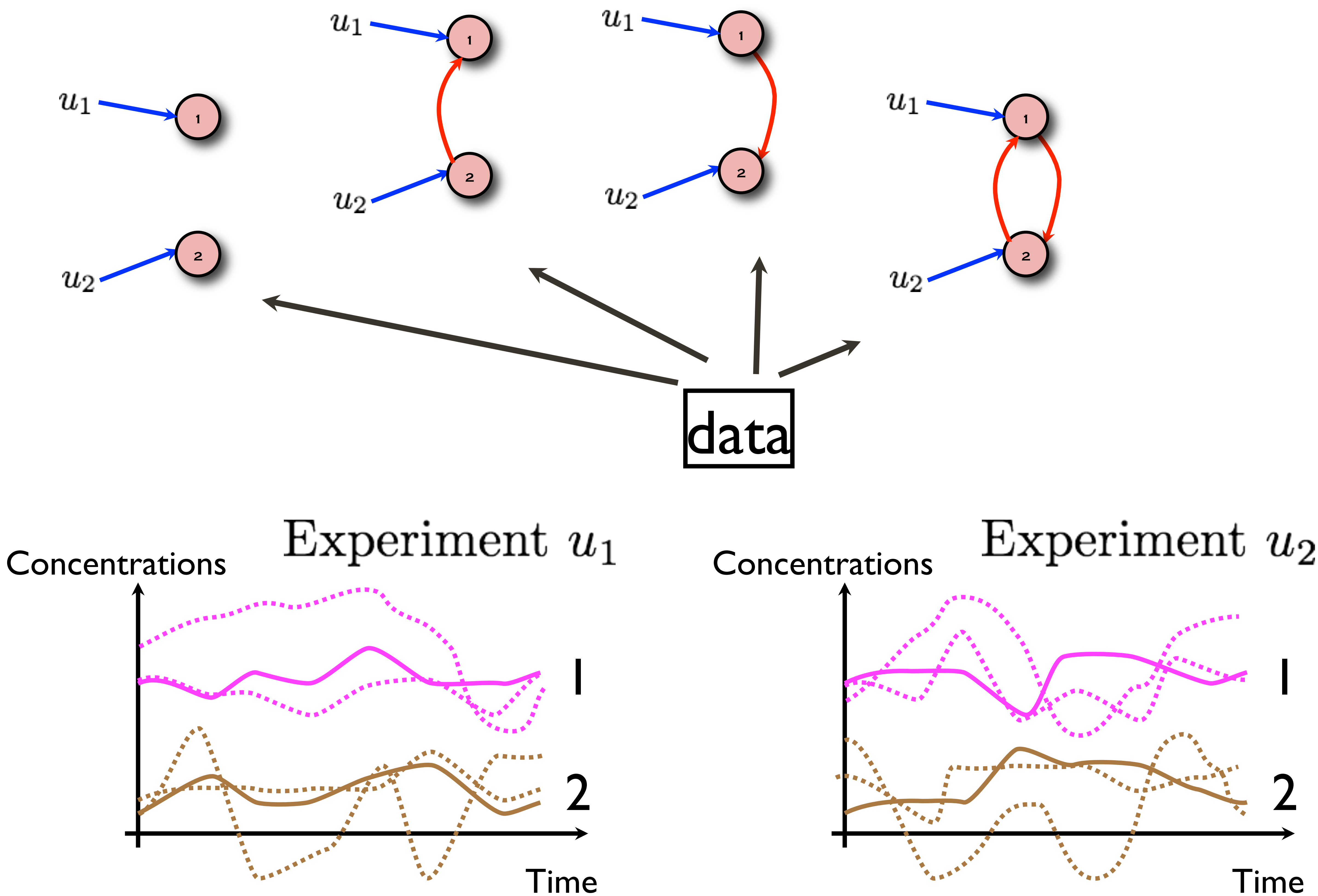
$$U = O(10^{-9})$$

$$U = O(10^{-7})$$

$$Q_{normalized} = \begin{bmatrix} 0 & 1 & .274 \\ .277 & 0 & 1 \\ 1 & .338 & 0 \end{bmatrix}$$

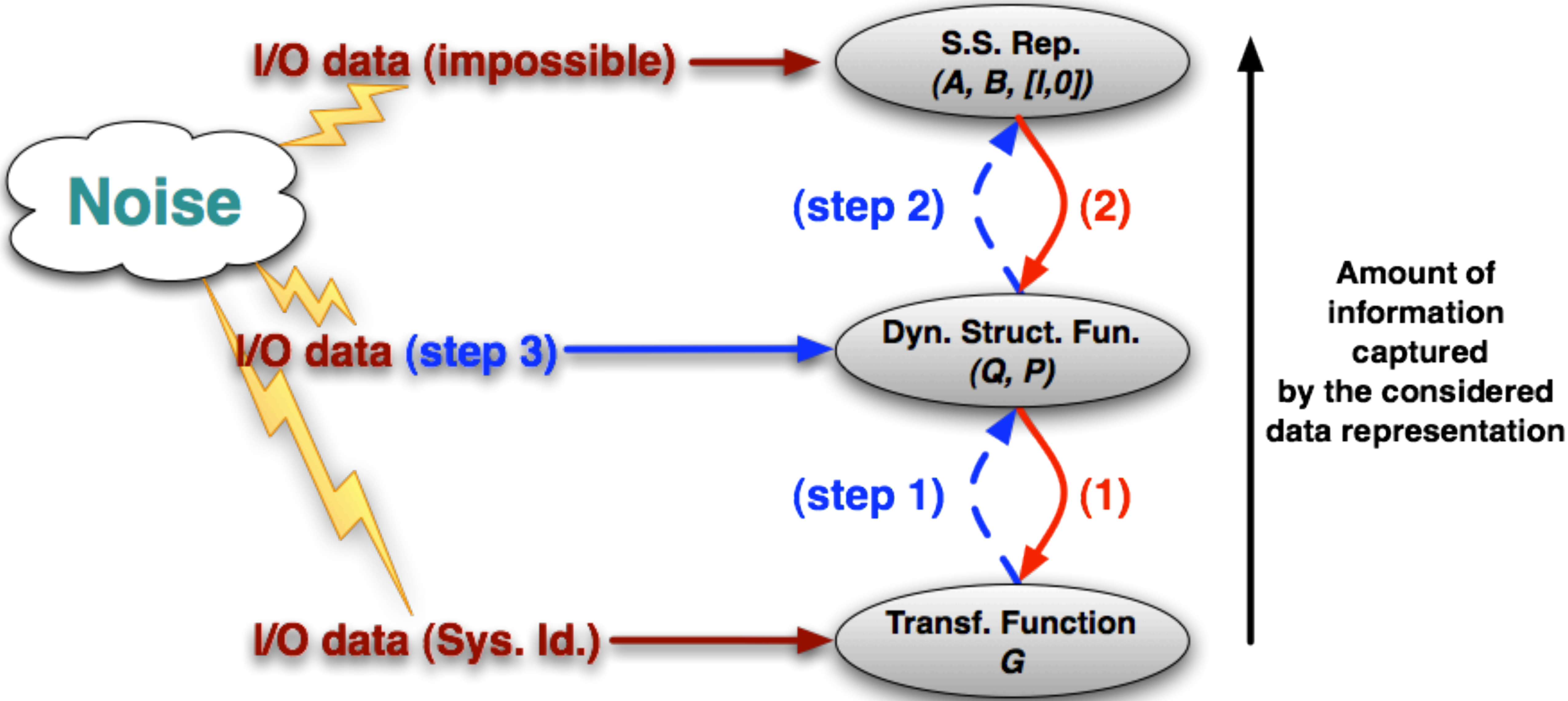
$$Q_{normalized} = \begin{bmatrix} 0 & 1 & .663 \\ 1 & 0 & .581 \\ .642 & 1 & 0 \end{bmatrix}$$

• Robustness



Yuan, et. al., Automatica 2011.
Hayden, Yuan, Goncalves, CDC 2012.

Conclusion



- Y. Yuan, "Decentralised network prediction and reconstruction algorithms," PhD Thesis, 2012. (available on www-control.eng.cam.ac.uk/~yy311) [Chapter 3]

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Thanks for your attention!