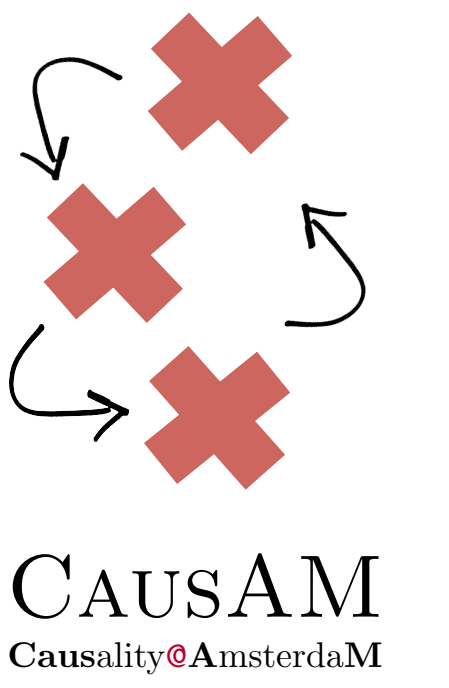


# Bridging the Gap between Random Differential Equations and Structural Causal Models

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## Abstract

In this work (Bongers and Mooij, 2018) we show how, and under which conditions, every equilibrium solution of the Random Differential Equation (RDE) can be described by a (cyclic) Structural Causal Model (SCM), while preserving the causal semantics. This enables the study of the equilibrium solutions of the RDE by applying the theory and statistical tools available for SCMs, for example, we can perform marginalizations and apply the (general) directed global Markov property (Bongers et al., 2018), as we illustrate by means of an example.

## Theory

### Random Dynamical Model (RDM):

$$\mathcal{R} := \begin{cases} \frac{d}{dt} \mathbf{X}_{\setminus K} = \mathbf{F}_{\setminus K}(\mathbf{X}, \mathbf{E}) \\ \mathbf{X}_K = \boldsymbol{\eta}_K \end{cases}$$

with  $\mathbf{F}_{\setminus K}: \mathcal{X} \times \mathcal{E} \rightarrow \mathcal{X}$  a function and the following stochastic processes on  $\mathbb{R}$ :

- $\mathbf{X}$  a sample-path solution
- $\boldsymbol{\eta}_K$  an intervened s.p.
- $\mathbf{E}$  an exogenous s.p.

### Structural Causal Model (SCM):

$$\mathcal{M} := \{ \mathbf{X}^* = \mathbf{f}^*(\mathbf{X}^*, \mathbf{E}^*) \}$$

with  $\mathbf{f}^*: \mathcal{X} \times \mathcal{E} \rightarrow \mathcal{X}$  the causal mechanism function and the following random variables:

- $\mathbf{X}^*$  a solution
- $\mathbf{E}^*$  an exogenous r.v.

A **perfect intervention** for some subset of variables  $I$  such that  $\lim_{t \rightarrow \infty} (\boldsymbol{\xi}_I)_t = \boldsymbol{\xi}_I^* \in \mathcal{X}_I$  is given by:

### Intervened RDM:

$$\mathcal{R}_{\text{do}(I, \boldsymbol{\xi}_I)} := \begin{cases} \frac{d}{dt} \mathbf{X}_{\setminus(I \cup K)} = \mathbf{F}_{\setminus(I \cup K)}(\mathbf{X}, \mathbf{E}) \\ \mathbf{X}_{I \cup K} = (\boldsymbol{\xi}_I, \boldsymbol{\eta}_{K \setminus I}) \end{cases}$$

### Intervened SCM:

$$\mathcal{M}_{\text{do}(I, \boldsymbol{\xi}_I^*)} := \begin{cases} \mathbf{X}_{\setminus I}^* = \mathbf{f}_{\setminus I}^*(\mathbf{X}^*, \mathbf{E}^*) \\ \mathbf{X}_I^* = \boldsymbol{\xi}_I^* \end{cases}$$

We call an RDM  $\mathcal{R}$  **steady**, if  $\mathbf{F}_{\setminus K}$ ,  $\mathbf{E}$ ,  $\boldsymbol{\eta}_K$  are (sample-path) continuous,  $\lim_{t \rightarrow \infty} \mathbf{E}_t = \mathbf{E}^*$  is a r.v. and  $\lim_{t \rightarrow \infty} (\boldsymbol{\eta}_K)_t = \boldsymbol{\eta}_K^* \in \mathcal{X}_K$ .

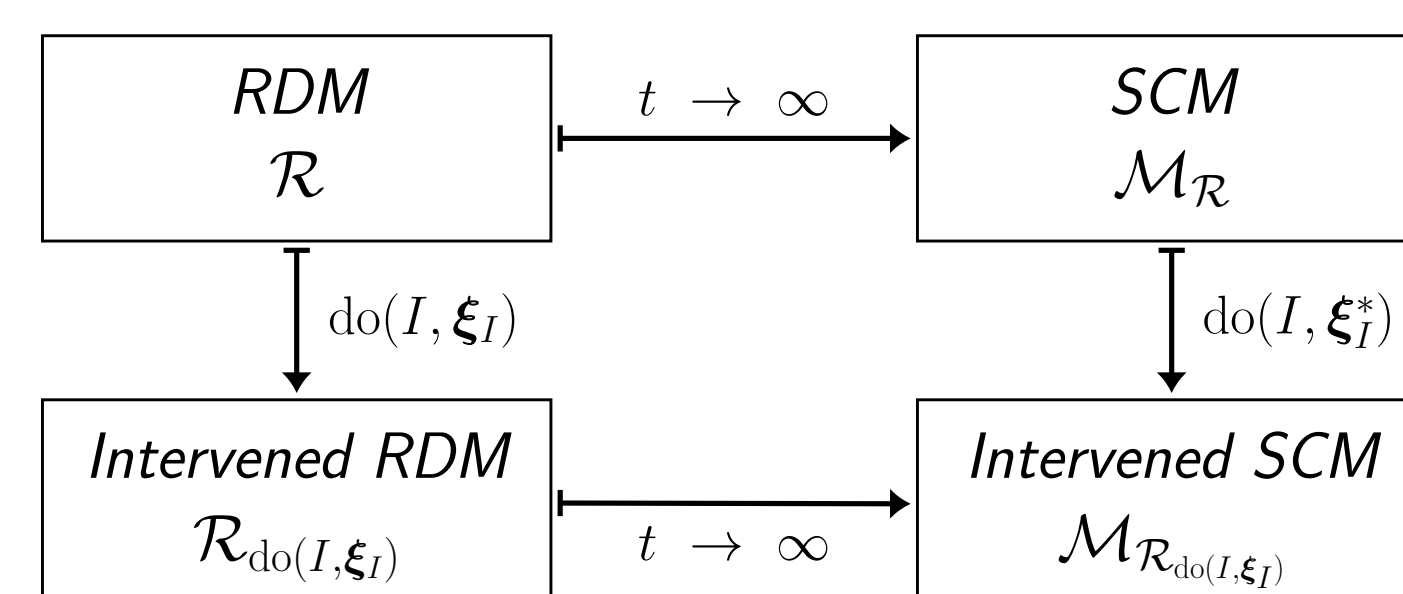
**Construct an SCM from a steady RDM:**  $\mathcal{R} \xrightarrow{t \rightarrow \infty} \mathcal{M}_{\mathcal{R}}$

where the causal mechanism  $\mathbf{f}^*: \mathcal{X} \times \mathcal{E} \rightarrow \mathcal{X}$  is defined by

$$\mathbf{f}^*(\mathbf{x}, \mathbf{e}) := (\mathbf{x}_{\setminus K} + \mathbf{F}_{\setminus K}(\mathbf{x}, \mathbf{e}), \boldsymbol{\eta}_K^*) \quad \text{with} \quad \boldsymbol{\eta}_K^* := \lim_{t \rightarrow \infty} (\boldsymbol{\eta}_K)_t \quad \text{and} \quad \mathbf{E}^* := \lim_{t \rightarrow \infty} \mathbf{E}_t.$$

**Theorem 1** Given a steady RDM  $\mathcal{R}$ . If there exists a sample-path solution  $\mathbf{X}$  of  $\mathcal{R}$  that equilibrates to  $\mathbf{X}^*$ , i.e.  $\lim_{t \rightarrow \infty} \mathbf{X}_t = \mathbf{X}^*$  is a r.v., then  $\mathbf{X}^*$  is a solution of the associated SCM  $\mathcal{M}_{\mathcal{R}}$ .

**Theorem 2** Perfect intervention commutes with the mapping from steady RDM to SCM, i.e.



## Chemical Kinetics

Enzyme reaction:  $S + E \xrightleftharpoons[k_r]{k_f} C \xrightarrow{k_c} P + E$

Random Dynamical Model: 
$$\begin{aligned} \frac{d}{dt} S &= k_i - k_f ES + k_r C \\ \frac{d}{dt} E &= -k_f ES + (k_r + k_c) C \\ \frac{d}{dt} C &= k_f ES - (k_r + k_c) C \\ \frac{d}{dt} P &= k_c C - k_o P \end{aligned}$$

Structural Causal Model: 
$$\begin{aligned} S &= k_i k_f^{-1} E^{-1} - k_r k_f^{-1} E^{-1} C \\ E &= k_f^{-1} (k_r + k_c) S^{-1} C \\ C &= k_f (k_r + k_c)^{-1} ES \\ P &= k_c k_o^{-1} C \end{aligned}$$

Intervened RDM: 
$$\begin{aligned} \frac{d}{dt} S &= k_i - k_f ES + k_r C \\ E &= \eta \\ \frac{d}{dt} C &= k_f ES - (k_r + k_c) C \\ \frac{d}{dt} P &= k_c C - k_o P \end{aligned}$$

Intervened SCM: 
$$\begin{aligned} S &= k_i k_f^{-1} E^{-1} - k_r k_f^{-1} E^{-1} C \\ E &= \eta \\ C &= k_f (k_r + k_c)^{-1} ES \\ P &= k_c k_o^{-1} C \end{aligned}$$

Functional graphs:

## Damped Coupled Harmonic Oscillator

Diagram of a damped coupled harmonic oscillator with masses  $m_1, \dots, m_5$  and springs  $l_0, \dots, l_5$  between fixed walls at  $Q=0$  and  $Q=L$ .

Random Dynamical Model: 
$$\begin{aligned} \frac{d}{dt} P_i &= k_i(Q_{i+1} - Q_i - l_i) - k_{i-1}(Q_i - Q_{i-1} - l_{i-1}) - \frac{b_i}{m_i} P_i \\ \frac{d}{dt} Q_i &= P_i / m_i \\ l_i &\sim \psi(L/6, \sigma, 0, L/3), \quad \text{where } \psi \text{ is the truncated normal distribution on } [0, L/3] \end{aligned}$$

Structural Causal Model: 
$$\begin{aligned} P_i &= k_i(Q_{i+1} - Q_i - l_i) - k_{i-1}(Q_i - Q_{i-1} - l_{i-1}) + (1 - \frac{b_i}{m_i}) P_i \\ Q_i &= Q_i + P_i / m_i \end{aligned}$$

Marginal SCM: 
$$Q_i = \frac{k_i}{k_i + k_{i-1}} (Q_{i+1} - l_i) + \frac{k_{i-1}}{k_i + k_{i-1}} (Q_{i-1} - l_{i-1})$$

Functional graph: SCM Functional graph: marginal SCM Functional graph: intervened SCM

d- and  $\sigma$ -separation  $\implies$  that  $Q_1 \perp\!\!\!\perp Q_5 | Q_3$  holds in the intervened model

## References

- Bongers, S. and Mooij, J. M. (2018). From random differential equations to structural causal models: the stochastic case. *arXiv.org preprint*, arXiv:1803.08784 [cs.AI].  
Bongers, S., Peters, J., Schölkopf, B., and Mooij, J. M. (2018). Theoretical aspects of cyclic structural causal models. *arXiv.org preprint*, arXiv:1611.06221v2 [stat.ME].